Sentaurus™ Device User Guide

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SYNOPSYS®

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About This Guide

The Synopsys Sentaurus™ Device tool is a full-featured, electrothermal, mixed-mode device and circuit simulator for one-dimensional, two-dimensional, and three-dimensional semiconductor devices. It incorporates advanced physical models and robust numeric methods for the simulation of most types of semiconductor device ranging from very deep-submicron silicon MOSFETs to large bipolar power structures. In addition, SiC and III–V compound homostructure and heterostructure devices are fully supported.

The user guide is divided into parts:

- Part I presents information about how to start Sentaurus Device and how it interacts with other Synopsys tools.
- Part II describes the physics in Sentaurus Device.
- Part III describes the physical models used in light-emitting diode simulations.
- Part IV presents the automatic grid generation facility and provides background information on the numeric methods used in Sentaurus Device.
- Part V describes the physical model interface, which provides direct access to certain models in the semiconductor transport equations and the numeric methods in Sentaurus Device.
- Part VI contains the appendices.

This guide assumes familiarity with working on UNIX-like systems and requires a basic understanding of semiconductor device physics and its terminology.

Related Publications

For additional information, see:

- The TCAD Sentaurus release notes, available on the Synopsys SolvNet® support site (see Accessing SolvNet on page xlii).
- Documentation available on SolvNet at https://solvnet.synopsys.com/DocsOnWeb.

Conventions

The following conventions are used in Synopsys documentation.

Convention	Description
Blue text	Identifies a cross-reference (only on the screen).
Bold text	Identifies a selectable icon, button, menu, or tab. It also indicates the name of a field or an option.
Courier font	Identifies text that is displayed on the screen or that the user must type. It identifies the names of files, directories, paths, parameters, keywords, and variables.
Italicized text	Used for emphasis, the titles of books and journals, and non-English words. It also identifies components of an equation or a formula, a placeholder, or an identifier.
Menu > **Command**	Indicates a menu command, for example, **File** > **New** (from the **File** menu, select **New**).

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Customer support is available through the Synopsys SolvNet customer support website and by contacting the Synopsys support center.

Accessing SolvNet

The SolvNet support site includes an electronic knowledge base of technical articles and answers to frequently asked questions about Synopsys tools. The site also gives you access to a wide range of Synopsys online services, which include downloading software, viewing documentation, and entering a call to the Support Center.

To access the SolvNet site:

1. Go to the web page at https://solvnet.synopsys.com.

2. If prompted, enter your user name and password. (If you do not have a Synopsys user name and password, follow the instructions to register.)

If you need help using the site, click **Help** on the menu bar.

Contacting Synopsys Support

If you have problems, questions, or suggestions, you can contact Synopsys support in the following ways:

- Go to the Synopsys Global Support Centers site on synopsys.com. There you can find e-mail addresses and telephone numbers for Synopsys support centers throughout the world.

- Go to either the Synopsys SolvNet site or the Synopsys Global Support Centers site and open a case online (Synopsys user name and password required).

Contacting Your Local TCAD Support Team Directly

Send an e-mail message to:

- support-tcad-us@synopsys.com from within North America and South America.

- support-tcad-eu@synopsys.com from within Europe.

- support-tcad-ap@synopsys.com from within Asia Pacific (China, Taiwan, Singapore, Malaysia, India, Australia).

- support-tcad-kr@synopsys.com from Korea.

- support-tcad-jp@synopsys.com from Japan.

Acknowledgments

Parts of Sentaurus Device were codeveloped by Integrated Systems Laboratory of ETH Zurich in the joint research project LASER with financial support by the Swiss funding agency CTI and in the joint research project VCSEL with financial support by the Swiss funding agency TOP NANO 21. The GEBAS Library was codeveloped by Integrated Systems Laboratory of ETH Zurich in the joint research project MQW with financial support by the Swiss funding agency TOP NANO 21.

The third-party software ARPACK (ARnoldi PACKage) by R. Lehoucq, K. Maschhoff, D. Sorensen, and C. Yang is used in Sentaurus Device (http://www.caam.rice.edu/software/ARPACK).

Sentaurus Device contains the QD library for double-double and quad-double floating-point arithmetic (http://crd-legacy.lbl.gov/~dhbailey/mpdist). The QD library requires the following copyright notice:

Sentaurus Device contains the ARPREC library for arbitrary floating-point arithmetic (http://crd-legacy.lbl.gov/~dhbailey/mpdist). The ARPREC library requires the following copyright notice:

Sentaurus Device uses the LAPACK linear algebra package (http://www.netlib.org/lapack), which requires the following copyright notice:

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Sentaurus Device uses code adapted from the SLATEC/FNLIB routines daie.f, daide.f, dbie.f, and dbide.f by Wayne Fullerton for the evaluation of exponentially scaled Airy functions and their derivatives.

Part I   Getting Started

This part of the *Sentaurus™ Device User Guide* contains the following chapters:

CHAPTER 1 Introduction to Sentaurus Device

This chapter describes how Sentaurus Device integrates into the TCAD tool suite and presents some complete simulation examples.

Functionality of Sentaurus Device

Sentaurus Device simulates numerically the electrical behavior of a single semiconductor device in isolation or several physical devices combined in a circuit. Terminal currents, voltages, and charges are computed based on a set of physical device equations that describes the carrier distribution and conduction mechanisms. A real semiconductor device, such as a transistor, is represented in the simulator as a 'virtual' device whose physical properties are discretized onto a nonuniform 'grid' (or 'mesh') of nodes.

Therefore, a virtual device is an approximation of a real device. Continuous properties such as doping profiles are represented on a sparse mesh and, therefore, are only defined at a finite number of discrete points in space. The doping at any point between nodes (or any physical quantity calculated by Sentaurus Device) can be obtained by interpolation. Each virtual device structure is described in the Synopsys TCAD tool suite by a TDR file containing the following information:

- The grid (or geometry) of the device contains a description of the various regions, that is, boundaries, material types, and the locations of any electrical contacts. It also contains the locations of all the discrete nodes and their connectivity.

- The data fields contain the properties of the device, such as the doping profiles, in the form of data associated with the discrete nodes. Figure 1 on page 4 shows a typical example: the doping profile of a MOSFET structure discretized by a mixed-element grid. By default, a device simulated in 2D is assumed to have a 'thickness' in the third dimension of $1 \ \mu m$.

The features of Sentaurus Device are many and varied. They can be summarized as:

- An extensive set of models for device physics and effects in semiconductor devices (drift-diffusion, thermodynamic, and hydrodynamic models).

- General support for different device geometries (1D, 2D, 3D, and 2D cylindrical).

- Mixed-mode support of electrothermal netlists with mesh-based device models and SPICE circuit models.
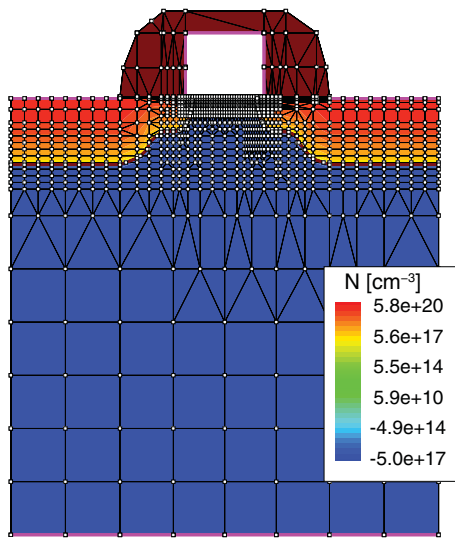
Figure 1   Two-dimensional doping profile that is discretized on the nodes of simulation grid

Nonvolatile memory simulations are accommodated by robust treatment of floating electrodes in combination with Fowler–Nordheim and direct tunneling, and hot-carrier injection mechanisms.

Hydrodynamic (energy balance) transport is simulated rigorously to provide a more physically accurate alternative to conventional drift-diffusion formulations of carrier conduction in advanced devices.

Floating semiconductor regions in devices such as thyristors and silicon-on-insulator (SOI) transistors (floating body) are handled robustly. This allows hydrodynamic breakdown simulations in such devices to be achieved with good convergence.

The mixed device and circuit capabilities give Sentaurus Device the ability to solve three basic types of simulation: single device, single device with a circuit netlist, and multiple devices with a circuit netlist (see Figure 2).

Single Device   Single Device With Circuit   Multiple Devices With Circuit
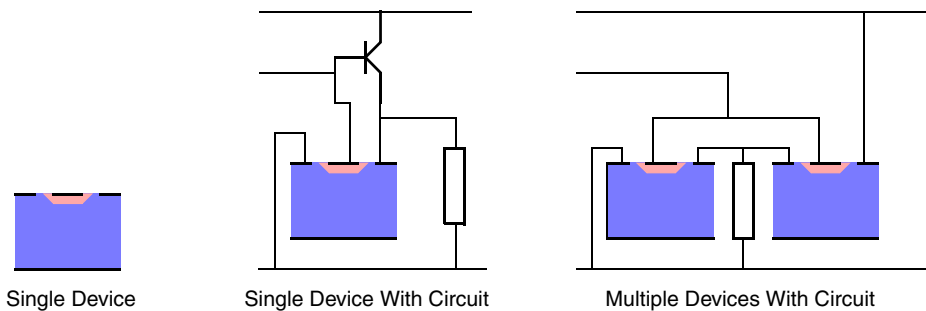
Figure 2   Three types of simulation

Multiple-device simulations can combine devices of different mesh dimensionality, and different physical models can be applied in individual devices, providing greater flexibility. In all cases, the circuit netlists can contain an electrical and a thermal section.

Creating and Meshing Device Structures

Device structures can be created in various ways, including 1D, 2D, or 3D process simulation (Sentaurus Process), 2D or 3D process emulation (Sentaurus Structure Editor), and 2D or 3D structure editors (Sentaurus Structure Editor).

Regardless of the means used to generate a virtual device structure, it is recommended that the structure be remeshed using Sentaurus Structure Editor (2D and 3D meshing with an interactive graphical user interface (GUI)) or Sentaurus Mesh (1D, 2D, and 3D meshing without a GUI) to optimize the grid for efficiency and robustness.

For maximum efficiency of a simulation, a mesh must be created with a minimum number of vertices to achieve the required level of accuracy. For any given device structure, the optimal mesh varies depending on the type of simulation.

It is recommended that to create the most suitable mesh, the mesh must be densest in those regions of the device where the following are expected:

- High current density (MOSFET channels, bipolar base regions)
- High electric fields (MOSFET channels, MOSFET drains, depletion regions in general)
- High charge generation (single event upset (SEU) alpha particle, optical beam)

For example, accurate drain current modeling in a MOSFET requires very fine, vertical, mesh spacing in the channel at the oxide interface (of the order $1\,\text{Å}$) when using advanced mobility models. For reliable simulation of breakdown at a drain junction, the mesh must be more concentrated inside the junction depletion region for good resolution of avalanche multiplication.

Generally, a total node count of 2000 to 4000 is reasonable for most 2D simulations. Large power devices and 3D structures require a considerably larger number of elements.

Tool Flow

In a typical device tool flow, the creation of a device structure by process simulation (Sentaurus Process) is followed by remeshing using Sentaurus Structure Editor or Sentaurus Mesh. In this scheme, control of mesh refinement is handled automatically through the file `_dvs.cmd`.

Sentaurus Device is used to simulate the electrical characteristics of the device. Finally, Sentaurus Visual is used to visualize the output from the simulation in 2D and 3D, and Inspect is used to plot the electrical characteristics.
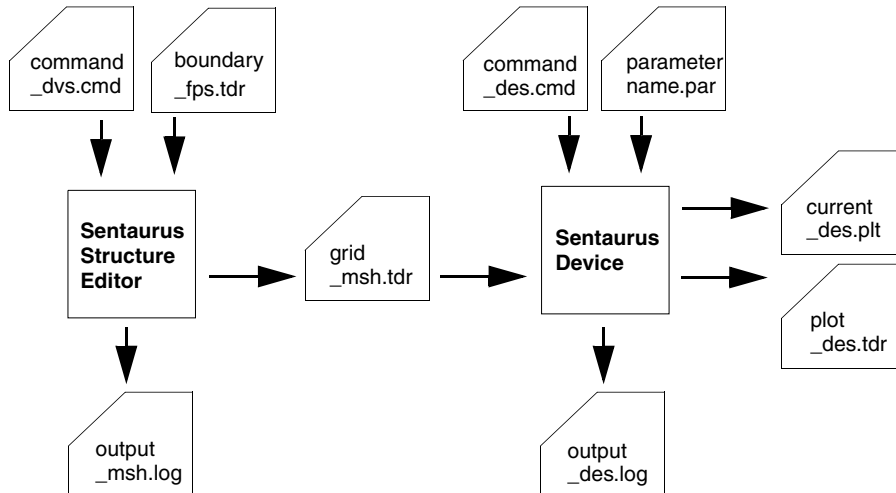
Figure 3   Typical tool flow with device simulation using Sentaurus Device

Starting Sentaurus Device

You can start Sentaurus Device from either the command line or Sentaurus Workbench.

From the Command Line

Sentaurus Device is driven by a command file and run by the command:

```
sdevice <command_filename>
```

Various options exist at start-up and are listed by using:

```
sdevice -h
```

By default, sdevice runs the latest version in the current release of Sentaurus Device. To run a particular version in the current release, use the command-line option -ver. For example:

```
sdevice -ver 1.4 nmos_des.cmd
```

starts version 1.4 of the latest release of Sentaurus Device.

To run the latest version in a particular release, use the command-line option `-rel`. For example:

```
sdevice -rel N-2017.09 nmos_des.cmd
```

starts the latest version available in release N-2017.09. To run a particular version in a particular release, combine `-ver` and `-rel`. For example:

```
sdevice -rel M-2016.12 -ver 1.2 nmos_des.cmd
```

starts Sentaurus Device, release M-2016.12, version 1.2.

When the release or the version requested is not installed, the available releases or versions are listed, and the program aborts.

Appendix D on page 1333 lists the command options of Sentaurus Device, which include:

`sdevice -versions`

Checks which versions are in the installation path.

`sdevice -P` and `sdevice -L`

Extract model parameter files (see Generating a Copy of Parameter File on page 32).

`sdevice --parameter-names`

Prints names of parameters that can be ramped (see Ramping Physical Parameter Values on page 78).

When Sentaurus Device starts, the command file is checked for correct syntax, and the commands are executed in sequence. Character strings starting with `*` or `#` are ignored by Sentaurus Device, so that these characters can be used to insert comments in the simulation command file.

From Sentaurus Workbench

Sentaurus Device is launched automatically through the Scheduler when working inside Sentaurus Workbench.

Sentaurus Workbench interprets `#` as a special marker for conditional statements (for example, `#if...`, `#elif...`, and `#endif...`).

Simulation Projects

The Sentaurus Device module of the TCAD Sentaurus Tutorial provides various projects demonstrating the capabilities of Sentaurus Device.

To access the TCAD Sentaurus Tutorial, open Sentaurus Workbench and either choose **Help > Training** or click the corresponding toolbar button.

Alternatively, to access the TCAD Sentaurus Tutorial, go to:

```
$STROOT/tcad/$STRELEASE/Sentaurus_Training/index.html
```

where the STROOT environment variable indicates where the Synopsys TCAD distribution has been installed, and STRELEASE indicates the Synopsys TCAD release number.

CHAPTER 2   # Specifying Physical Devices

This chapter describes how to specify physical devices.

Before performing a simulation, Sentaurus Device needs to know which device will actually be simulated. This chapter describes what Sentaurus Device needs to know and how to specify it. This includes obvious information, such as the size and shape of the device, the materials of which the device is made, and the doping profiles. It also includes less obvious aspects such as which physical effects must be taken into account, and by which models and model parameters this should be performed.

Reading a Structure

A device is defined by its shape, material composition, and doping. This information is defined on a grid and contained in a TDR file that you specify with the keyword `Grid` in the `File` section of the command file, for example:

```
File {
   Grid = "mosfet.tdr"
   ...
}
```

The following keywords affect the interpretation of the geometry in the `Grid` file:

- `CoordinateSystem` in the global `Math` section specifies the coordinate system that is used for explicit coordinates in the Sentaurus Device command file. Many features such as current plot statements (see Tracking Additional Data in the Current File on page 110) or `LatticeParameters` in the parameter file (see Crystal and Simulation Coordinate Systems on page 781) use explicit coordinates, and they are based on an implicit assumption regarding the orientation of the device. By specifying the following keyword, you can indicate the required orientation of the device:

   ```
   Math {
      CoordinateSystem { <option> }
   }
   ```

Table 1   Options of the CoordinateSystem keyword

Option	Description
AsIs	(Default) This option specifies that the coordinate system of the device is compatible with the explicit coordinates used in the Sentaurus Device command file. No transformation is applied to the structure.

Table 1   Options of the CoordinateSystem keyword (Continued)

Option	Description
DFISE	In 2D, the x-axis points across the surface, and the y-axis points down into the device. In 3D, the x-axis and y-axis span the surface of the device, and the z-axis points upwards away from the device.
UCS	The unified coordinate system (UCS) uses the convention of the simulation coordinate system as established by Sentaurus Process. The x-axis always points down into the device. In 2D, the y-axis runs across the surface of the device. In 3D, the z-axis is added to obtain a right-handed coordinate system.

If the coordinate system of the device is incompatible with the specification in the `Math` section, Sentaurus Device automatically transforms the device into the required coordinate system.

- `Cylindrical` in the global `Math` section specifies that the device is simulated using cylindrical coordinates. In this case, a 3D device is specified by a 2D mesh and the vertical or horizontal axis around which the device is rotated.

- `AreaFactor` in the global `Physics` section specifies a multiplier for currents and charges. For 1D or 2D simulations, it typically specifies the extension of the device in the remaining one or two dimensions. In simulations that exploit the symmetry of the device, it can also be used to account for the reduction of the simulated device compared to the real device. `AreaFactor` is also available in the `Electrode` and `Thermode` sections, with the same meaning; if both `AreaFactors` are present, Sentaurus Device multiplies them.

TDR units are taken into account when loading from a `.tdr` file. Thereby, the units read from files are converted to the appropriate units used in Sentaurus Device. The TDR unit is ignored in the case of a conversion failure. Use the keyword `IgnoreTdrUnits` in the `Math` section to disregard TDR units during loading. This applies not only to the `Grid` file, but also to other loaded files (see Save and Load on page 157).

Abrupt and Graded Heterojunctions

Sentaurus Device supports both abrupt and graded heterojunctions, with an arbitrary mole fraction distribution. In the case of abrupt heterojunctions, Sentaurus Device treats discontinuous datasets properly by introducing double points at the heterointerfaces.

This option is switched on automatically when thermionic emission (see Thermionic Emission Current on page 763) is selected, or when the keyword `HeteroInterface` is specified in the `Physics` section of a selected heterointerface. By default, this double points option is switched off.

NOTE   The keyword `HeteroInterface` provides equilibrium conditions (continuous quasi-Fermi potentials) for the double points. It does not provide realistic physics at the interface for high-current regimes. Using the `HeteroInterface` option without thermionic emission or a tunneling model is discouraged.

To illustrate the double points option, Figure 4 shows the conduction band near an abrupt heterointerface. The wide line shows a case without double points, which requires a very fine mesh to avoid a large barrier error (δE_C).
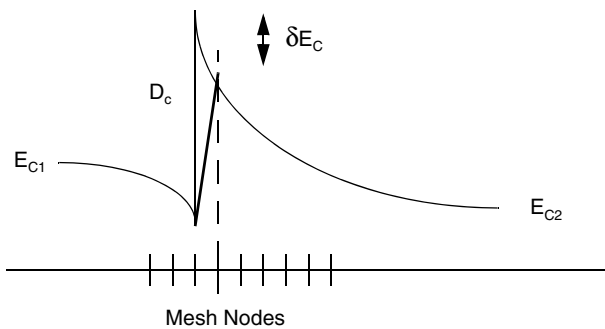
Figure 4   Band edge at a heterointerface with and without double points

Doping Specification

Sentaurus Device relies on the `Variables` section of the file `datexcodes.txt` to determine its doping species. A variable is identified as a doping species by a `doping` field that shows whether it is an acceptor or a donor. Chemical concentrations are linked to their corresponding active concentrations by an `active` field. Similarly, ionized concentrations are specified by an `ionized` field.

A typical declaration would be:

```
BoronConcentration, BoronChemicalConcentration {
   doping = acceptor (
      active = BoronActiveConcentration
      ionized = BoronMinusConcentration
   )
   ...
}

BoronActiveConcentration {
   ...
}
```

```
BoronMinusConcentration {
   ...
}
```

It is also possible to limit doping species to certain substrate materials. For example, to restrict `SiliconConcentration` as a donor for GaN substrates only, you would specify the following:

```
SiliconConcentration, SiliconChemicalConcentration {
   doping = donor (
      active = SiliconActiveConcentration
      ionized = SiliconPlusConcentration
      material = GaN
   )
}
```

The TCAD Sentaurus tool suite provides a default `datexcodes.txt` file in the directory `$STROOT_LIB` (or `$STROOT/tcad/$STRELEASE/lib`). Many common doping species are already predefined in this file. To add user-defined doping species or to modify an existing specification, you can use a `datexcodes.txt` file in the local directory. The local `datexcodes.txt` file only needs to contain the variables that you want to add or modify.

If the incomplete ionization model is activated (see Chapter 13 on page 277), the model parameters of the user-defined species must be specified in the `Ionization` section of the material parameter file.

Sentaurus Device loads doping distributions from the `Grid` file specified in the `File` section (see Reading a Structure on page 9) and reads the following datasets:

- Net doping (`DopingConcentration` in the `Grid` file)
- Total doping (`TotalConcentration` in the `Grid` file)
- Concentrations of individual species

Sentaurus Device supports the following rules of doping specification:

- Sentaurus Device takes the net doping dataset from the file if this dataset is present. Otherwise, net doping is recomputed from the concentrations of the separate species. To force the recomputation of the net doping based on individual species, use the keyword `ComputeDopingConcentration` in the global `Math` section.
- The same rule is applied for the total doping dataset.

  NOTE Total concentration, which originates from process simulators (for example, Sentaurus Process), is the sum of the chemical concentrations of dopants. However, if the total concentration is recomputed inside Sentaurus Device, active concentrations are used.

- Sentaurus Device takes the active concentration of a dopant if it is in the `Grid` file (for example, `BoronActiveConcentration`). Otherwise, the chemical dopant concentration is used (for example, `BoronConcentration`).

To perform any simulation, Sentaurus Device must prepare four major doping arrays:

- The net doping concentration, $N_{net} = N_{D,0} - N_{A,0}$.
- $N_{D,0}$ and $N_{A,0}$, the donor and acceptor concentrations.
- The total doping concentration, $N_{tot} = N_{D,0} + N_{A,0}$.

After loading the doping file, Sentaurus Device uses the following scheme to compute the doping arrays:

1. If the `Grid` file does not have any species: N_{net} is initialized from `DopingConcentration`, N_{tot} is initialized from `TotalConcentration` or $|N_{net}|$ if `TotalConcentration` was not read, $N_{D,0} = (N_{tot} + N_{net})/2$, and $N_{A,0} = (N_{tot} - N_{net})/2$.

2. If the `Grid` file has individual species: $N_{A,0}$ and $N_{D,0}$ are computed as the sum of individual donor and acceptor concentrations, N_{net} is initialized from `DopingConcentration` or $N_{D,0} - N_{A,0}$ if `DopingConcentration` was not read, and N_{tot} is initialized from `TotalConcentration` or $N_{A,0} + N_{D,0}$ if `TotalConcentration` was not read.

3. Doping concentration is also affected if the `Physics` section includes trap specifications with the `Add2TotalDoping` or `Add2TotalDoping(ChargedTraps)` option (see Options to Include Traps in Doping on page 469 for a description of these options).

Material Specification

Sentaurus Device supports all materials that are declared in the `datexcodes.txt` file (see Utilities User Guide, Chapter 1 on page 1). The following search strategy is observed to locate the `datexcodes.txt` file:

- Either `$STROOT_LIB/datexcodes.txt` or `$STROOT/tcad/$STRELEASE/lib/datexcodes.txt` if the environment variable `STROOT_LIB` is not defined (lowest priority)
- `$HOME/datexcodes.txt` (medium priority)
- `datexcodes.txt` in local directory (highest priority)

Definitions in later files replace or add to the definitions in earlier files.

User-Defined Materials

New materials can be defined in a local `datexcodes.txt` file. To add a new material, add its description to the `Materials` section of `datexcodes.txt`:

```
Materials {
   Silicon {
      label = "Silicon"
      group = Semiconductor
      color = #ffb6c1
   }
   Oxide {
      label = "SiO2"
      group = Insulator
      color = #7d0505
   }
   ...
}
```

The `label` value is used as a legend in visualization tools.

The `group` value identifies the type of new material. The available values are:

```
Conductor
Insulator
Semiconductor
```

The field `color` defines the color of the material in visualization tools. This field must have the syntax:

```
color = #rrggbb
```

where `rr`, `gg`, and `bb` denote hexadecimal numbers representing the intensity of red, green, and blue, respectively. The values of `rr`, `gg`, and `bb` must be in the range `00` to `ff`.

Table 2   Sample values for color

Color code	Color	Color code	Color
#000000	Black	#ffffff	White
#ff0000	Red	#40e0d0	Turquoise
#00ff00	Green	#7fff00	Chartreuse
#0000ff	Blue	#b03060	Maroon
#ffff00	Yellow	#ff7f50	Coral

Table 2   Sample values for color (Continued)

Color code	Color	Color code	Color
`#ff00ff`	Magenta	`#da70d6`	Orchid
`#00ffff`	Cyan	`#e6e6fa`	Lavender

Mole-Fraction Materials

Sentaurus Device reads the file `Molefraction.txt` to determine mole fraction–dependent materials. The following search strategy is used to locate this file:

1. Sentaurus Device looks for `Molefraction.txt` in the current working directory.

2. If the environment variables `STROOT` and `STRELEASE` are defined, Sentaurus Device tries to read the file:

   `$STROOT/tcad/$STRELEASE/lib/Molefraction.txt`

3. If these previous strategies are unsuccessful, Sentaurus Device uses the built-in defaults that follow.

The default `Molefraction.txt` file has the following content:

```
# Ge(x)Si(1-x)
SiliconGermanium (x=0) = Silicon
SiliconGermanium (x=1) = Germanium

# Al(x)Ga(1-x)As
AlGaAs (x=0) = GaAs
AlGaAs (x=1) = AlAs

# In(1-x)Al(x)As
InAlAs (x=0) = InAs
InAlAs (x=1) = AlAs

# In(1-x)Ga(x)As
InGaAs (x=0) = InAs
InGaAs (x=1) = GaAs

# Ga(x)In(1-x)P
GaInP (x=0) = InP
GaInP (x=1) = GaP

# InAs(x)P(1-x)
InAsP (x=0) = InP
InAsP (x=1) = InAs
```

```
# GaAs(x)P(1-x)
GaAsP (x=0) = GaP
GaAsP (x=1) = GaAs

# Hg(1-x)Cd(x)Te
HgCdTe (x=0) = HgTe
HgCdTe (x=1) = CdTe

# In(1-x)Ga(x)As(y)P(1-y)
InGaAsP (x=0, y=0) = InP
InGaAsP (x=1, y=0) = GaP
InGaAsP (x=1, y=1) = GaAs
InGaAsP (x=0, y=1) = InAs
```

To add a new mole fraction–dependent material, the material (and its side and corner materials) must first be added to `datexcodes.txt`. Afterwards, `Molefraction.txt` can be updated.

Quaternary alloys are specified by their corner materials in the file `Molefraction.txt`. For example, the 2:2 III–V quaternary alloy $In_{1-x}Ga_xAs_yP_{1-y}$ is given by:

```
InGaAsP (x=0, y=0) = InP
InGaAsP (x=1, y=0) = GaP
InGaAsP (x=1, y=1) = GaAs
InGaAsP (x=0, y=1) = InAs
```

and the 3:1 III–V quaternary alloy $Al_xIn_yGa_{1-x-y}As$ is defined by:

```
AlInGaAs (x=0, y=0) = GaAs
AlInGaAs (x=1, y=0) = AlAs
AlInGaAs (x=0, y=1) = InAs
```

When the corner materials of an alloy have been specified, Sentaurus Device determines the corresponding side materials automatically. In the case of $In_{1-x}Ga_xAs_yP_{1-y}$, the four side materials are $InAs_xP_{1-x}$, $GaAs_xP_{1-x}$, $Ga_xIn_{1-x}P$, and $In_{1-x}Ga_xAs$. Similarly, for $Al_xIn_yGa_{1-x-y}As$, the three side materials are $In_{1-x}Al_xAs$, $Al_xGa_{1-x}As$, and $In_{1-x}Ga_xAs$.

> **NOTE** All side and corner materials must appear in `datexcodes.txt`, and their mole dependencies must be specified in `Molefraction.txt` (see Material Specification on page 13).

> **NOTE** If it cannot parse the file `Molefraction.txt`, Sentaurus Device reverts to the defaults shown above. This may lead to unexpected simulation results.

Mole-Fraction Specification

In Sentaurus Device, the mole fraction of a compound semiconductor or insulator is defined in two ways:

- In the `Grid` file (`<name>.tdr`) of the device structure
- Internally, in the `Physics` section of the command file

If the mole fraction is loaded from the `.tdr` file and an internal mole fraction specification is also applied, the loaded mole fraction values are overwritten in the regions specified in the `MoleFraction` sections of the command file.

The internal mole fraction distribution is described in the `MoleFraction` statement inside the `Physics` section:

```
Physics { ...
   MoleFraction(<MoleFraction parameters>)
}
```

The parameters for the mole fraction specification and grading options are described in

The specification of an `xFraction` is mandatory in the `MoleFraction` statement for binary or ternary compounds; a `yFraction` is also mandatory for quaternary materials. If the `MoleFraction` statement is inside a default `Physics` section, the `RegionName` must be specified. If it is inside a region-specific `Physics` section, by default, it is applied only to that region. If a `MoleFraction` statement is inside a material-specific `Physics` section and the `RegionName` is not specified, this composition is applied to all regions containing the specified material. If `RegionName` is specified inside a region-specific and material-specific `Physics` section, this specification is used instead of the default regions.

> **NOTE** Similar to all statements, only one `MoleFraction` statement is allowed inside each `Physics` section. By default, grading is not included.

An example of a mole fraction specification is:

```
Physics {
  MoleFraction(RegionName = ["Region.3" "Region.4"]
    xFraction=0.8
    yFraction=0.7
    Grading(
       (xFraction=0.3 GrDistance=1
          RegionInterface=("Region.0" "Region.3"))
       (xFraction=0.2 yFraction=0.1 GrDistance=1
          RegionInterface=("Region.0" "Region.5"))
       (yFraction=0.4 GrDistance=1
```

```
                RegionInterface=("Region.0" "Region.3"))
        )
    )
}
Physics (Region = "Region.6") {
    MoleFraction(xFraction=0.1 yFraction=0.7 GrDistance=0.01)
}
```

Physical Models and the Hierarchy of Their Specification

The `Physics` section is used to select the models that are used to simulate a device. Table 233 on page 1427 lists the keywords that are available, and Part II and Part III discuss the models in detail.

Physical models can be specified globally, per region or material, per interface, or per electrode.

Some models (for example, the hydrodynamic transport model) can only be activated for the whole device. Regionwise or materialwise specifications are syntactically possible, but Sentaurus Device silently ignores them. Likewise, some specifications are syntactically possible for all locations, but they are semantically valid only for interfaces or bulk regions. In the tables in Appendix G on page 1377, the validity of specifications is indicated in the description column by characters in parentheses. For example, (g) denotes models that can be activated only for the entire device, but not for individual parts of it.

Some specifications are syntactically possible everywhere, but are valid for certain materials only. For example, `Mobility` is only valid in semiconductors.

Region-Specific and Material-Specific Models

In Sentaurus Device, different physical models for different regions and materials within a device structure can be specified. The syntax for this feature is:

```
Physics (material="material") {
    <physics-body>
}
```

or:

```
Physics (region="region-name") {
    <physics-body>
}
```

This feature is also available for the `Math` section:

```
Math (material="material") {
   <math-body>
}
```

or:

```
Math (region="region-name") {
   <math-body>
}
```

A `Physics` section without any region or material specifications is considered the default section.

> **NOTE** You can edit region names in Sentaurus Structure Editor (see Sentaurus™ Structure Editor User Guide, Changing the Name of a Region on page 109).

The `Physics` (and `Math`) sections for different locations are related as follows:

- Physical models defined in the global `Physics` section (that is, in the section without any region or material specifications) are applied in all regions of the device.
- Physical models defined in a material-specific `Physics` section are added to the default models for all regions containing the specified material.
- The same applies to the physical models defined in a region-specific `Physics` section: all regionwise defined models are added to the models defined in the default section.

> **NOTE** If for a region, both a region-specific `Physics` section and a material-specific `Physics` section for the material of the region are present, the region-specific declaration overrides the material-specific declaration, that is, the region-specific `Physics` section will not inherit any models from the material-specific section.

For example:

```
Physics {<Default models>}
Physics (Material="GaAs") {<GaAs models>}
Physics (Region="Emitter"){<Emitter models>}
```

If the `"Emitter"` region is made of GaAs, the models in this region are `<Default models>` and `<Emitter models>`, that is, whatever `<GaAs models>` contains is ignored in region `"Emitter"`.

For some models, the model specification and numeric values of the parameters are defined in the `Physics` sections. Examples of such models are `Traps` and the `MoleFraction`

specifications. For these models, the specifications in region or material `Physics` sections overwrite previously defined values of the corresponding parameters.

If in the default `Physics` section, `xMoleFraction` is defined for a given region and, afterward, is defined for the same region again, in a region or material `Physics` section, the default definition is overwritten. The hierarchy of the parameter specification is the same as discussed previously.

Interface-Specific Models

A special set of models can be activated at the interface between two different materials or two different regions. In Table 233 on page 1427, pure interface models are flagged with '(i)' in the description column.

As physical phenomena at an interface are not the same as in the bulk of a device, not all models are allowed inside interface-specific `Physics` sections. For example, it is not possible to define any mobility models or bandgap narrowing at interfaces.

> **NOTE** Although the `Recombination(surfaceSRH)` statement and the `GateCurrent` statement describe pure interface phenomena, they can be defined in a region-specific `Physics` section. In this case, the models are applied to all interfaces between this region and all adjacent insulator regions. If specified in the global `Physics` section, these models are applied to all semiconductor–insulator interfaces.

Interface models are specified in interface-specific `Physics` sections. Their respective parameters are accessible in the parameter file. The syntax for specification of an interface model is:

```
Physics (MaterialInterface="material-name1/material-name2") {
   <physics-body>
}
```

or:

```
Physics (RegionInterface="region-name1/region-name2") {
   <physics-body>
}
```

The following is an example illustrating the specification of fixed charges at the interface between the materials oxide and aluminum gallium arsenide (AlGaAs):

```
Physics(MaterialInterface="Oxide/AlGaAs") {
   Traps(Conc=-1.e12 FixedCharge)
}
```

If no region interface `Physics` section is present for a given region interface, the material interface section is used if present. If the material interface `Physics` section is missing as well, built-in defaults are used. Similar to what holds for regions and materials, if a region interface section is present, it is used for the region interface, ignoring material interface settings completely, even when a material interface `Physics` section is present. However, other than for regions and materials, the global `Physics` section is not used automatically to determine interface `Physics` settings.

Electrode-Specific Models

Electrode-specific `Physics` sections can be defined, for example:

```
Physics(Electrode="Gate"){
   Schottky
   eRecVel = <float>
   hRecVel = <float>
   Workfunction = <float>
}
```

Physical Model Parameters

Most physical models depend on parameters that can be adjusted in a file given by `Parameter` in the `File` section:

```
File {
   Parameter = <string>
   ...
}
```

The name of the parameter file conventionally has the extension .par.

Model parameters are split into sets, where a particular set corresponds to a particular physical model. The available parameter sets and the individual parameters they contain are described along with the description of the related model (see Part II and Part III).

Parameters can be specified globally, materialwise, regionwise, material interface–wise, region interface–wise, and electrode-wise. The following example shows each of these possibilities:

```
LatticeHeatCapacity {
   cv = 1.1
}
Material = "Silicon" {
   LatticeHeatCapacity {
      cv = 1.63
```

```
      }
   }
   Region = "Oxide" {
      LatticeHeatCapacity {
         cv = 1.67
      }
   }
   MaterialInterface = "Silicon/Oxide" {
      LatticeHeatCapacity {
         cv = -1
      }
   }
   RegionInterface = "Oxide/Bulk" {
      LatticeHeatCapacity {
         cv = -2
      }
   }
   Electrode = "gate" {
      LatticeHeatCapacity {
         cv = -3
      }
   }
```

As for the models themselves, not all parameters are valid in all locations, even though it is syntactically possible to specify them. For example, the heat capacity is not used for interfaces and electrodes. Therefore, it does not matter that the values provided in the example above are nonsensical.

To specify parameters for multiple parameter sets for the same location, put all these specifications together into one section for that location, as in the following example for dielectric permittivity and heat capacity:

```
   Material = "Silicon" {
      Epsilon{
         epsilon= 11.6
      }
      LatticeHeatCapacity {
         cv = 1.63
      }
   }
```

Parameter files support an `Insert` statement to insert other parameter files. Inserted files themselves can use `Insert`. You can change parameters after an `Insert` statement. This is useful to provide standard values through the inserted file and to make the changes to those standards explicit. `Insert` is used as in the following example:

```
   Material = "Silicon" { Insert = "Silicon.par" }
```

Search Strategy for Parameter Files

Sentaurus Device uses the following strategy to search for inserted files, from highest to lowest priority as follows:

1. Local directory.

2. The `ParameterPath` variable in the `File` section can specify a list of releases, for example:

   ```
   File {
      ParameterPath = "2016.03 2016.12 2017.09"
   }
   ```

   In this case, the following directories are added to the search path:

   ```
   $STROOT/tcad/$STRELEASE/lib/sdevice/MaterialDB/2016.03
   $STROOT/tcad/$STRELEASE/lib/sdevice/MaterialDB/2016.12
   $STROOT/tcad/$STRELEASE/lib/sdevice/MaterialDB/2017.09
   ```

3. Sentaurus Device checks whether the environment variable `SDEVICEDB` is defined. This variable must contain a directory or a list of directories separated by whitespace or colons, for example:

   ```
   SDEVICEDB="/home/usr/lib /home/tcad/lib"
   ```

   Sentaurus Device scans the directories in the given order until the inserted file is found.

   NOTE　The environment variable `SDEVICEDB` also is used for the insert directive in Sentaurus Device command files (see Inserting Files on page 134).

4. The default library directory:

   ```
   $STROOT/tcad/$STRELEASE/lib/sdevice/MaterialDB
   ```

In all cases, Sentaurus Device prints the path to the actual file and displays an error message if it cannot be found.

   NOTE　The insert directive is also available for command files (see Inserting Files on page 134).

Parameters for Composition-Dependent Materials

The following parameter sets provide mole fraction dependencies. All models are available for compound semiconductors only, except where otherwise noted:

- `Epsilon` (also available for compound insulators)
- `LatticeHeatCapacity` (also available for compound insulators)
- `Kappa` (lattice thermal conductivity, also available for compound insulators)
- `EnergyRelaxationTime`
- `Bandgap`
- `Bennett` (bandgap narrowing)
- `delAlamo` (bandgap narrowing)
- `OldSlotboom` (bandgap narrowing)
- `Slotboom` (bandgap narrowing)
- `JainRoulston` (bandgap narrowing)
- `eDOSMass`
- `hDOSMass`
- `ConstantMobility`
- `DopingDependence` (mobility model)
- `HighFieldDependence` (mobility model)
- `TransferredElectronEffect2` (mobility model)
- `Enormal` (mobility model)
- `ToCurrentEnormal` (mobility model)
- `PhuMob` (mobility model)
- `ThinLayerMobility`
- `StressMobility` (hSixBand model parameters)
- `vanOverstraetendeMan` (impact ionization model)
- `MLDAQMModel`
- `SchroedingerParameters`
- `Band2BandTunneling`
- `DirectTunneling` (for semiconductor–insulator interfaces only)
- `AbsorptionCoefficient`
- `QWStrain` (see Electronic Band Structure for Wurtzite Crystals on page 967 and Syntax for Quantum-Well Strain on page 977)
- `RefractiveIndex` (also available for compound insulators)

- Radiative recombination

- Shockley–Read–Hall recombination

- Auger recombination

- Piezoelectric polarization

- `QuantumPotentialParameters`

- Deformation potential (elasticity modulus, the parameters for the electron band: `xis`, `dbs`, `xiu`, `xid` and, for hole band: `adp`, `bdp`, `ddp`, `dso`)

- `SHEDistribution`

- `ComplexRefractiveIndex`

- `BandstructureParameters` (see Electronic Band Structure for Wurtzite Crystals on page 967)

Sentaurus Device supports the suppression of the mole fraction dependence of a given model and the use of a fixed (mole fraction–independent) parameter set instead. To suppress mole fraction dependency, specify the (fixed) values for the parameter (for example, `Eg0=1.53`) and omit all other coefficients associated with the interpolation over the mole fraction (for example, `Eg0(1)`, `B(Eg0(1))`, and `C(Eg0(1))`) from this section of the parameter file. It is not necessary to set them to zero individually.

NOTE When specifying a fixed value for one parameter of a given model, all other parameters for the same model must be fixed.

In summary, if the mole fraction dependence of a given model is suppressed, the parameter specification for this model is performed in exactly the same manner as for mole fraction–independent material.

Ternary Semiconductor Composition

To illustrate a calculation of mole fraction–dependent parameter values for ternary materials, consider one mole interval from x_{i-1} to x_i. For mole fraction value (x) of this interval, to compute the parameter value (P), Sentaurus Device uses the expression:

$$P = P_{i-1} + A \cdot \Delta x + B_i \cdot \Delta x^2 + C_i \cdot \Delta x^3$$

$$A = \frac{\Delta P_i}{\Delta x_i} - B_i \cdot \Delta x_i - C_i \cdot \Delta x_i^2$$

$$\Delta P_i = P_i - P_{i-1} \tag{1}$$

$$\Delta x_i = x_i - x_{i-1}$$

$$\Delta x = x - x_{i-1}$$

where P_i, B_i, C_i, x_i are values defined in the parameter file for each mole fraction interval, $x_0 = 0$, P_0 is the parameter value (at $x = 0$) specified using the same manner as for mole

fraction–independent material (for example, `Eg0=1.53`). As in the formulas above, you are not required to specify coefficient A of the polynomial because it is easily recomputed inside Sentaurus Device.

In the case of undefined parameters (these can be listed by printing the parameter file), Sentaurus Device uses linear interpolation using two parameter values of side materials (for $x = 0$ and $x = 1$):

$$P = (1-x)P_{x0} + xP_{x1} \tag{2}$$
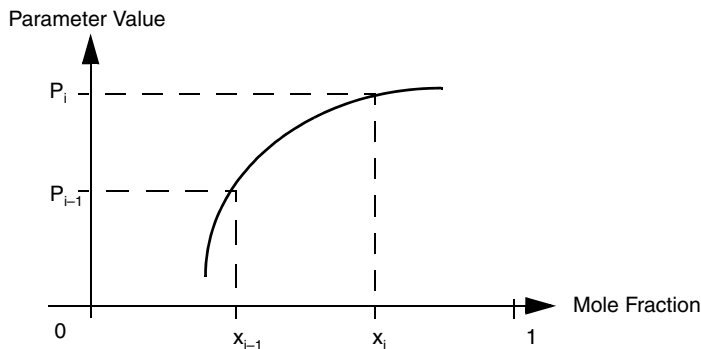
Figure 5   Parameter value as a function of mole fraction

Example 1: Specifying Electric Permittivity

This example provides the specification of dielectric permittivity for $Al_xGa_{1-x}As$:

```
Epsilon
{ *  Ratio of the permittivities of material and vacuum
        epsilon = 13.18      # [1]
* Mole fraction dependent model.
* The linear interpolation is used on interval [0,1].
        epsilon(1) = 10.06   # [1]
}
```

A linear interpolation is used for the dielectric permittivity, where `epsilon` specifies the value for the mole fraction $x = 0$, and `epsilon(1)` specifies the value for $x = 1$.

Example 2: Specifying Band Gap

This example provides a specification of the bandgap parameters for $Al_xGa_{1-x}As$. A polynomial approximation, up to the third degree, describes the mole fraction–dependent band parameters on every mole fraction interval. In the following example, two intervals are used, namely, `[Xmax(0), Xmax(1)]` and `[Xmax(1), Xmax(2)]`. The parameters `Eg0`, `Chi0`, ... correspond to the values for $X = $ `Xmax(0)`; while the parameters `Eg0(1)`, `Chi0(1)`, ...

correspond to the values for $X =$ `Xmax(1)` and, finally, `Eg0(2)`, `Chi0(2)`, ... correspond to the values for $X =$ `Xmax(2)`.

The coefficients A and F of the polynomial:

$$F + A(X - \texttt{Xmin}(I)) + B(X - \texttt{Xmin}(I))^2 + C(X - \texttt{Xmin}(I))^3 \tag{3}$$

are determined from the values at both ends of the intervals, while the coefficients B and C must be specified explicitly. You can introduce additional intervals:

```
Bandgap *temperature dependent*
{ * Eg = Eg0 - alpha T^2 / (beta + T) + alpha Tpar^2 / (beta + Tpar)
  * Eg0 can be overwritten in below bandgap narrowing models,
  * if any of the BGN model is chosen in physics section.
  * Parameter 'Tpar' specifies the value of lattice
  * temperature, at which parameters below are defined.
      Eg0 = 1.42248      # [eV]
      Chi0 = 4.11826     # [eV]
      alpha = 5.4050e-04 # [eV K^-1]
      beta = 2.0400e+02  # [K]
      Tpar = 3.0000e+02  # [K]
  * Mole fraction dependent model.
  * The following interpolation polynomial can be used on interval
  [Xmin(I),Xmax(I)]:
  * F(X) = F(I-1)+A(I)*(X-Xmin(I))+B(I)*(X-Xmin(I))^2+C(I)*(X-Xmin(I))^3,
  * where Xmax(I), F(I), B(I), C(I) are defined below for each interval.
  * A(I) is calculated for a boundary condition F(Xmax(I)) = F(I).
  * Above parameters define values at the following mole fraction:
      Xmax(0) = 0.0000e+00     # [1]
  * Definition of mole fraction intervals, parameters, and coefficients:
      Xmax(1) = 0.45           # [1]
      Eg0(1)  = 1.98515        # [eV]
      B(Eg0(1)) = 0.0000e+00   # [eV]
      C(Eg0(1)) = 0.0000e+00   # [eV]
      Chi0(1) = 3.575          # [eV]
      B(Chi0(1)) = 0.0000e+00  # [eV]
      C(Chi0(1)) = 0.0000e+00  # [eV]
      alpha(1) = 4.7727e-04    # [eV K^-1]
      B(alpha(1)) = 0.0000e+00 # [eV K^-1]
      C(alpha(1)) = 0.0000e+00 # [eV K^-1]
      beta(1) = 1.1220e+02     # [K]
      B(beta(1)) = 0.0000e+00  # [K]
      C(beta(1)) = 0.0000e+00  # [K]
      Xmax(2) = 1              # [1]
      Eg0(2)  = 2.23           # [eV]
      B(Eg0(2)) = 0.143        # [eV]
      C(Eg0(2)) = 0.0000e+00   # [eV]
      Chi0(2) = 3.5            # [eV]
```

```
        B(Chi0(2)) = 0.0000e+00  # [eV]
        C(Chi0(2)) = 0.0000e+00  # [eV]
        alpha(2) = 4.0000e-04    # [eV K^-1]
        B(alpha(2)) = 0.0000e+00 # [eV K^-1]
        C(alpha(2)) = 0.0000e+00 # [eV K^-1]
        beta(2) = 0.0000e+00     # [K]
        B(beta(2)) = 0.0000e+00  # [K]
        C(beta(2)) = 0.0000e+00  # [K]
    }
```

Quaternary Semiconductor Composition

Sentaurus Device supports 1:3, 2:2, and 3:1 III–V quaternary alloys. A 1:3 III–V quaternary alloy is given by:

$$AB_x C_y D_z \tag{4}$$

where A is a group III element, and B, C, and D are group V elements (usually listed according to increasing atomic number). Conversely, a 3:1 III–V quaternary alloy can be described as:

$$A_x B_y C_z D \tag{5}$$

where A, B, and C are group III elements, and D is a group V element.

The composition variables x, y, and z are nonnegative, and they are constrained by:

$$x + y + z = 1 \tag{6}$$

An example would be $Al_x Ga_y In_{1-x-y} As$, where $1 - x - y$ corresponds to z.

Sentaurus Device uses the symmetric interpolation scheme proposed by Williams *et al.* [1] to compute the parameter value $P(A_x B_y C_z D)$ of a 3:1 III–V quaternary alloy as a weighted sum of the corresponding ternary values:

$$P(A_x B_y C_z D) = \frac{xyP(A_{1-u}B_u D) + yzP(B_{1-v}C_v D) + xzP(A_{1-w}C_w D)}{xy + yz + xz} \tag{7}$$

where:

$$u = \frac{1-x+y}{2}, v = \frac{1-y+z}{2}, w = \frac{1-x+z}{2} \tag{8}$$

The parameter values $P(AB_xC_yD_z)$ for 1:3 III–V quaternary alloys are computed similarly. A general 2:2 III–V quaternary alloy is given by:

$$A_xB_{1-x}C_yD_{1-y} \tag{9}$$

where A and B are group III elements, and C and D are group V elements. The composition variables x and y satisfy the inequalities $0 \le x \le 1$ and $0 \le y \le 1$. As an example, the material $In_{1-x}Ga_xAs_yP_{1-y}$ is mentioned.

The parameters $P(A_xB_{1-x}C_yD_{1-y})$ of a 2:2 III–V quaternary alloy are determined by interpolation between the four ternary side materials:

$$P(A_xB_{1-x}C_yD_{1-y}) = \frac{x(1-x)(yP(A_xB_{1-x}C) + (1-y)P(A_xB_{1-x}D)) + y(1-y)(xP(AC_yD_{1-y}) + (1-x)P(BC_yD_{1-y}))}{x(1-x) + y(1-y)} \tag{10}$$

The interpolation of model parameters for quaternary alloys is also discussed in the literature [2][3][4][5]. A comprehensive survey paper is available [6].

Default Model Parameters for Compound Semiconductors

It is important to understand how the default values for different physical models in different materials are determined. The approach used in Sentaurus Device is summarized here. For example, consider the material `Material`. Assume that no default parameters are defined for this material and a given physical model `Model`.

In this case, use the command `sdevice -P:Material` to see for which models specific default parameters are predefined in the material `Material`:

1. Silicon parameters are used, by default, in the model `Model` if the material `Material` is mole fraction independent.

2. If `Material` is a compound material and dependent on the mole fraction x, the default values of the parameters for the model `Model` are determined by a linear interpolation between the values of the respective parameters of the corresponding 'pure' materials (that is, materials corresponding to $x = 0$ and $x = 1$). For example, for $Al_xGa_{1-x}As$, values of the parameters of GaAs and AlAs are used in the interpolation formula.

3. If `Material` is a quaternary material and dependent on x and y, an interpolation formula, which is based on the values of all corresponding ternary materials, is used. For example, for InGaAsP, the values of four materials (InAsP, GaAsP, GaInP, and InGaAs) are used in the interpolation procedure to obtain the default values of the parameters.

Additional details for each model and specific materials are found in the comments of the parameter file.

Combining Parameter Specifications

Sentaurus Device has built-in values for many parameters, can read parameters from files in a default location, and can read a user-supplied parameter file that can specify parameters for various locations. This section discusses the rules for combining all these specifications.

Parameter handling is affected by the presence of the flag `DefaultParametersFromFile` (specified in the global `Physics` section) and the value of `ParameterInheritance` (specified in the global `Math` section). By default, `ParameterInheritance=Flatten`; by setting `ParameterInheritance=None`, the rules for combining parameter specifications can be altered.

Materialwise Parameters

To determine materialwise parameters, follow these steps:

1. The parameters are initialized from built-in values. These values can depend on the material. For many materials, no appropriate built-in values exist, and silicon values are used instead.

2. If the `DefaultParametersFromFile` flag is present, Sentaurus Device reads the default parameter file for the material. This file can add parameters (for example, add intervals to a mole fraction specification) or overwrite built-in values (for details, see Default Parameters on page 35).

3. If `ParameterInheritance=Flatten` and specifications outside any location-specific section are present, they can add or overwrite the parameter values obtained through the previous two steps, and they also contribute to a separate, global, default parameter set.

4. If your parameter file contains a section for the material, specifications in this section can add to or overwrite the parameter values obtained through the previous three steps. If `ParameterInheritance=None`, specifications outside any location-specific section are handled as if they occurred in a section for the material silicon.

Materialwise specifications in your parameter file are read even when the material is not contained in the structure to be simulated. This is useful, for example, to provide parameters for corner and side materials for materials that are present in the structure.

Apart from corner and side materials, materialwise parameters are rarely used directly; physical bulk models access parameters regionwise, not materialwise. However, materialwise settings can affect regionwise parameters. The next section explains this in detail.

Regionwise Parameters

When your parameter file does not contain a section for a certain region, the parameter values for this region are the same as for the material of the region. In this case, if `ParameterInheritance=None`, the regionwise parameters are discarded entirely and the material parameters are accessed instead. If `ParameterInheritance=Flatten`, the region parameters are a copy of the material parameters (the subtle distinction of these two cases becomes important only when ramping parameters).

If your parameter file does contain a section for a certain region, the parameters for this region are initialized executing Steps 1 and 2 as for the materialwise parameters, using the material of the region to select the built-in values and the default parameter file. If `ParameterInheritance=Flatten`, and a section for this material is present in your parameter file, Steps 3 and 4 are taken as well. Finally, in any case, the section for the region is evaluated and can add to or overwrite the values previously obtained.

> **NOTE** If `ParameterInheritance=None` and a section for a region is present in your parameter file, none of the settings for any parameter in the section for the material of the region (if such a section exists) has an effect on the parameters for that region. In other words, if `ParameterInheritance=None`, the region parameters do not 'inherit' user settings from the material parameters.

Material Interface–Wise Parameters

Material interface–wise parameters are handled similarly to materialwise parameters, simply replace the term 'material' by 'material interface' in the description of the handling of materialwise parameters.

Region Interface–Wise Parameters

Region interface–wise parameters are handled similarly to regionwise parameters, and the relation between region interface–wise parameters and material interface–wise parameters is analogous to the relation between regionwise and materialwise parameters. As an additional complication, if `ParameterInheritance=None` and neither a section for the region interface nor for its material interface is present in your parameter file, the region interface parameters are discarded, and the parameters for material silicon are accessed instead.

Electrode-Wise Parameters

Electrode-wise parameters are handled similarly to materialwise parameters, simply replace the term 'material' by 'electrode' in the description of the handling of materialwise parameters.

Generating a Copy of Parameter File

To redefine a parameter value for a particular material, a copy of the default parameter file must be created. To do this, the command `sdevice -P` prints the parameter file for silicon, with insulator properties. Table 3 lists the principal options for the command `sdevice -P`.

Table 3   Principal options for generating parameter file

Option	Description
`-P:All`	Prints a copy of the parameter file for all materials. Materials are taken from the file `datexcodes.txt`.
`-P:Material`	Prints model parameters for the specified material.
`-P:Material:x`	Prints model parameters for the specified material for mole fraction `x`.
`-P:Material:x:y`	Prints model parameters for the specified material for mole fractions `x` and `y`.
`-P filename`	Prints model parameters for materials and interfaces used in the command file `filename`.
`-r`	Reads parameters from default locations (see Search Strategy for Parameter Files on page 23) before printing parameters. This is analogous to using the `DefaultParametersFromFile` flag (see Materialwise Parameters on page 30).

For regionwise and materialwise parameter specifications, any model and parameter from the default section is usable, even if it is not printed for the particular material.

For mole fraction–dependent parameters, for people, it is difficult to read a parameter file and to obtain the final values of parameters (for example, the band gap) for a particular composition mole fraction. By using the command `sdevice -M <inputfile.cmd>`, Sentaurus Device creates a `models-M.par` file that will contain regionwise parameters with only constant values (instead of the polynomial coefficients) for regions where the composition mole fraction is constant. For regions where the composition is not a constant, Sentaurus Device prints the default material parameters.

As an alternative to the command `sdevice -P`, Sentaurus Device provides the command `sdevice -L`, which supports the same options as described in Table 3 on page 32 for `sdevice -P`. However, rather than generating a single file, it creates separate files for each material and each material interface. Typically, these files are edited and used to provide default parameters (see Default Parameters on page 35).

For example, assume the command file `pp1_des.cmd` is for a simple silicon MOSFET with four electrodes, one silicon region, and one oxide region. By using the command:

```
sdevice -L pp1_des.cmd
```

a parameter file is created in the current directory for each material, material interface, and electrode found in `nmos_mdr.tdr`. In this example, the appropriate files are `Silicon.par`, `Oxide.par`, `Oxide%Silicon.par`, and `Electrode.par`.

In addition, the following `models.par` file is created in the current directory:

```
Region = "Region0" { Insert = "Silicon.par" }
Region = "Region1" { Insert = "Oxide.par" }
RegionInterface = "Region1/Region0" { Insert = "Oxide%Silicon.par" }
Electrode = "gate" { Insert = "Electrode.par" }
Electrode = "source" { Insert = "Electrode.par" }
Electrode = "drain" { Insert = "Electrode.par" }
Electrode = "substrate" { Insert = "Electrode.par" }
```

This `models.par` file can be renamed. It is only used in the simulation if it is specified in the `File` section of the command file of Sentaurus Device:

```
File {...
   Parameter = "models.par"
   ...
```

Undefined Physical Models

For a nonsilicon simulation, the default behavior of Sentaurus Device is to use silicon parameters for models that are not defined in a material used in the simulation. It is useful for noncritical models, but it can lead to confusion, for example, if the semiconductor band gap is not defined, and Sentaurus Device uses that of silicon. Therefore, Sentaurus Device has a list of critical models and stops the simulation, with an error message, if these models are not defined.

> **NOTE** The model is defined in a material if it is present in the default parameter file of Sentaurus Device for the material or it is specified in a user-defined parameter file.

Table 4 lists the critical models (with names from the parameter file of Sentaurus Device) with materials where these models are checked.

Table 4   List of critical models

Model	Insulator	Semiconductor	Conductor
Auger		x	
Bandgap		x	
ConstantMobility		x	
DopingDependence		x	

Table 4   List of critical models (Continued)

Model	Insulator	Semiconductor	Conductor
eDOSmass hDOSmass		x	
Epsilon	x	x	
Kappa	x	x	x
RadiativeRecombination		x	
RefractiveIndex	x	x	
Scharfetter		x	
SchroedingerParameters	x	x	

The models `Bandgap`, `DOSmass`, and `Epsilon` are checked always. For other models, this check is performed for each region, but only if appropriate models in the `Physics` section and equations in the `Solve` section are activated. The thermal conductivity model `Kappa` is checked only if the lattice temperature equation is included.

Drift-diffusion or hydrodynamic simulations activate the checking mobility models `ConstantMobility` and `DopingDependence` (with appropriate models in the `Physics` section).

> **NOTE**   This checking procedure can be switched off by the keyword `-CheckUndefinedModels` in the `Math` section.

The models `eDOSmass` and `hDOSmass` also must be defined for insulators to support tunneling (see). Only the following specifications are acceptable for insulators:

```
eDOSmass {
   Formula = 1
   a = 0
   ml = 0
   mm = <effective mass>    # default 0.42
}

hDOSmass {
   Formula = 1
   a = 0
   b = 0
   c = 0
   d = 0
   e = 0
   f = 0
   g = 0
```

```
    h = 0
    i = 0
    mm = <effective mass>    # default 1
}
```

NOTE   In general, the models `eDOSmass` and `hDOSmass` only need to be
specified for user-specified insulators. The correct values are predefined
for standard insulators.

Default Parameters

Sentaurus Device provides built-in default parameters for many models and materials.
However, Sentaurus Device also offers the option to overwrite the built-in values with default
parameters from files. This option is activated by `DefaultParametersFromFile` in the
global `Physics` section:

```
Physics {
   DefaultParametersFromFile
   ...
}
```

Table 5   File names that are used to initialize default parameters

Location of parameters	File name
Materials	`<material>.par`, for example, `Silicon.par`, `GaAs.par`
Material interfaces	`<material1>%<material2>.par`, for example, `InAlAs%AlGaAs.par` (Instead of %, a comma or space can also be used.)
Contacts	`Contact.par` or `Electrode.par`

Sentaurus Device uses the same search strategy as for inserted files (see Physical Model
Parameters on page 21). Sentaurus Device ships with a selection of parameter files in the
directory `$STROOT/tcad/$STRELEASE/lib/sdevice/MaterialDB`. This directory also
contains release-specific subdirectories, for example:

```
$STROOT/tcad/$STRELEASE/lib/sdevice/MaterialDB/2016.03
$STROOT/tcad/$STRELEASE/lib/sdevice/MaterialDB/2016.12
$STROOT/tcad/$STRELEASE/lib/sdevice/MaterialDB/2017.09
```

You can request that the parameter files from a specific release are taken by specifying the
`ParameterPath` variable in the `File` section:

```
File {
   ParameterPath = "2017.09"
}
```

If a matching file is not found, the built-in default parameters are used unaltered. Check the log file of Sentaurus Device to see which files were actually used.

Named Parameter Sets

Some models in Sentaurus Device support the use of parameter sets that can be named. For example, `EnormalDependence` is the unnamed parameter set used with the Lombardi mobility model. In the parameter file, you can write the following to declare a parameter set for the Lombardi mobility model with the name `myset`:

```
EnormalDependence "myset" {
   B = 3.6100e+07 , 1.5100e+07    # [cm/s]
   C = 1.7000e+04 , 4.1800e+03    # [cm^(5/3)/(V^(2/3)s)]
   ...
}
```

Typically, named parameter sets are used to store alternative parameterizations for a model. They can be selected from the command file by specifying the name with `ParameterSetName` as an option to a model that supports this feature. For example:

```
Physics {
   Mobility (
      PhuMob
      Enormal( Lombardi (ParameterSetName="myset") )
      HighFieldSaturation
   )
}
```

If `ParameterSetName` is not specified, the unnamed parameter set associated with the model is used by default.

Table 6   Models that support named parameter sets

Model name		Parameter set (unnamed)
eQuantumPotential hQuantumPotential		QuantumPotentialParameters
Mobility eMobility hMobility	Enormal(Lombardi) ToCurrentEnormal(Lombardi)	EnormalDependence
	ThinLayer(Lombardi)	EnormalDependence ThinLayerMobility
	Enormal(IALMob) ToCurrentEnormal(IALMob)	IALMob
	ThinLayer(IALMob)	IALMob ThinLayerMobility
	HighFieldSaturation eHighFieldSaturation hHighFieldSaturation Diffusivity eDiffusivity hDiffusivity	HighFieldDependence HydroHighFieldDependence
Piezo(Mobility)	Tensor eTensor hTensor	Piezoresistance
	Factor eFactor hFactor	Piezoresistance EffectiveStressModel
Recombination(Band2Band)		Band2BandTunneling

Auto-Orientation Framework

Some models in Sentaurus Device support an auto-orientation framework that automatically switches between different named parameter sets for model evaluation, based on the surface orientation of the nearest interface.

When the AutoOrientation option is activated for a model, by default, Sentaurus Device looks for and uses parameter sets named "100", "110", and "111" corresponding to surface orientations of {100}, {110}, and {111}. If the nearest interface orientation is {110}, for example, the model is evaluated using the parameter set "110". For surface orientations that fall between {100}, {110}, and {111}, the named parameter set that most closely corresponds to the actual surface orientation is used.

Models that support the auto-orientation framework include:

■ Density-gradient quantization model (`eQuantumPotential`, `hQuantumPotential`)

■ `Lombardi` and `IALMob` mobility models

■ `HighFieldSaturation` and `Diffusivity`

■ `ThinLayer` mobility model

■ Piezoresistance models (`Tensor`, `eTensor`, `hTensor`, `Factor`, `eFactor`, `hFactor`)

■ `EffectiveStressModel` (`Factor`, `eFactor`, `hFactor`)

In the `Plot` section of the command file, the quantities `InterfaceOrientation` and `NearestInterfaceOrientation` can be specified to see the orientation that is used, at each interface face vertex and at every vertex, respectively, when auto-orientation is enabled for a model.

Changing Orientations Used With Auto-Orientation

The auto-orientation framework can be modified to use surface orientations other than {100}, {110}, and {111}. This is accomplished by providing a definition for `AutoOrientation` in the `Math` section of the command file:

```
Math {
    AutoOrientation=(ori₁, ori₂, ...)
}
```

In the above specification, the ori_i values are three-digit integers that represent Miller indices for families of equivalent planes (a cubic lattice structure is assumed). For example, to modify `AutoOrientation` to use the surface orientations {100}, {110}, {111}, and {211}, specify:

```
Math {
    AutoOrientation=(100, 110, 111, 211)
}
```

In this case, models that support `AutoOrientation` will switch between the parameter sets named `"100"`, `"110"`, `"111"`, and `"211"`, depending on the surface orientation of the nearest interface.

Auto-Orientation Smoothing

By default, the switch from one parameter set to another when using auto-orientation occurs abruptly. To enable a smooth transition between different parameter sets, specify a nonzero value for the auto-orientation smoothing distance in the `Math` section:

```
Math {
    AutoOrientationSmoothingDistance = 0.005    # [micrometers]
}
```

The smoothing distance is an approximate measure of the distance over which the transition between different parameter sets will occur. For convenience, specifying `AutoOrientationSmoothingDistance < 0` uses the average interface vertex spacing as the smoothing distance. In many cases, this is a reasonable choice.

When auto-orientation smoothing is used, weights are calculated at each vertex for each orientation-dependent parameter set based on the proximity to the different supported surface orientations:

$$w_i(\text{vertex}) \ = \ \sum_{j=1}^{N_i} \left(\frac{A_j}{A_{\text{total}}} \right) \exp\left(-\frac{d_j - d_{\text{min}}}{d_{\text{smooth}}} \right) \ , \ i = 100, \ 110, \ ... \tag{11}$$

The summation is over all interface vertices associated with orientation i:

- d_{min} is the minimum distance to the interface.
- d_j is the distance to the interface vertex j.
- d_{smooth} is the smoothing distance.
- A_j is the area associated with the interface vertex j.
- A_{total} is the total interface area.

At each vertex, very small weights are set to zero, and the remaining weights are normalized so that their sum is equal to one.

During model evaluation, the weights for each orientation at a vertex are used to obtained a weighted average of the quantity being calculated.

In the `Plot` section of the command file, the quantity `AutoOrientationSmoothing` can be specified to see the vertices where auto-orientation smoothing is used and the dominant orientation at those vertices.

References

[1]　C. K. Williams *et al.*, "Energy Bandgap and Lattice Constant Contours of III-V Quaternary Alloys of the Form $A_xB_yC_zD$ or $AB_xC_yD_z$," *Journal of Electronic Materials*, vol. 7, no. 5, pp. 639–646, 1978.

[2]　T. H. Glisson *et al.*, "Energy Bandgap and Lattice Constant Contours of III-V Quaternary Alloys," *Journal of Electronic Materials*, vol. 7, no. 1, pp. 1–16, 1978.

[3]　M. P. C. M. Krijn, "Heterojunction band offsets and effective masses in III–V quaternary alloys," *Semiconductor Science and Technology*, vol. 6 , no. 1, pp. 27–31, 1991.

[4] S. Adachi, "Band gaps and refractive indices of AlGaAsSb, GaInAsSb, and InPAsSb: Key properties for a variety of the 2–4-mm optoelectronic device applications," *Journal of Applied Physics*, vol. 61, no. 10, pp. 4869–4876, 1987.

[5] R. L. Moon, G. A. Antypas, and L. W. James, "Bandgap and Lattice Constant of GaInAsP as a Function of Alloy Composition," *Journal of Electronic Materials*, vol. 3, no. 3, pp. 635–644, 1974.

[6] I. Vurgaftman, J. R. Meyer, and L. R. Ram-Mohan, "Band parameters for III–V compound semiconductors and their alloys," *Journal of Applied Physics*, vol. 89, no. 11, pp. 5815–5875, 2001.

Mixed-Mode Sentaurus Device

This chapter describes the specification of circuits and compact devices.

Overview

Sentaurus Device is a single-device simulator, and a mixed-mode device and circuit simulator. A single-device command file is defined through the mesh, contacts, physical models, and solve command specifications.

For a multidevice simulation, the command file must include specifications of the mesh (`File` section), contacts (`Electrode` section), and physical models (`Physics` section) for each device. A circuit netlist must be defined to connect the devices (see Figure 6), and solve commands must be specified that solve the whole system of devices.

Netlist

```
File {...}
Electrode {...}
Physics {...}
```

```
File {...}
Electrode {...}
Physics {...}
```

Single Device   **Multiple Devices**
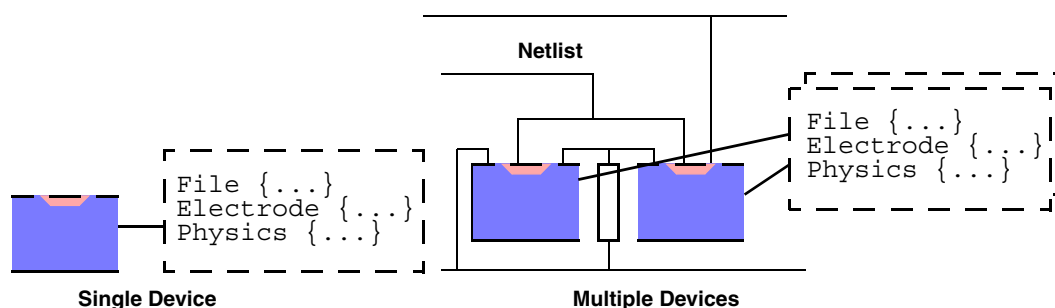
Figure 6   Each device in a multidevice simulation is connected with a circuit netlist

The `Device` command defines each physical device. A command file can have any number of `Device` sections. The `Device` section defines a device, but a `System` section is required to create and connect devices.

Sentaurus Device also provides a number of compact models for use in mixed-mode simulations.

Sentaurus Device supports different ways of specifying compact models:

- `System` section of the command file

  Electrical and thermal circuits can be defined in the `System` section. Initial conditions for the circuit nodes can be specified, as well as `Plot` statements to generate output (see System Section on page 55).

- Netlist file

  Netlist files support a subset of the Synopsys HSPICE® language. They can be used to specify parameter sets and instances of SPICE and HSPICE models (see Netlist Files on page 45).

- SPICE circuit files

  SPICE circuit files (extension `.scf`) are available for SPICE and HSPICE models, as well as for built-in models. Both parameter sets and instances can be specified (see SPICE Circuit Files on page 51).

- Compact circuit files

  Compact circuit files (extension `.ccf`) support the compact model interface in Sentaurus Device. Devices and parameter sets for user-defined models must be specified in compact circuit files. Instances may appear either in compact circuit files or in the `System` section of the command file (see User-Defined Circuit Models on page 63).

Compact Models

Sentaurus Device provides four different types of models:

- SPICE

  These include compact models from Berkeley SPICE 3 Version 3F5. The BSIM3v3.2, BSIM4.1.0, and BSIMPDv2.2.2 MOS models are also available (see Table 8 on page 43).

- HSPICE

  Several frequently used HSPICE models are provided (see Table 9 on page 44).

- Built-in

  There are several special-purpose models (see Table 7 on page 43).

- User-defined

  A compact model interface (CMI) is available for user-defined models. These models are implemented in C++ and linked to Sentaurus Device at runtime. No access to the source code of Sentaurus Device is necessary (see User-Defined Circuit Models on page 63).

This section describes the incorporation of compact models in mixed-mode simulations. The *Compact Models User Guide* provides references for the different model types.

Hierarchical Description of Compact Models

In Sentaurus Device, the compact models comprise three levels:

- Device

  This describes the basic properties of a compact model and includes the names of the model, electrodes, thermodes, and internal variables; and the names and types of the internal states and parameters. The devices are predefined for SPICE models and built-in models. For user-defined models, you must specify the devices.

- Parameter set

  Each parameter set is derived from a device. It defines default values for the parameters of a compact model. Usually, a parameter set defines parameters that are shared among several instances. Most SPICE and built-in models provide a default parameter set, which can be directly referenced in a circuit description. For more complicated models, such as MOSFETs, you can introduce new parameter sets.

- Instance

  Instances correspond to the elements in the Sentaurus Device circuit. Each instance is derived from a parameter set. If necessary, an instance can override the values of its parameters.

For SPICE and built-in models, you define parameter sets and instances. For user-defined models, it is possible (and required) to introduce new devices. This is described in the *Compact Models User Guide*.

Table 7 lists the built-in models, whereas Table 8 and Table 9 on page 44 present an overview of the available SPICE and HSPICE models.

Table 7   Built-in models in Sentaurus Device

Model	Device	Default parameter set
Electrothermal resistor	`Ter`	`Ter_pset`
Parameter interface	`Param_Interface_Device`	`Param_Interface`
SPICE temperature interface	`Spice_Temperature_Interface_Device`	`Spice_Temperature_Interface`

Table 8   SPICE models in Sentaurus Device

Model	Device	Default parameter set
Resistor	`Resistor`	`Resistor_pset`
Capacitor	`Capacitor`	`Capacitor_pset`
Inductor	`Inductor`	`Inductor_pset`

Table 8   SPICE models in Sentaurus Device (Continued)

Model	Device	Default parameter set
Coupled inductors	`mutual`	`mutual_pset`
Voltage-controlled switch	`Switch`	`Switch_pset`
Current-controlled switch	`CSwitch`	`CSwitch_pset`
Voltage source	`Vsource`	`Vsource_pset`
Current source	`Isource`	`Isource_pset`
Voltage-controlled current source	`VCCS`	`VCCS_pset`
Voltage-controlled voltage source	`VCVS`	`VCVS_pset`
Current-controlled current source	`CCCS`	`CCCS_pset`
Current-controlled voltage source	`CCVS`	`CCVS_pset`
Junction diode	`Diode`	`Diode_pset`
Bipolar junction transistor	`BJT`	`BJT_pset`
Junction field-effect transistor	`JFET`	`JFET_pset`
MOSFET	`Mos1`	`Mos1_pset`
	`Mos2`	`Mos2_pset`
	`Mos3`	`Mos3_pset`
	`Mos6`	`Mos6_pset`
	`BSIM1`	`BSIM1_pset`
	`BSIM2`	`BSIM2_pset`
	`BSIM3`	`BSIM3_pset`
	`BSIM4`	`BSIM4_pset`
	`B3SOI`	`B3SOI_pset`
GaAs MESFET	`MES`	`MES_pset`

Table 9   HSPICE models in Sentaurus Device

Model	Device
HSPICE Level 1	`HMOS_L1`
HSPICE Level 2	`HMOS_L2`
HSPICE Level 3	`HMOS_L3`
HSPICE Level 28	`HMOS_L28`

Table 9   HSPICE models in Sentaurus Device (Continued)

Model	Device
HSPICE Level 49	HMOS_L49
HSPICE Level 53	HMOS_L53
HSPICE Level 54	HMOS_L54
HSPICE Level 57	HMOS_L57
HSPICE Level 59	HMOS_L59
HSPICE Level 61	HMOS_L61
HSPICE Level 62	HMOS_L62
HSPICE Level 64	HMOS_L64
HSPICE Level 68	HMOS_L68
HSPICE Level 69	HMOS_L69
HSPICE Level 72	HMOS_L72
HSPICE Level 73	HMOS_L73
HSPICE Level 76	HMOS_L76

Netlist Files

Sentaurus Device accepts HSPICE netlists that are provided in a separate file. A netlist is specified in the `System` section as follows:

```
System {
   Netlist = "spice_netlist.sp"
}
```

Sentaurus Device can process only a subset of the HSPICE netlist syntax. The recognized syntax is described in the following sections.

Structure of Netlist File

The first line of a netlist file is assumed to be a title line and is always ignored:

```
.TITLE 'amplifier netlist'
```

The title line is followed by a sequence of HSPICE statements, and the netlist is terminated by an optional `.END` statement:

```
.END
```

Everything after the final `.END` statement is ignored.

The netlist parser is case insensitive, except for string literals or file names in `.INCLUDE` statements:

```
.PARAM s = str('This is a case sensitive string.')
.INCLUDE 'Case/Sensitive/Filename'
```

Comments

A line starting with either the `$` or `*` character is a comment line, for example:

```
* This is a comment.
```

You can use in-line comments after the `$` character:

```
R1 1 2 R=100  $ drain resistor
```

Continuation Lines

Use a `+` character in the first column to indicate a continuation line:

```
R1 1 0
+ R=500
```

The INCLUDE Statement

Use the `.INCLUDE` statement to include another netlist in the current netlist:

```
.INCLUDE models.sp
```

Numeric Constants

You can enter numbers in one of the following formats:

- Integer
- Floating point

- Floating point with an integer exponent
- Integer with a scale factor
- Floating point with a scale factor listed in Table 10.

Table 10   Scale factors

Scale factor	Description	Multiplying factor
t	tera	10^{12}
g	giga	10^{9}
meg or x	mega	10^{6}
k	kilo	10^{3}
mil	one-thousandth of an inch	$25.4 \cdot 10^{-6}$
m	milli	10^{-3}
u	micro	10^{-6}
n	nano	10^{-9}
p	pico	10^{-12}
f	femto	10^{-15}
a	atto	10^{-18}

NOTE   The scale factor `a` is not a scale factor in a character string that contains `amps`. For example, the expression `20amps` is interpreted as 20 amperes of current, not as `20e-18mps`.

Examples

```
7
-4.5
3e8
-1.2e-9
6k
-8.9meg
```

Parameters and Expressions

Parameters in HSPICE are names that you associate with a value. Numeric and string parameters are supported:

```
.PARAM a = 4
.PARAM b = '2*a + 7'
```

```
.PARAM s = str('This is a string')
.PARAM t = str(s)
```

The following built-in mathematical functions are supported:

```
sin, cos, tan, asin, acos, atan, sinh, cosh, tanh, abs, sqrt, pow, pwr, log,
log10, exp, db, int, nint, sgn, sign, floor, ceil, min, max
```

Subcircuits

Reusable cells can be specified as subcircuits. The general definition is given by:

```
.SUBCKT name n1 n2 ... [param1=val] [param2=val] ...
.ENDS
```

or:

```
.MACRO name n1 n2 ... [param1=val] [param2=val] ...
.EOM
```

String parameters are supported as well:

```
.SUBCKT name n1 n2 ... [param=str('string')] ...
.ENDS
```

Examples

```
.PARAM P5=5 P2=10

.SUBCKT SUB1 1 2 P4=4
  R1 1 0 P4
  R2 2 0 P5
  X1 1 2 SUB2 P6=7
  X2 1 2 SUB2
.ENDS

.MACRO SUB2 1 2 P6=11
  R1 1 2 P6
  R2 2 0 P2
.EOM

X1 1 2 SUB1 P4=6

X2 3 4 SUB2 P6=15
```

Model Statements

A `.MODEL` statement has the following general syntax:

```
.MODEL model_name type [level=num]
+ [pname1=val1] [pname2=val2] ...
```

Table 11   Recognized model types

Type	Description	Type	Description
c	Capacitor model	npn	NPN BJT model
csw	Current-controlled switch	pjf	P-channel JFET model
d	Diode model	pmf	P-channel MESFET
l	Mutual inductor model	pmos	P-channel MOSFET model
njf	N-channel JFET model	pnp	PNP BJT model
nmf	N-channel MESFET	r	Resistor model
nmos	N-channel MOSFET model	sw	Voltage-controlled switch

Examples

```
.MODEL mod1 NPN BF=50 IS=1e-13 VFB=50 PJ=3 N=1.05

.MODEL mod2 PMOS LEVEL=72
+ aigbinv = 0.0111
+ at = -0.00156
```

Elements

Element names must begin with a specific letter for each element type.

Table 12   Supported HSPICE element types

First letter	Element	Example
c	Capacitor	Cbypass 1 0 10pf
d	Diode	D7 3 9D1
e	Voltage-controlled voltage source	Ea 1 2 3 4 K
f	Current-controlled current source	Fsub n1 n2 vin 2.0
g	Voltage-controlled current source	G12 4 0 3 0 10
h	Current-controlled voltage source	H3 4 5 Vout 2.0

Table 12   Supported HSPICE element types (Continued)

First letter	Element	Example
i	Current source	`IA 2 6 1e-6`
j	JFET or MESFET	`J1 7 2 3 model_jfet w=10u l=10u`
k	Linear mutual inductor	`K1 L1 L2 0.98`
l	Linear inductor	`Lx a b 1e-9`
m	MOS transistor	`M834 1 2 3 4 N1`
q	Bipolar transistor	`Q5 3 6 7 8 pnp1`
r	Resistor	`R10 21 10 1000`
v	Voltage source	`V1 8 0 5`
x	Subcircuit call	`X1 2 4 17 31 MULTI WN=100 LN=5`

Table 13   Supported Berkeley SPICE element types

First letter	Element	Example
s	Voltage-controlled switch	`S1 1 2 3 4 SWITCH1 ON`
w	Current-controlled switch	`W1 1 2 VCLOCK SWITCHMOD1`
z	GaAs MESFET	`Z1 7 2 3 ZM1 AREA=2`

Physical Devices

Sentaurus Device supports an extension of the HSPICE netlist format so that physical devices can be specified within an HSPICE netlist. An `.SDEVICE` command declares the name of the physical device and its contacts:

```
.SDEVICE device_name drain gate source bulk
```

Instances of a physical device can be inserted into the netlist using the subcircuit command:

```
x1 d g s b device_name
```

An `.SDEVICE` statement and a subcircuit instantiation are equivalent to the following specification in the `System` section of a Sentaurus Device command file:

```
System {
   device_name x1 (drain=d gate=g source=s bulk=b)
}
```

NOTE   HSPICE names are case insensitive, and the netlist parser converts all identifiers to lowercase. As a consequence, physical devices in Sentaurus Device must be specified in lowercase as well.

Netlist Commands

A limited set of netlist commands is recognized.

To make node names global across all subcircuits, use a `.GLOBAL` statement:

```
.GLOBAL node1 node2 node3 ...
```

Use the `.OPTION PARHIER` statement to specify scoping rules:

```
.OPTION PARHIER=GLOBAL|LOCAL
```

Other HSPICE netlist commands, which have not been explicitly mentioned already, are ignored.

SPICE Circuit Files

Compact models can be specified in an external SPICE circuit file, which is recognized by the extension `.scf`. The declaration of a parameter set can be:

```
PSET pset
   DEVICE dev
   PARAMETERS
   parameter0 = value0
   parameter1 = value1
   ...
END PSET
```

This declaration introduces the parameter set `pset` that is derived from the device `dev`. It assigns default values for the given parameters. The device `dev` should have already declared the parameter names. Furthermore, the values assigned to the parameters must be of the appropriate type.

Table 14   Parameters types in SPICE circuit files

Parameter type	Example	Parameter type	Example
char	c = 'n'	char[]	cc = ['a' 'b' 'c']
double	d = 3.14	double[]	dd = [1.2 -3.4 5e6]

Table 14   Parameters types in SPICE circuit files (Continued)

Parameter type	Example	Parameter type	Example
`int`	`i = 7`	`int[]`	`ii = [1 2 3]`
`string`	`s = "hello world"`	`string[]`	`ss = ["hello" "world"]`

Similarly, the circuit instances can be declared as:

```
INSTANCE inst
   PSET pset
   ELECTRODES e0 e1 ...
   THERMODES t0 t1 ...
   PARAMETERS
      parameter0 = value0
      parameter1 = value1
      ...
END INSTANCE
```

According to this declaration, the instance `inst` is derived from the parameter set `pset`. Its electrodes are connected to the circuit nodes `e0`, `e1`, ..., and its thermodes are connected to `t0`, `t1`, ...

This instance also defines or overrides parameter values.

See Compact Models User Guide, Syntax of Compact Circuit (.ccf) Files on page 174 for the complete syntax of the input language for SPICE circuit files.

Example

Consider the following simple rectifier circuit:
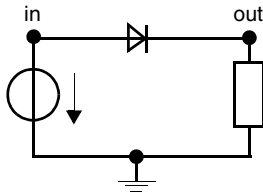
The circuit comprises three compact models and can be defined in the file `rectifier.scf` as:

```
PSET D1n4148
   DEVICE Diode
   PARAMETERS
      is = 0.1p   // saturation current
      rs = 16     // Ohmic resistance
```

```
      cjo = 2p    // junction capacitance
      tt = 12n    // transit time
      bv = 100    // reverse breakdown voltage
      ibv = 0.1p  // current at reverse breakdown voltage
  END PSET

  INSTANCE v
    PSET Vsource_pset
    ELECTRODES in 0
    PARAMETERS sine = [0 5 1meg 0 0]
  END INSTANCE

  INSTANCE d1
    PSET D1n4148
    ELECTRODES in out
    PARAMETERS temp = 30
  END INSTANCE

  INSTANCE r
    PSET Resistor_pset
    ELECTRODES out 0
    PARAMETERS resistance = 1000
  END INSTANCE
```

The parameter set `D1n4148` defines the parameters shared by all diodes of type `1n4148`.
Instance parameters are usually different for each diode, for example, their operating
temperature.

> **NOTE** A parameter set must be declared before it can be referenced by an
> instance.

The *Compact Models User Guide* further explains the SPICE parameters in this example. The
command file for this simulation can be:

```
File {
    SPICEPath = ". lib spice/lib"
}
System {
    Plot "rectifier" (time() v(in) v(out) i(r 0))
}
Solve {
    Circuit
    NewCurrentPrefix = "transient_"
    Transient (InitialTime = 0 FinalTime = 0.2e-5
          InitialStep = 1e-7 MaxStep = 1e-7) {Circuit}
}
```

The `SPICEPath` in the `File` section is assigned a list of directories. All directories are scanned
for `.scf` files (SPICE circuit files).

Check the log file of Sentaurus Device to see which circuit files were found and used in the simulation.

The `System` section contains a `Plot` statement that produces the plot file `rectifier_des.plt`. The simulation time, the voltages of the nodes `in` and `out`, and the current from the resistor `r` into the node `0` are plotted. The `Solve` section describes the simulation. The keyword `Circuit` denotes the circuit equations to be solved.

The instances in a circuit also can appear directly in the `System` section of the command file, for example:

```
System {
   Vsource_pset v (in 0) {sine = (0 5 1meg 0 0)}
   D1n4148 d1 (in out) {temp = 30}
   Resistor_pset r (out 0) {resistance = 1000}

   Plot "rectifier" (time() v(in) v(out) i(r 0))
}
```

Device Section

The `Device` sections of the command file define the different device types used in the system to be simulated. Each device type must have an identifier name that follows the keyword `Device`. Each `Device` section can include the `Electrode`, `Thermode`, `File`, `Plot`, `Physics`, and `Math` sections. For example:

```
Device "resist" {
   Electrode {
   ...
   }
   File {
   ...
   }
   Physics {
   ...
   }
...
}
```

If information is not specified in the `Device` section, information from the lowest level of the command file is taken (if defined there), for example:

```
# Default Physics section
Physics{
...
}
```

```
Device resist {
   # This device contains no Physics section
   # so it uses the default set above
   Electrode{
   ...
   }
   File{
   ...
   }
}
```

System Section

The System section defines the netlist of physical devices and circuit elements to be solved. The netlist is connected through circuit nodes. By default, a circuit node is electrical, but it can be declared to be electrical or thermal:

```
Electrical { enode0 enode1 ... }
Thermal { tnode0 tnode1 ... }
```

Each electrical node is associated with a voltage variable, and each thermal node is associated with a temperature variable. Node names are numeric or alphanumeric. The node 0 is predefined as the ground node (0 V).

Compact models can be defined in HSPICE netlist files (see Netlist Files on page 45) or in SPICE circuit files (see SPICE Circuit Files on page 51). However, instances of compact models can also appear directly in the System section of the command file:

```
parameter-set-name instance-name (node0 node1 ...) {
   <attributes>
}
```

The order of the nodes in the connectivity list corresponds to the electrodes and thermodes in the SPICE device definition (refer to the *Compact Models User Guide*).

The connectivity list is a list of contact-name=node-name connections, separated by white space. Contact-name is the name of the contact from the grid file of the given device, and node-name is the name of the circuit netlist node as previously defined in the definition of a circuit element.

Physical devices are defined as:

```
device-type instance-name (connectivity list) {<attributes>}
```

The connectivity list of a physical device explicitly establishes the connection between a contact and node. For example, the following defines a physical diode and circuit diode:

```
Diode_pset circuit_diode (1 2) {...}                # circuit diode
Diode243   device_diode (anode=1 cathode=2) {...}   # physical diode
```

Both diodes have their anode connected to node `1` and their cathode connected to node `2`. In the case of the circuit diode, the device specification defines the order of the electrodes (see Compact Models User Guide, Syntax of Compact Circuit (.ccf) Files on page 174). Conversely, the connectivity for the physical diode must be given explicitly. The names `anode` and `cathode` of the contacts are defined in the grid file of the device. The device types of the physical devices must be defined elsewhere in the command file (with `Device` sections) or an external .device file.

The `System` section can contain the initial conditions of the nodes. Three types of initialization can be specified:

- Fixed values (`Set`)
- Fixed until transient (`Initialize`)
- Initialized only for the first solve (`Hint`)

In addition, the `Unset` command is available to free a node after a `Set` command. The fixed value set by a `Set` command remains fixed during all subsequent simulations until a `Set` or an `Unset` command is used in the `Solve` section or the node itself becomes a `Goal` of a `Quasistationary`.

The `System` section can also contain `Plot` statements to generate plot files of node values, currents through devices, and parameters of internal circuit elements. For a simple case of one device without circuit connections (besides resistive contacts), the keyword `System` is not required because the system is implicit and trivial given the information from the `Electrode`, `Thermode`, and `File` sections at the base level.

Physical Devices

A physical device is instantiated using a previously defined device type, name, connectivity list, and optional parameters, for example:

```
device_type instance-name (<connectivity list>) {
   <optional device parameters>
}
```

If no extra device parameters are required, the device is specified without braces, for example:

```
device-type instance-name (<connectivity list>)
```

The device parameters overload the parameters defined in the device type. As for a device type of Sentaurus Device, the parameters can include `Electrode`, `Thermode`, `File`, `Plot`, `Physics`, and `Math` sections.

> **NOTE**   Electrodes have `Voltage` statements that set the voltage of each electrode. If the electrodes are connected to nodes through the connectivity list, these values are only hints (as defined by the keyword `Hint`) for the first Newton solve, but do not set the electrodes to those values as with the keyword `Set`. By default, an electrode that is connected to a node is floating.
>
> Electrodes must be connected to electrical nodes and thermodes to thermal nodes. This enables electrodes and thermodes to share the same contact name or number.

Circuit Devices

SPICE instances can be declared in HSPICE netlist files (see Netlist Files on page 45) or in SPICE circuit files as discussed in SPICE Circuit Files on page 51. They can also appear directly in the `System` section of the command file, for example:

```
pset inst (e0 e1 ... t0 t1 ...) {
   parameter0 = value0
   parameter1 = value1
   ...
}
```

This declaration in the command file provides the same information as the equivalent declaration in an HSPICE netlist file or a SPICE circuit file.

Array parameters must be specified with parentheses, not braces, for example:

```
dd = (1.2 -3.4 5e6)
ss = ("hello" "world")
```

Certain SPICE models have internal nodes that are accessible through the form `instance_name.internal_node`. For example, a SPICE inductance creates an internal node `branch`, which represents the current through the instance. Therefore, the expression `v(l.branch)` can be used to gain access to the current through the inductor `l`. This is useful for plotting internal data or initializing currents through inductors (refer to the *Compact Models User Guide* for a list of the internal nodes for each model).

Electrical and Thermal Netlist

Sentaurus Device allows both electrical and thermal netlists to coexist in the same system, for example:

```
System {
   Thermal (ta tc t300)
   Set (t300 = 300)
   Hint (ta = 300 tc = 300)

   Isource_pset i (a 0) {dc = 0}
   PRES pres ("Anode"=a "Cathode"=0 "Anode"=ta "Cathode"=tc)
   Resistor_pset ra (ta t300) {resistance = 1}
   Resistor_pset rc (tc t300) {resistance = 1}

   Plot "pres" (v(a) t(ta) t(tc) h(pres ta) h(pres tc) i(pres 0))
}
```

The current source `i` drives a resistive physical device `pres`. This device has two contacts `Anode` and `Cathode` that are connected to the circuit nodes `a` and `0`, and are also used as thermodes, which are connected to the heat sink `t300` through two thermal resistors `ra` and `rc`.

The `Plot` statement accesses the voltage of the node `a`, the temperature of the nodes `ta` and `tc`, the heat flux from `pres` into `ta` and `tc`, and the current from `pres` into the ground node `0`.

Many SPICE models provide a temperature parameter for electrothermal simulations. In Sentaurus Device, a temperature parameter is connected to the thermal circuit by a parameter interface.
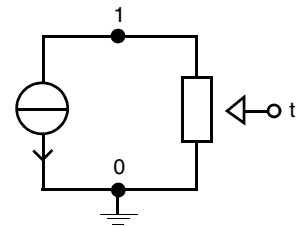
For example, in this simple circuit, the resistor `r` is a SPICE semiconductor resistor whose resistance depends on the value of the temperature parameter `temp`:

$$r_0 = \text{rsh} \cdot \frac{l - \text{narrow}}{w - \text{narrow}}$$

(12)

$$r(\text{temp}) = r_0 \cdot (1 + \text{tc}_1 \cdot (\text{temp} - \text{tnom}) + \text{tc}_2 \cdot (\text{temp} - \text{tnom})^2)$$

To feed the value of the thermal node `t` as a parameter into the resistor `r`, a parameter interface is required:

```
System {
   Thermal (t)
   Set (t = 300)

   Isource_pset i (1 0) {dc = 1}
```

```
      cres_pset r (1 0) {temp = 27 l = 0.01 w = 0.001}
      Param_Interface rt (t) {parameter = "r.temp" offset = -273.15}

      Plot "cres" (t(t) p(r temp) i(r 0) v(1))
  }
```

The parameter set `cres_pset` for the resistor `r` is defined in an external SPICE circuit file:

```
  PSET cres_pset
     DEVICE Resistor
     PARAMETERS
        rsh = 1
        narrow = 0
        tc1 = 0.01
        tnom = 27
  END PSET
```

The parameter interface `rt` updates the value of `temp` in `r` when the variable `t` is changed. This is the general mechanism in Sentaurus Device, which allows a circuit node to connect to a model parameter.

> **NOTE** It is important to declare the parameter interface after the instance to which it refers. Otherwise, Sentaurus Device cannot establish the connection between the parameter interface and the instance.

Temperatures in Sentaurus Device are defined in kelvin. SPICE temperatures are measured in degree Celsius. Therefore, an offset of –273.15 must be used to convert kelvin to degree Celsius.

The parameter `Spice_Temperature` in the `Math` section is used to initialize the global SPICE circuit temperature at the beginning of a simulation. It cannot be used to change the SPICE temperature later. To modify the SPICE temperature during a simulation, a so-called SPICE temperature interface must be used.

A SPICE temperature interface has one contact that can be connected to an electrode or a thermode. When the value u of the electrode or thermode changes, the global SPICE temperature is updated according to:

$$\text{Spice temperature} = \text{offset} + c_1 u + c_2 u^2 + c_3 u^3 \tag{13}$$

By default, $\text{offset} = c_2 = c_3 = 0$ and $c_1 = 1$. Therefore, the SPICE temperature interface ensures that the global SPICE temperature is identical to the value u.

In the following example, a SPICE temperature interface is used to ramp the global SPICE temperature from $300\,\text{K}$ to $400\,\text{K}$:

```
System {
   Set (st = 300)
   Spice_Temperature_Interface ti (st) { }
}
Solve {
   Quasistationary (Goal {Node = st Value = 400} DoZero
      InitialStep = 0.1 MaxStep = 0.1) {
      Coupled {Circuit}
      }
}
```

Set, Unset, Initialize, and Hint

The keywords `Set`, `Initialize`, and `Hint` are used to set nodes to a specific value.

`Set` establishes the node value. This value remains fixed during all subsequent simulations until a `Set` or an `Unset` command is used in the `Solve` section (see Mixed-Mode Electrical Boundary Conditions on page 69), or the node becomes a `Goal` of a `Quasistationary`, which controls the node itself (see Quasistationary in Mixed Mode on page 80). For a set node, the corresponding equation (that is, the current balance equation for electrical nodes and the heat balance equation for thermal nodes) is not solved, unlike an unset node.

> **NOTE** The `Set` and `Unset` commands exist in the `Solve` section. These act like the `System`-level `Set` but allow more flexibility (see System Section on page 55).

The `Set` command can also be used to change the value of a parameter in a compact model. For example, the resistance of the resistor `r1` changes to $1000\,\Omega$:

```
Set (r1."resistance" = 1000)
```

`Initialize` is similar to the `Set` statement except that node values are kept only during nontransient simulations. When a transient simulation starts, the node is released with its actual value, that is, the node is unset.

> **NOTE** The keyword `Initialize` can be used with an internal node to set a current through an inductor before a transient simulation. For example, the keyword:
>
> ```
> Inductor_pset L2 (a b){ inductance = 1e-5 }
> Initialize (L2.branch = 1.0e-4)
> ```

Hint provides a guess value for an unset node for the first Newton step only. The numeric value is given in volt, ampere, or kelvin. A current value only makes sense for internal current nodes in circuit devices. The commands are used as follows:

```
Set ( <node> = <float> <node> = <float> ... )
Unset (<node> <node> ... )
Initialize ( <node> = <float> <node> = <float> ... )
Hint ( <node> = <float> <node> = <float> ... )
```

For example:

```
Set ( anode = 5 )
```

System Plot

The System section can contain any number of Plot statements to print voltages at nodes, currents through devices, or circuit element parameters. The output is sent to a given file name. If no file name is provided, the output is sent to the standard output file and the log file. The Plot statement is:

```
Plot (<plot command list>)
Plot <filename> (<plot command list>)
```

where <plot command list> is a list of nodes or plot commands as defined in Table 205 on page 1399.

> **NOTE** Plot commands are case sensitive.

Two examples are:

```
Plot (a b i(r1 a) p(r1 rT) p(v0 "sine[0]"))
Plot "plotfile" (time() v(a b) i(d1 a))
```

> **NOTE** The Plot command does not print the time by default. When plotting a transient simulation, the time() command must be added.

AC System Plot

An ACPlot statement in the System section can be used to modify the output in the Sentaurus Device AC plot file:

```
System {
   ACPlot (<plot command list>)
}
```

The `<plot command list>` is the same as the system plot command discussed in System Plot on page 61.

If an `ACPlot` statement is present, the given quantities are plotted in the Sentaurus Device AC plot file with the results from the AC analysis. Otherwise, only the voltages at the AC nodes are plotted with the results from the AC analysis.

File Section

In the `File` section, one of the following can be specified:

- Output file name and the small-signal AC extraction file name (keywords `Output` and `ACExtract`)
- Sentaurus Device directory path (keyword `DevicePath`)
- Search path for SPICE models and compact models (keywords `SPICEPath` and `CMIPath`)
- Default file names for the devices

The syntax for these keywords is shown in Table 185 on page 1381.

The variables `Output` and `ACExtract` can be assigned a file name. Only a file name without an extension is required. Sentaurus Device automatically appends a predefined extension:

```
File {
   Output = "mct"
   ACExtract = "mct"
}
```

The variables `DevicePath`, `SPICEPath`, and `CMIPath` represent search paths. They must be assigned a list of directories for which Sentaurus Device searches, for example:

```
File {
   DevicePath = "../devices:/usr/local/tcad/devices:."
   SPICEPath = ". lib lib/spice"
   CMIPath = ". libcmi"
}
```

Device files (extension .device) in `DevicePath` are loaded. The devices found can then be used in the `System` section.

SPICE circuit files (extension .scf) in `SPICEPath` are parsed and added to the `System` section of the command file.

The compact circuit files (extension `.ccf`) and the corresponding shared object files (extension `.so.arch`) in `CMIPath` are parsed and are added to the `System` section of the command file.

Device-specific keywords are defined under the file entry in the `Device` section.

SPICE Circuit Models

Sentaurus Device supports SPICE circuit models for mixed-mode simulations. These models are based on Berkeley SPICE 3 Version 3F5. Several frequently used HSPICE models are also available. A detailed description of the SPICE models can be found in the *Compact Models User Guide*.

User-Defined Circuit Models

Sentaurus Device provides a compact model interface (CMI) for user-defined circuit models. The models are implemented in C++ by you and linked to Sentaurus Device at runtime. Access to the source code of Sentaurus Device is not required.

To implement a new user-defined model:

1. Provide a corresponding equation for each variable in the compact model. For electrode voltages, compute the current flowing from the device into the electrode. For an internal model variable, use a model equation.

2. Write a formal description of the new compact model. This compact circuit file is read by Sentaurus Device before the model is loaded.

3. Implement a set of interface subroutines C++. Sentaurus Device provides a runtime environment.

4. Compile the model code into a shared object file, which is linked at runtime to Sentaurus Device. A `cmi` script executes this compilation.

5. Use the variable `CMIPath` in the `File` section of the command file to define a search path.

6. Reference user-defined compact models in compact circuit files (with the extension `.ccf`) or directly in the `System` section of the command file.

Mixed-Mode Math Section

The following SPICE circuit parameters can be specified in the global `Math` section:

```
Spice_Temperature = ...
Spice_gmin = ...
```

The value of `Spice_Temperature` denotes the global SPICE circuit temperature. Its default value is 300.15 K. The parameter `Spice_gmin` refers to the minimum conductance in SPICE. The default value is $10^{-12}\,\Omega^{-1}$.

Using Mixed-Mode Simulation

In Sentaurus Device, mixed-mode simulations are handled as a direct extension of single device simulations.

From Single-Device File to Multidevice File

The command file of Sentaurus Device accepts both single-device and multidevice problems. Although the two forms of input look different, they fit in the same input syntax pattern. This is possible because the command file has multiple levels of definitions and there is a built-in default mechanism for the `System` section.

```
File {...}
Electrode {...}          } Global
  ...

Device <type> {
  File {...}
  Electrode {...}        } Device
  ...
}

System {
  <type> <name> {
  File {...}
  Electrode {...}        } Instance
  }
}
```

Figure 7   Three levels of device definition

The complete input syntax allows for three levels of device definition: global, device, and instance (see Figure 7 on page 64). The three levels are linked in that the global level is the default for the device level and instance level.

By default, if no `Device` section exists, a single device is created with the content of a global device. If no `System` section exists, one is created with this single device. In this way, single devices are converted to multidevice problems with a single device and no circuit.

> **NOTE** The device that is created by default has the name " " (that is, an empty string).

This translation process can be performed manually by creating a `Device` and `System` section with a single entry (see Figure 8).

```
Electrode {
   {name="anode" Voltage=0}
   {name="cathode" Voltage=1}
}

File {
   Grid = "diode.tdr"
   Output = "diode"
}
```

```
File {
   Output = "diode"
}
Device diode {
   Electrode {
      {name="anode" Voltage=0}
      {name="cathode" Voltage=1}
   }
   File {
      Grid = "diode.tdr"
   }
}

System {
   diode diode1 ...
}
```
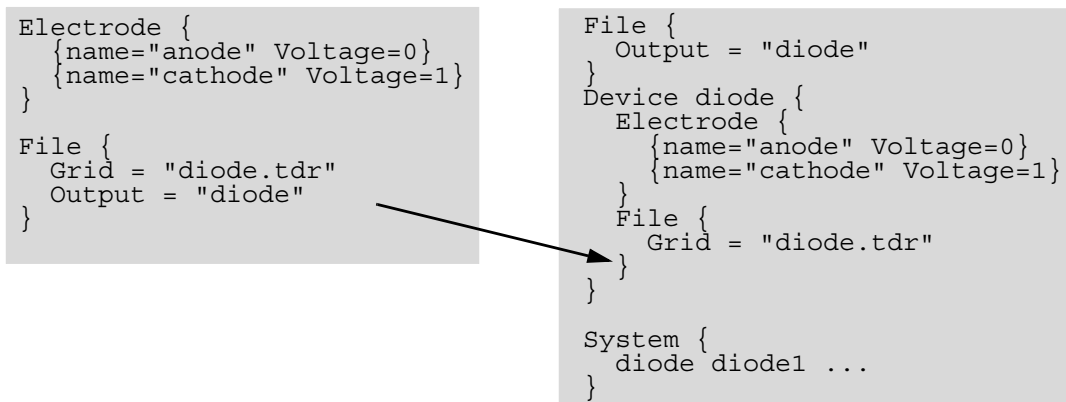
Figure 8   Translating a single device syntax to mixed-mode form

The `Solve` section can also be converted if the flag `NoAutomaticCircuitContact` is used (see Figure 9).

```
Math {
 NoAutomaticCircuitContact
}
Solve {
 Coupled {Poisson Contact Circuit}
 Coupled {Poisson Contact Circuit Electron Hole}
}
```

```
Solve {
 Poisson
 Coupled {Poisson Electron Hole}
}
```
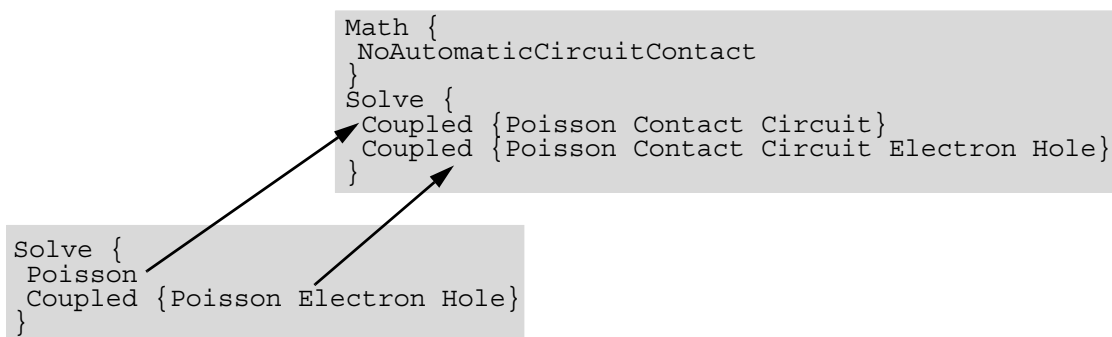
Figure 9   Translating a default solve syntax to a NoAutomaticCircuitContact form

In this case, all occurrences of the keyword `Poisson` must be expanded to the three keywords `Poisson Contact Circuit`.

File-Naming Convention: Mixed-Mode Extension

A `File` section can be defined at all levels of a command file. Therefore, a default file name can be potentially included by more than one device, for example:

```
Device res {
   File { Save="res" ... }
   ...
}
System {
   res r1
   res r2
}
```

Both `r1` and `r2` use the save device parameters set up in the definition of `res`. Therefore, they have in principle the same default for `Save` (that is, `res`). Since it is impractical to save both devices under the same name, names of device instances (that is, `r1` and `r2`) are concatenated to the file name to produce the files `res.r1` and `res.r2`. This process of file name extension is performed for the file parameters `Save`, `Current`, `Path`, and `Plot`, and is also performed when the file name is copied from the global default to a device type declaration.

In practice, the following possibilities exist:

- The file name is defined at the instance level, in which case, it is unchanged.

- The file name is defined at the device type level, in which case, the instance name is concatenated to the original file name.

- The file name is defined at the global command file level, in which case, the device name and instance name are concatenated to the original file name.

Table 15   Summary of file modifications for Save, Current, Path, and Plot commands

Level	File name format
Instance	`<given name>`
Device	`<given name>.<instance name>`
Global	`<given name>.<device type>.<instance name>`

CHAPTER 4   Performing Numeric Experiments

This chapter describes how to perform numeric experiments.

Performing a simulation is the virtual analog to performing an experiment in the real world. This chapter describes how to specify the parameters that constitute such an *experiment*, in particular, bias conditions and their variation. It also describes how to perform important types of experiment that involve periodic signals, such as small-signal analysis. Some experiments described here have no real-world analogy, for example, continuous change of physical parameters and device-internal quantities.

Specifying Electrical Boundary Conditions

Electrical boundary conditions are specified in the `Electrode` section. Only one `Electrode` section must be defined for each device. Each electrode is defined in a subsection enclosed by braces and must include a name and default voltage. For example, a complete `Electrode` section is:

```
Electrode {
    { name = "source" Voltage = 1.0 Current = 1e-3}
    { name = "drain"  Voltage = 0.0 }
    { name = "gate"   Voltage = 0.0 Material = "PolySi"(P=6.0e19) }
}
```

Table 206 on page 1399 lists all keywords that can be specified for each electrode. Keywords that relate to the physical properties of electrodes are discussed in Electrical Boundary Conditions on page 201.

Contacts in the `Electrode` section can be specified alternatively by a user-defined regular expression instead of a well-defined name. In this case, all the matching contacts in the structure file (TDR file) will be given the properties defined by the contact with the matching pattern. For example, in a device with nine drain contacts named `drain1` ... `drain9`, you can define them simultaneously with:

```
Electrode {
    ...
    { name = regexp("drain[1-9]")  Voltage = 0.0 }
    ...
}
```

The regular expressions must be specified following the rules defined by the `boost::regex` library with Perl regular expression syntax enabled [1].

Internally, Sentaurus Device matches the regular expressions defined in the `Electrode` section against the contacts in the structure file as a preprocessing step before the simulation. The list of matched structure contacts is expanded as valid contacts, and the simulation proceeds as usual. When structure contacts are matched by more than a regular expression, the last defined in the `Electrode` section succeeds. When a contact is specified in the standard way using the `Name` keyword and also is matched by a regular expression, the last defined in the `Electrode` section succeeds.

You can specify time-dependent boundary conditions, by providing a list of voltage–time pairs. For example:

```
{ name = "source" voltage = (5 at 0, 10 at 1e-6) }
```

specifies the voltage at `source` to be $5\,\text{V}$ at $0\,\text{s}$, increasing linearly to $10\,\text{V}$ at $1\,\mu\text{s}$. In addition, you can specify a separate 'static' voltage, for example:

```
{ name = "source" voltage = 0 voltage = (5 at 0, 10 at 1e-6) }
```

This combination is useful where an initial quasistationary command ramps `source` from $0\,\text{V}$ to $5\,\text{V}$, before `source` increases to $10\,\text{V}$ during a subsequent transient analysis.

The parameters `Charge` and `Current` determine the boundary condition type as well as the value for an electrode By default, electrodes have a voltage boundary condition type. The keyword `Current` changes the boundary to current type, and the keyword `Charge` changes it to charge type. Note that for current boundary conditions, you still must specify `Voltage`; this value is used as an initial guess when the simulation begins, but it has no impact on the final results. `Charge` and `Current` support time-dependent specifications in the same manner as explained for `Voltage`.

Changing Boundary Condition Type During Simulation

The `Set` command in the `Solve` section changes the boundary condition type for an electrode. To change the boundary condition of a current contact `<name>` to voltage type, use `Set(<name> mode voltage)`. To change the boundary condition of a voltage contact `<name>` to current type or charge type, use `Set(<name> mode current)` or `Set(<name> mode charge)`, respectively. To change the boundary condition of a charge contact `<name>` to voltage type, use `Set(<name> mode voltage)`. Changing the boundary condition of a current contact `<name>` directly to charge type or from a charge contact `<name>` directly to current type is not allowed. For example, use:

```
Solve { ...
   Set ("drain" mode current)
```

```
    ...
  }
```

to change the boundary condition for the voltage contact `drain` from voltage type to current type. If the boundary condition for `drain` was of current type before the `Set` command is executed, nothing happens.

The `Set` command does not change the value of the voltages and currents at the electrodes. The boundary value for the new boundary condition type results from the solution previously obtained for the bias point at which the `Set` command appears.

An alternative method to change the boundary condition type of a contact is to use the `Quasistationary` statement (see Quasistationary Ramps on page 74). This alternative is usually more convenient. However, a goal value for the boundary condition must be specified, whereas the `Set` command allows you to fix the current, charge, or voltage at a contact to a value reached during the simulation, even if this value is not known beforehand.

Mixed-Mode Electrical Boundary Conditions

In mixed-mode simulations, an additional possibility to specify electrical boundary conditions is to connect electrodes to a circuit (see Electrical and Thermal Netlist on page 58).

The `Set` command in the `Solve` section can be used to determine the boundary conditions at circuit nodes (see Set, Unset, Initialize, and Hint on page 60). The `Set` command takes a list of nodes with optional values as parameters. If a value is given, the node is set to that value. If no value is given, the node is set to its current value. The nodes are set until the end of the Sentaurus Device run or the next `Unset` command with the specified node.

The `Unset` command takes a list of nodes and 'frees' them (that is, the nodes are floating). In practice, the `Set` command is used in the `Solve` section to establish a complex system of steps, circuit region by circuit region.

The SPICE voltage and current sources use vector parameters to define the properties of various source types. For example:

```
System {
   Vsource_pset v0 (n1 n0) { sine = (0.5 1 10 0 0) }
}
```

defines a voltage source with an offset $vo = sine[0] = 0.5\,V$, an amplitude $va = sine[1] = 1\,V$, a frequency $freq = sine[2] = 10\,Hz$, a delay $td = sine[3] = 0\,s$, and a damping factor $theta = sine[4] = 0\,s^{-1}$. Components of such vectors can be set in the `Solve` section.

The following example sets the offset of the sine voltage source `v0` to $0.75\ \mathrm{V}$:

```
Solve { ...
   Set (v0."sine[0]" = 0.75) ...
}
```

Specifying Thermal Boundary Conditions

The `Thermode` section defines the thermal contacts of a device. The `Thermode` section is defined in the same way as the `Electrode` section. By default, the temperature specified with `Temperature` is the temperature of the thermode. If, in addition, `Power` (in $\mathrm{W/cm^2}$) is specified in the `Thermode` section, a heat flux boundary condition is imposed instead, and the specified temperature serves as an initial guess only, for example:

```
Thermode {
   { Name = "top"    Temperature = 350 }
   { Name = "bottom" Temperature = 300 Power = 1e6 }
}
```

Thermal contacts in the `Electrode` section can be specified alternatively by a user-defined regular expression instead of a well-defined name. In this case, all the matching thermal contacts in the structure file (TDR file) will be given the properties defined by the thermal contact with the matching pattern. The matching process is similar to that of electrical contacts (see Specifying Electrical Boundary Conditions on page 67).

Time-dependent thermal boundary conditions are specified using the same syntax as for electrical boundary conditions (see Specifying Electrical Boundary Conditions on page 67).

Table 209 on page 1402 lists the keywords available for the `Thermode` section. Thermal Boundary Conditions on page 226 discusses the physical options. In mixed-mode device simulation, an additional possibility to specify thermal boundary conditions is to connect thermodes to a thermal circuit (see Electrical and Thermal Netlist on page 58).

> **NOTE** Only thermodes with a thermal resistive boundary condition can be
> connected to a circuit. Thermodes with a heat flux boundary condition
> are not available for circuit connections.

Table 16   Various thermode declarations

Command statement	Description
`{ Name = "surface"  Temperature = 310` `  SurfaceResistance = 0.1 }`	This is a thermal resistive boundary condition with $0.1\text{cm}^2\text{K/W}$ thermal resistance, which is specified at the thermode 'surface.'
`{ Name = "body"   Temperature = 300` `  Power = 1e6 }`	Heat flux boundary condition.

`{ Name = "bulk"   Temperature = 300`
`  Power = 1e5`
`  Power = (1e5 at 0, 1e6 at 1e-4,`
`          1e3 at 2e-4) }`
	Thermode with time-dependent heat flux boundary condition.

Break Criteria: Conditionally Stopping the Simulation

Sentaurus Device prematurely terminates a simulation if certain values exceed a given limit. This feature is useful during a nonisothermal simulation to stop the calculations when the silicon starts to melt or to stop a breakdown simulation when the current through a contact exceeds a predefined value.

The following values can be monitored during a simulation:

- Contact voltage (inner voltage)
- Contact current
- Lattice temperature
- Current density
- Electric field (absolute value of field)
- Device power

It is possible to specify values to a lower bound and an upper bound. Similarly, a bound can be specified on the absolute value. The break criteria can have a global or sweep specification. If the break is in sweep, you can have multiple break criteria in one simulation. The break can be specified in a single device and in mixed mode.

Global Contact Break Criteria

The limits for contact voltages and contact currents can be specified in the global `Math` section:

```
Math {
   BreakCriteria {
      Voltage (Contact = "drain" absval = 10)
```

```
      Current (Contact = "source" minval = -0.001 maxval = 0.002)
   }
   ...
}
```

In this example, the stopping criterion is met if the absolute value of the inner voltage at the drain exceeds $10\,\mathrm{V}$. In addition, Sentaurus Device terminates the simulation if the source current is less than $-0.001\,\mathrm{A/\mu m}$ or greater than $0.002\,\mathrm{A/\mu m}$.

> **NOTE** The unit depends on the device dimension. It is $\mathrm{A/\mu m}^2$ for 1D, $\mathrm{A/\mu m}$ for 2D, and A for 3D devices.

Global Device Break Criteria

The device power is equal to $P = \sum_k I_k \cdot V_k$, where:

- k is the index of a device contact.

- I_k is the current.

- V_k is the inner or outer voltage at this contact.

Examples of the device power criteria are:

```
Math {
   BreakCriteria { DevicePower( Absval=6e-5) }
   BreakCriteria { OuterDevicePower( Absval=6e-5) }
   BreakCriteria { InnerDevicePower( Absval=2e-6) }
   ...
}
```

The keywords `DevicePower` and `OuterDevicePower` are synonyms. In this example, the stopping criterion is met if the absolute value of the outer power exceeds $6\times10^{-5}\,\mathrm{W/\mu m}$ or the inner power exceeds $2\times10^{-6}\,\mathrm{W/\mu m}$.

The break criteria for lattice temperature, current density, and electric field can be specified by region and material. If no region or material is given, the stopping criteria apply to all regions. A sample specification is:

```
Math (material = "Silicon") {
   BreakCriteria {
      LatticeTemperature (maxval = 1000)
      CurrentDensity (maxval = 1e7)
   }
   ...
}
Math (region = "Region.1") {
   BreakCriteria {
```

```
         ElectricField (maxval = 1e6)
      }
      ...
   }
```

Sentaurus Device terminates the simulation if the lattice temperature in silicon exceeds $1000\,\mathrm{K}$, the current density in silicon exceeds $10^7\,\mathrm{A/cm^2}$, or the electrical field in the region `Region.1` exceeds $10^6\,\mathrm{V/cm}$.

An upper bound for the lattice temperature can also be specified in the `Physics` section, for example:

```
   Physics {
      LatticeTemperatureLimit = 1693 # melting point of Si
      ...
   }
```

> **NOTE** The break criteria of the lattice temperature are only valid for nonisothermal simulations, that is, the keyword `Temperature` must appear in the corresponding `Solve` section.

Sweep-Specific Break Criteria

Sweep-specific break criteria can be specified as an option of `Quasistationary`, `Transient`, and `Continuation`:

```
   solve {
      Quasistationary(
         BreakCriteria {
            Current(Contact = "drain" AbsVal = 1e-8)
            DevicePower(Absval = 1e-5)
         }
         Goal { Name="drain" Voltage = 5 }
      )
      { coupled { poisson electron hole } }

      Quasistationary(
         BreakCriteria { CurrentDensity( AbsVal = 0.1) }
         Goal { Name = "gate" Voltage = 2 }
      )
      { coupled { poisson electron hole } }
      ...
   }
```

This example contains multiple break criteria. As soon as either the drain current or the device power exceeds the limit, Sentaurus Device stops the first `Quasistationary` computations

and switches to the second `Quasistationary`. As soon as the current density exceeds its limit, Sentaurus Device exits this section and switches to the next section.

Mixed-Mode Break Criteria

All the abovementioned break criteria are also available in mixed mode. In this case, the `BreakCriteria` section must contain the circuit device name (an exception are voltage criteria on circuit nodes). Examples of the break criteria conditions in mixed mode are:

```
Quasistationary(
   BreakCriteria {
      # mixed-mode variables
      Voltage( Node = a MaxVal = 10)
      Current( DevName = resistor Node = b MinVal = -1e-5)

      # device variables
      Voltage(DevName = diode Contact = "anode" MaxVal=10)
      LatticeTemperature(DevName = mos MaxVal=1000)
      ElectricField(DevName = mos MaxVal=1e6)
      DevicePower(DevName = resistor AbsVal=1e-5)
   }
   ...
)
```

Quasistationary Ramps

The `Quasistationary` command ramps a device from one solution to another through the modification of its boundary conditions (such as contact voltages) or parameter values.

The simulation continues by iterating between the modification of the boundary conditions or parameter values, and re-solving the device (see Figure 10). The command to re-solve the device at each iteration is given with the `Quasistationary` command.
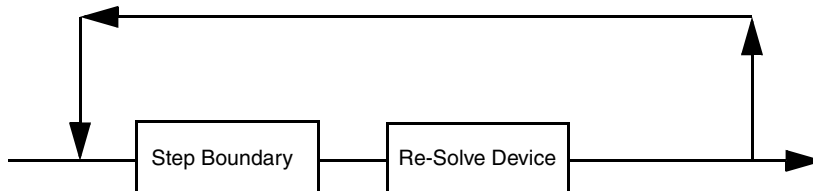
Figure 10   Quasistationary ramp

Ramping Boundary Conditions

To ramp boundary conditions, such as voltages on electrodes, the `Quasistationary` command is:

```
Quasistationary ( <parameter-list> ) { <solve-command> }
```

The possibilities for `<parameter-list>` are summarized in Table 197 on page 1394. `<solve-command>` is `Coupled`, `Plugin`, `ACCoupled`, `HBCoupled`, or possibly another `Quasistationary`.

For example, ramping a drain voltage of a device to $5\,\mathrm{V}$ is performed by:

```
Quasistationary( Goal {Voltage=5 Name=Drain } ){
   Coupled { Poisson Electron Hole }
}
```

Internally, the `Quasistationary` command works by ramping a variable t from 0.0 to 1.0. The voltage at the contact changes according to the formula $V = V_0 + t(V_1 - V_0)$, where V_0 is the initial voltage and V_1 is the final voltage, which is specified in the `Goal` statement.

Control of the stepping is expressed in terms of the t variable. The control is not made over contact values because more than one contact can be ramped simultaneously.

The step control parameters are `MaxStep`, `MinStep`, `InitialStep`, `Increment`, and `Decrement` in `<parameter-list>`:

- `MaxStep` and `MinStep` limit the step size.
- `InitialStep` controls the size of the first step of the ramping. The step size is automatically augmented or reduced depending on the rate of success of the inner solve command.
- The rate of increase is controlled by the number of performed Newton iterations and by the factor `Increment`.
- The step size is reduced by the factor `Decrement`, when the inner solve fails. The ramping process aborts when the step becomes smaller than `MinStep`.
- If the dynamic nonlocal path band-to-band model is activated, the `NonlocalPath` section can be included (see Handling of Derivatives on page 442).

Each contact has a type, which can be voltage, current, or charge. Each `Quasistationary` command has a goal, which can also be voltage, current, or charge. If the goal and contact type do not match, Sentaurus Device changes the contact type to match the goal. However, Sentaurus Device cannot change a contact of charge type to current type, or a contact of current type to charge type.

Contacts in the `Goal` section of each `Quasistationary` can be specified alternatively by a user-defined regular expression instead of a well-defined name. In this case, all the matching valid contacts in the `Electrode` section will be ramped.

For example, the following statement will ramp all contacts named `d1` ... `d9` to 5 V:

```
Quasistationary( Goal {Voltage=5 Name=Regexp("d[1-9]") } ){
   Coupled { Poisson Electron Hole }
}
```

For more details on the matching process, see Specifying Electrical Boundary Conditions on page 67.

The initial value (for $t = 0$) is the current or voltage computed for the contact before the `Quasistationary` command starts. Contacts keep their boundary condition type after the `Quasistationary` command finishes. To change the boundary condition type of a contact explicitly, use the `Set` command (see Changing Boundary Condition Type During Simulation on page 68).

If all equations to be solved in a `Quasistationary` also have been solved in the solve statement immediately before, Sentaurus Device omits the point $t = 0$, as the solution is already known. Otherwise, this point is computed at the beginning of the `Quasistationary`. You can explicitly force or prevent this point from being computed using `DoZero` or `-DoZero` in the `<parameter-list>`.

Ramping Quasi-Fermi Potentials in Doping Wells

Electron and hole quasi-Fermi potentials in specified doping wells can also be ramped in a `Quasistationary` statement. This is a quick and robust way to deplete doping wells without having to solve the continuity equation for the carrier to be depleted. Its main application is in CMOS image sensor (CIS) and charge-coupled device (CCD) simulations.

To ramp a quasi-Fermi potential, specify the keyword `WellContactName` or `DopingWell` followed by `eQuasiFermi` or `hQuasiFermi` in the `Goal` section of the `Quasistationary` command:

```
Goal { [ WellContactName = <contact name> | DopingWell(<point coordinates>)]
   [eQuasiFermi = <value> | hQuasiFermi = <value>] }
```

The `DopingWell` specification is more general and can be used for both semiconductor wells with or without contacts (buried wells). In this case, the coordinates of a point in the well must be given to select the well (see code above).

When the semiconductor well where the quasi-Fermi potential is ramped is connected to a contact, the `WellContactName` specification can be used. Now, the contact associated with the well must be specified to select the well (see code above).

The starting value of the `Goal` for the quasi-Fermi potential ramping in the specified well is taken as the well averaged value of the quasi-Fermi potential at the end of the previous `Quasistationary` command. This starting value can be changed using a `Set` statement:

```
Solve {
   Set(DopingWell(0.5 0.5) eQuasiFermi=5.0)
   Quasistationary(... Goal {DopingWell(0.5 0.5) eQuasiFermi=10.0})
      ) {Coupled {poisson hole}}
}
```

The `Set` statement has the same options and syntax as the `Goal` statement above.

In mixed-mode simulations, the feature still can be used for each device separately. In this case, the keywords `DopingWell` and `WellContactName` must be prefixed by the device name:

```
System {
   MOSCAP1 "mc1" (
      "gate_contact" = gate1
      "substrate_contact" = sub
   )
   ...
}

Solve {
   Set(mc1.DopingWell(0.5 0.5) eQuasiFermi=5.0)
   Quasistationary(...
      Goal {mc1.DopingWell(0.5 0.5) eQuasiFermi=10.0}

   ) {Coupled {poisson hole circuit}}
}
```

In addition, Sentaurus Device supports multiple-well ramping, activated by the keyword `DopingWells` with an option in parentheses. The syntax is:

```
Quasistationary(...
   Goal {DopingWells([Region=<region> | Material=<material> | Semiconductor])
      eQuasiFermi=<value>}
) {Coupled {poisson hole}}
```

As can be seen from this syntax description, wells in a region, wells having the same material, or all semiconductor wells in the device can be ramped to a specified value of the electron or hole quasi-Fermi potential. A well is considered to be in a region if it has one or more vertices in common with the region. A well belongs to a region even if it is not entirely in the region.

For multiple-well ramping, the `Set` command is used to change the quasi-Fermi potential in a group of wells before a `Quasistationary` ramping:

```
Set(DopingWells([Region=<region> | Material=<material> | Semiconductor])
   eQuasiFermi=5.0)
```

In the case of mixed-mode simulations, `DopingWells` must be prefixed with the device instance name and a `"."` similar to single-well syntax.

Electron and hole quasi-Fermi potentials can be simultaneously ramped using multiple `Goal` statements and solving for the Poisson equation only.

When the continuity equation has been solved for a carrier whose quasi-Fermi potential is to be ramped, the initial value of the quasi-Fermi potential for all vertices in the well is computed from the carrier density in the point specified when the well was defined. For multiple-well ramping, the same scheme applies well-wise.

Ramping Physical Parameter Values

A `Quasistationary` command allows parameters from the parameter file of Sentaurus Device to be ramped. The `Goal` statement has the form:

```
Goal { [ Device = <device> ]
   [ Material = <material> | MaterialInterface = <interface> |
   Region = <region> | RegionInterface = <interface> ]
   Model = <model> Parameter = <parameter> Value = <value> }
```

Specifying the device and location (material, material interface, region, or region interface) is optional. However, the model name and parameter name must always be specified.

A list of model names and parameter names is obtained by using:

```
sdevice --parameter-names
```

This list of parameters corresponds to those in the Sentaurus Device parameter file, which can be obtained by using `sdevice -P` (see Generating a Copy of Parameter File on page 32).

The following command produces a list of model names and parameter names that can be ramped in the command file:

```
sdevice --parameter-names <command file>
```

Sentaurus Device reads the devices in the command file and reports all parameter names that can be ramped. However, no simulation is performed. The models in Table 17 on page 79 contain command file parameters that can be ramped.

Table 17   Command file parameters

Model name	Parameters
DeviceTemperature	Temperature
GalvanicTransport	MagneticFieldx, MagneticFieldy, MagneticFieldz
Optics	Wavelength, Intensity, Theta, Phi, Polarization
PEPolarization	activation
RadiationBeam	Dose, DoseRate, DoseTSigma, DoseTime_end, DoseTime_start
Strain	StrainXX, StrainXY, StrainXZ, StrainYY, StrainYZ, StrainZZ
Stress	StressXX, StressXY, StressXZ, StressYY, StressYZ, StressZZ
Traps(<index>)	Conc, EnergyMid, EnergySig, eGfactor, eJfactor, eXsection, hGfactor, hJfactor, hXsection

> **NOTE**   Certain models such as traps must be specified with an index, for example:
>
> ```
> Model="Traps(1)"
> ```

The index denotes the exact model for which a parameter should be ramped. Usually, Sentaurus Device assigns an increasing index starting with zero for each optical beam, trap, and so on. However, the situation becomes more complex if material and region specifications are present. To confirm the value of the index, using the following command is recommended:

```
sdevice --parameter-names <command file>
```

Mole fraction–dependent parameters can be ramped. For example, if the parameter p is mole fraction–dependent, the parameter names listed in Table 18 can appear in a `Goal` statement.

Table 18   Mole fraction–dependent parameters as Quasistationary Goals

Parameter in Goal statement	Description
Parameter=p	Parameter p in non-mole fraction–dependent materials.
Parameter="p(0)" Parameter="p(1)" ...	Interpolation value of p at Xmax(0), Xmax(1), …
Parameter="B(p(1))" Parameter="C(p(1))" Parameter="B(p(2))" Parameter="C(p(2))" ...	Quadratic and cubic interpolation coefficients of p in intervals [Xmax(0), Xmax(1)], [Xmax(1), Xmax(2)], …

Mole fraction–dependent parameters can be ramped in all materials. In mole fraction–dependent materials, the interpolation values $p(\ldots)$ and the interpolation

coefficients `B(p(...))` and `C(p(...))` must be ramped. In a non-mole fraction–dependent material, only the parameter `p` can be ramped.

If a parameter is not found, Sentaurus Device issues a warning, and the corresponding goal statement is ignored.

Parameters in PMI models can also be ramped.

To ramp optical parameters, see .

Quasistationary in Mixed Mode

The `Quasistationary` command is extended in mixed mode to include goals on nodes and circuit model parameters. shows the syntax of these goals.

The goal is usually used on a node that has been fixed with the `Set` or `Initialize` command in the `System` section. The keyword `Goal{Node=<string> Voltage=<float>}` assigns a new target voltage to a specified node. For example, the node `a` is set to $1\,\text{V}$ and ramped to $10\,\text{V}$:

```
System {
   Resistor_pset r1(a 0){resistance = 1}
   Set(a=1)
}

Solve {
   Circuit
   Quasistationary( Goal{Node=a Voltage=10} ){ Circuit }
}
```

A goal on circuit model parameters can be used to change the configuration of a system. The keyword `Goal{Parameter=<i-name>.<p-name> value=<float>}` assigns a new target value to a specified parameter `p-name` of a device instance `i-name`. Any circuit model parameter can be changed.

For example, the resistor `r1` is ramped from $1\,\Omega$ to $0.1\,\Omega$, and the offset of the sine voltage source is ramped to $1.5\,\text{V}$:

```
System {
   Resistor_pset r1(a 0){resistance = 1}
   Vsource_pset v0 (n1 n0) { sine = (0.5 1 10 0 0) }
   Set(a=1)
}

Solve {
   Circuit
```

```
Quasistationary(
    Goal { Parameter = r1."resistance" Value = 0.1 }
    Goal { Parameter = v0."sine[0]"    Value = 1.5 })
    { Circuit }
}
```

NOTE   When a node is used in a goal, it is set during the quasistationary simulation. At the end of the ramp, the node reverts to its previous 'set' status, that is, if it was not set before, it is not set afterward. This can cause unexpected behavior in the `Solve` statement following the `Quasistationary` statement. Therefore, it is better to set the node in the `Quasistationary` statement using the `Set` command.

Saving and Plotting During a Quasistationary

Data can be saved and plotted during a `Quasistationary` ramping process by using the `Plot` command. `Plot` is placed with the other `Quasistationary` parameters, for example:

```
Quasistationary(
    Goal {Voltage=5 Name=Drain}
    Plot {Range = (0 1) Intervals=5})
      {Coupled{ Poisson Electron Hole }}
```

In this example, six plot files are saved at five intervals: $t = 0, 0.2, 0.4, 0.6, 0.8$, and 1.0.

Another way to plot data is with `Plot` in the `Quasistationary` body rather than inside the `Quasistationary` parameters (see When to Plot on page 123). `Plot` is added after the equations to solve, such as:

```
Quasistationary( Goal {Voltage=5 Name=Drain } ){
    Coupled { Poisson Electron Hole }
    Plot ( Time= ( 0.2; 0.4; 0.6; 0.8; 1.0 ) NoOverwrite )
}
```

Extrapolation

The `Quasistationary` command can use extrapolation to predict the next solution based on the values of the previous solutions. Extrapolation can be switched on globally in the `Math` section:

```
Math { Extrapolate }
```

Alternatively, it can be switched on for a specific `Quasistationary` command only:

```
Quasistationary (
   Goal { ... }
   Extrapolate
) { Coupled { Poisson Electron Hole } }
```

By default, Sentaurus Device uses linear extrapolation, but you also can request higher order extrapolation. For example, quadratic extrapolation is obtained by specifying:

```
Extrapolate (Order = 2)
```

The extrapolation information is preserved between `Quasistationary` commands, and it also is saved and loaded automatically by the `Save` and `Load` commands. A subsequent `Quasistationary` command can use this extrapolation information if the following conditions are met:

1. The previous and current `Quasistationary` commands have the same number of goals.

2. The previous and current `Quasistationary` commands ramp the same quantities.

3. The previous and current `Quasistationary` commands are contiguous, that is, for all goals, the current initial value is equal to the goal value in the previous command.

4. Multiple goals are ramped at the same rate in the current `Quasistationary` command compared to the previous `Quasistationary` command. As an example, assume that all contact voltages have zero initial values. Then, the following two `Quasistationary` commands satisfy this condition:

```
Quasistationary (
   Goal { Name = "gate"   Voltage = 1 }
   Goal { Name = "drain"  Voltage = 2 }
) { Coupled { Poisson Electron Hole } }

Quasistationary (
   Goal { Name = "gate"   Voltage = 3 }
   Goal { Name = "drain"  Voltage = 6 }
) { Coupled { Poisson Electron Hole } }
```

On the other hand, the following two `Quasistationary` commands violate this condition:

```
Quasistationary (
   Goal { Name = "gate"   Voltage = 1 }
   Goal { Name = "drain"  Voltage = 2 }
) { Coupled { Poisson Electron Hole } }

Quasistationary (
   Goal { Name = "gate"   Voltage = 3 }
   Goal { Name = "drain"  Voltage = 10 }
) { Coupled { Poisson Electron Hole } }
```

In the second `Quasistationary` command, the drain voltage is ramped at a higher rate than the gate voltage. Therefore, the extrapolation information from the previous `Quasistationary` command cannot be used.

5. The values of the solution variables have not changed between the two `Quasistationary` commands, for example, by a `Load` command.

If the extrapolation information from a previous `Quasistationary` command can be used successfully, the following message appears in the log file:

```
Reusing extrapolation from a previous quasistationary
```

The `Quasistationary` options in Table 19 control the handling of extrapolation information.

Table 19   Extrapolation options

Option	Description
ReadExtrapolation	Tries to use the extrapolation information from a previous command if it is available and compatible. This is the default.
-ReadExtrapolation	Do not use the extrapolation information from a previous command.
StoreExtrapolation	Stores the extrapolation information internally at the end of the command, so that it will be available for a subsequent command, or can be written to a save or plot file. This is the default.
-StoreExtrapolation	Do not store the extrapolation information internally at the end of the command.

Continuation Command

The `Continuation` command enables automated tracing of arbitrarily shaped $I(V)$ curves of complicated device phenomena such as breakdown or latchup. Simulation of these phenomena usually requires biasing conditions tracing a multivalued $I(V)$ curve with abrupt changes. The implementation is based on a dynamic load-line technique [2] adapting the boundary conditions along the traced $I(V)$ curve to ensure convergence. An external load resistor is connected to the device electrode at which the $I(V)$ curve is traced, the device being indirectly biased through the load resistance. The boundary condition consists of an external voltage applied to the other end of the load resistor not connected to device. By monitoring the slope of the traced $I(V)$ curve, an optimal boundary condition (external voltage) is determined by adjusting the load line so it is orthogonal to the local tangent of the $I(V)$ curve. The boundary conditions are generated automatically by the algorithm without prior knowledge of the $I(V)$ curve characteristics.

An important part of the continuation method consists of computing the slope in each point of the $I(V)$ curve. This is equivalent with computing the inverse of the device differential resistance when a small-voltage perturbation is applied to the contact undergoing continuation.

The simulation advances to the next operating point if the solution has converged. Before moving to the next step, the load line is recalibrated so that it is orthogonal to the local tangent of the $I(V)$ curve. This ensures an optimal boundary condition. A user-defined window specifies the limits for curve tracing. The tracing window is specified by user-defined lower and upper values for the voltage and current of the operating point at the continuation electrode: `MinVoltage`, `MaxVoltage`, `MinCurrent`, and `MaxCurrent`. The simulation ends when the operating point is outside the tracing window.

The continuation method is activated by using the keyword `Continuation` in the `Solve` section. Some control parameters must be given in parentheses in the same way as for the `Plugin` statement, for example:

```
Continuation (<Control Parameters>) {
   Coupled (iterations=15) { poisson electron hole }
}
```

Table 188 on page 1386 summarizes the control parameters of the `Continuation` command. The method works with both single-device and mixed-mode setups, with only one electrode undergoing continuation at a time.

The first step of the continuation is always a voltage-controlled step. For this, you must supply an initial voltage step in the control parameter list using the `InitialVstep` statement. The continuation proceeds automatically until the values given by any of the `MinVoltage`, `MaxVoltage`, `MinCurrent`, or `MaxCurrent` parameters are exceeded. In addition, the parameters `Increment`, `Decrement`, `Error` and `Digits` can be specified. Their definitions are the same as for `Transient` and `Quasistationary` statements except that they measure the $I(V)$ curve arc length.

In the regions where the $I(V)$ curve becomes vertical (close to current boundary condition) and the current extends over several orders of magnitude for almost the same applied voltage, another parameter, `MinVoltageStep`, may need to be adjusted. `MinVoltageStep` is the minimum-allowed voltage difference between two adjacent operating points on the $I(V)$ curve. In such cases, increasing the parameter value produces a smoother curve over the vertical range.

Tracing successfully an $I(V)$ curve with the continuation method depends on how accurately the local slope of the traced $I(V)$ curve is computed. As slope computation involves using inverted Jacobian and current derivatives at the electrode, an accurate computation of the contact current and a low numeric noise in Jacobian are prerequisites for continuation.

At low-biasing voltages, current at the continuation electrode is very small and, in general, noisy. This leads to an inaccurate computation of the slope, which in turn causes the continuation method to backtrace. To overcome this problem, Sentaurus Device allows you to divide the continuation window into two regions separated by a threshold current with a value specified by the parameter `Iadapt`. The lower region is a low-current range where the slope

computation is inaccurate, and the upper region is now the region where the continuation method is expected to work as designed.

From `MinCurrent` to `Iadapt` (the lower region of the simulation window), the adaptive algorithm is switched off and a fixed-value resistor is used instead. In this range, the simulation proceeds as a voltage ramping through a fixed-value resistor attached to the continuation electrode. Because no slope computation is necessary, the sensitivity of the simulation to current noise is eliminated. When the current increases to the value specified by `Iadapt`, the adaptive continuation is switched on and the curve tracing proceeds as previously described. The default value for the fixed resistor used in the lower region is $0.001\ \Omega$, and it can be changed by either using the continuation parameter `Rfixed` or specifying the `Resist` keyword in the `Electrode` section of the continuation electrode.

An example of a `Solve` entry for continuation is:

```
Electrode {
   ...
   {Name="collector" Voltage=0.0}
}

Solve { ...
   Continuation ( Name="collector" InitialVstep=-0.001
                  MaxVoltage=0 MaxCurrent=0
                  MinVoltage=-10 MinCurrent=-1e-3
                  Iadapt=-1e-13) {
                  Coupled (iterations=10) { poisson electron hole }
   }
}
```

This specifies that the $I(V)$ curve must be traced at the electrode `"collector"`. The initial voltage-controlled step is $-0.001\,\mathrm{V}$, the voltage range is $-10\mathrm{V}$ to $0\mathrm{V}$, and the current range is $-1\mathrm{mA}$ to $0\,\mathrm{A}$. The adaptive algorithm is switched on when the current reaches $-1.0 \times 10^{-13}\,\mathrm{A}$ to avoid low-current regime noise.

The step along the traced $I(V)$ curve is controlled primarily by the convergence. The step increases by a factor `Increment` if the problem has converged. When the problem does not converge, the step is cut by a factor `Decrement` and the problem is re-solved. The step cut continues until the problem converges. The continuation parameters `Increment` and `Decrement` are available for adjustment in the `Continuation` section, and the default values are 2.0 for `Increment` and 1.5 for `Decrement`.

Sentaurus Device also allows a more complex step control based on both convergence and curve smoothness. This is activated by specifying the keyword `Normalized` in the `Continuation` section. The angle between the last two segments on the $I(V)$ is computed in a local scaled I–V plane, with the scaling factors depending on the current point on the $I(V)$ curve. If the angle is smaller than the continuation parameter `IncrementAngle`, the step

increases by the factor `Increment`. If the angle is greater than `IncrementAngle` but smaller than `DecrementAngle`, the step is kept constant. Finally, if the angle is greater than `DecrementAngle`, the step decreases by the factor `Decrement`. Default values for `IncrementAngle` and `DecrementAngle` are 2.5 and 5 degrees, respectively.

A few more options are available for limiting the step (arclength) along the traced $I(V)$ curve. By specifying the continuation parameter `MaxVstep`, the step along the $I(V)$ curve is limited to an upper value such that the step projection on the V-axis is smaller in absolute value than `MaxVstep`. This option is particularly useful for a low-voltage range when a curve with more points is needed. In the higher-current range, one of the continuation parameters `MaxIstep`, `MaxIfactor`, or `MaxLogIfactor` can be used to limit the step along the curve. When `MaxIstep` is specified, the step is limited such that the step projection on the I-axis is smaller in absolute value than `MaxIstep`. `MaxIfactor` specifies how many times the current is allowed to increase for two adjacent points on the $I(V)$ curve. Similarly, `MaxLogIfactor` specifies by how many orders of magnitude the current is allowed to increase for two adjacent points on the $I(V)$ curve. `MaxVstep` can be combined with one of `MaxIstep`, `MaxIfactor`, or `MaxLogIfactor`.

In mixed mode, the continuation method allows you to have all other contacts except the continuation contact connected in a circuit. The continuation contact should not be connected to any circuit node. In this case, the `Name` keyword in the `Continuation` section specifying the continuation contact name is replaced by `dev_inst.Name`, where `dev_inst` represents the device instance of the respective contact. For example, for device mos1 with electrodes named source, drain, gate, and substrate undergoing continuation on the drain electrode, the possible syntax is:

```
Device mos1 {
   Electrode {
      {Name="source" Voltage=0.0}
      {Name="drain" Voltage=0.0}
      {Name="gate" Voltage=0.0}
      {Name="substrate" Voltage=0.0}
   }
   ...
}

System {
   mos1 d1 (source=s1 gate=g1 substrate=s1)
   set (s1=0 g1=0 b1=0)
}

Solve {
   ...
   Continuation(d1.Name="drain"
      ...
      ) {Coupled {Poisson Electron Hole}}
}
```

In mixed-mode simulations, sometimes the continuation electrode must be biased to a certain voltage using a `Quasistationary` simulation before the continuation starts. In mixed mode, because the continuation electrode is not allowed to be connected to any node, special syntax must be used to avoid biasing the contact as a node.

For example, in the above syntax, the drain electrode needs to be biased to $3\,\text{V}$ before the continuation. Instead of `Name`, the `Contact` keyword is used to identify the drain contact:

```
Quasistationary ( InitialStep=1e-3
   ...
   Goal {Contact=d1."drain" Voltage=3}
) {Coupled {Poisson Electron Hole}}
```

Transient Command

The `Transient` command is used to perform a transient time simulation. The command must start with a device that has already been solved. The simulation continues by iterating between incrementing time and re-solving the device (see Figure 11). The command to solve the device at each iteration is given with the `Transient` command.
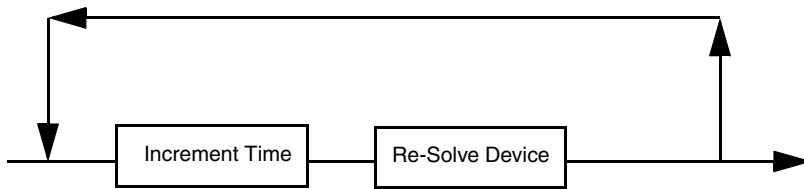
Figure 11   Transient simulation

The syntax of the `Transient` command is:

```
Transient ( <parameter-list> ) { <solve-command> }
```

lists the possible parameters.

In the above command, `<solve-command>` is `Coupled` or `Plugin`.

An example of performing a transient simulation for $10\,\mu\text{s}$ is:

```
Transient( InitialTime = 0.0 FinalTime=1.0e-5 ){
   Coupled { Poisson Electron Hole }
}
```

The `Transient` command allows you to overwrite time-step control parameters, which have default values or are globally defined in the `Math` section. The error control parameters that are accepted by the `Transient` command are listed in .

The parameters `TransientError`, `TransientErrRef`, and `TransientDigits` control the error over the transient integration method. This differs from the error control for the `Coupled` command, which only controls the error of each nonlinear solution. As with the error parameters for the `Coupled` command, the transient error controls can be both absolute and relative. Absolute values are parameterized according to equation–variable type.

The plot controls of the `Transient` command are the same as for the `Quasistationary` command, except the *t* is the real time (in seconds), and is not restricted to an interval from 0 to 1.

`Plot` can be given as a `Transient` parameter, for example:

```
Transient( InitialTime = 0.0 FinalTime = 1.0e-5
   Plot { Range = (0 3.0e-6) Intervals=3 } )
   { Coupled { Poisson Electron Hole } }
```

This example saves four plot files at `t = 0.0`, `1.0e-6`, `2.0e-6`, and `3.0e-6`. Alternatively, `Plot` can be put into the `Transient` solve command (see When to Plot on page 123):

```
Transient( InitialTime = 0.0 FinalTime = 1.0e-5 )
   { Coupled{ Poisson Electron Hole }
   Plot ( Time=( 1.0e-6; 2.0e-6; 3.0e-6 ) NoOverwrite )
}
```

Numeric Control of Transient Analysis

A set of keywords is available in the `Math` section to control transient simulation. Sentaurus Device uses implicit discretization of nonstationary equations and supports two discretization schemes: the trapezoidal rule/backward differentiation formula (TRBDF), which is the default, and the simpler backward Euler (BE) method. To select a particular transient method, specify `Transient=<transient-method>`, where `<transient-method>` can be `TRBDF` or `BE`.

In transient simulations, in addition to numeric errors of the nonlinear equations, discretization errors due to the finite time-step occur (see Transient Simulation on page 1032). By default, Sentaurus Device does not control the time step to limit this discretization error (that is, that time step depends only on convergence of Newton iterations).

To activate time-step control, `CheckTransientError` must be specified. For time-step control, Sentaurus Device uses a separate set of criteria, but as with Newton iterations, the control of both relative and absolute errors is performed. Relative transient error $\varepsilon_{R,tr}$ is defined similarly to ε_R in Eq. 32, p. 138:

$$\varepsilon_{R,tr} = 10^{-\texttt{TransientDigits}} \tag{14}$$

Similarly, for $x_{\text{ref,tr}}$ and $\varepsilon_{\text{A,tr}}$, the equation:

$$x_{\text{ref,tr}} = \frac{\varepsilon_{\text{A,tr}}}{\varepsilon_{\text{R,tr}}} x^* \tag{15}$$

is valid. The keyword `TransientDigits` must be used to specify relative error $\varepsilon_{\text{R,tr}}$ in transient simulations. An absolute error in time-step control can be specified by either the keyword `TransientError` ($\varepsilon_{\text{A,tr}}$) or `TransientErrRef` ($x_{\text{ref,tr}}$), and their values can be defined independently for each equation variable. The same flag as in Newton iteration control, `RelErrControl`, is used to switch to unscaled (`TransientErrRef`) absolute error specification.

For simulations with floating gates, Sentaurus Device can monitor the errors in the floating-gate charges as well. The details are described in Floating Gates on page 1035.

> **NOTE** All transient parameters in the `Math` section, except `Transient`, can be overwritten in the `Transient` command of the `Solve` section (see Transient Command on page 87).

Time-Stepping

A transient simulation computes the status of the system or device as a function of time for a finite time range, specified by `InitialTime` and `FinalTime`, by advancing from a status at a given time to the status at a later time point. The time step is chosen dynamically. The time step is bounded by `MinStep` and `MaxStep` from below and above, respectively; while `InitialStep` specifies the first time step at start time.

If the computation of the system status for a given time step fails, the time step is reduced iteratively until either the system status can be computed successfully or the minimum time step is reached. In the later case, the `Transient` terminates with an error. The factor by which a step is reduced can be set with the `Decrement` keyword.

After a successful computation of the system status, the time step is typically increased, depending on the computational effort for the actual time step. The maximum factor by which a step is increased can be controlled with the `Increment` keyword.

The effective time step can be smaller than the advancing time step, for example, if time points are specified for plotting, where a system status must be computed. However, these effective time steps do not reduce the advancing time step, that is, the subsequent effective time step may be as large as the advancing time step. You can bound (from above) the advancing time step at certain conditions by specifying turning points as a parameter in the `Transient`.

These conditions can be a list of arbitrary time points or time ranges (see Table 201 on page 1396), for example:

```
Transient ( ...
   TurningPoints (
      ( Condition ( Time ( 1.e-7 ; 2.e-7 ; 3.e-7 ) ) Value = 1.1e-9 )
      ( Condition ( Time ( Range = (1.e-7 2.e-7 ) ) ) Value = 2.1e-9 )
   )
)
```

The advancing time step is limited by the specified `Value` (in seconds) for the corresponding `Condition`. Here, the first condition limits the value for a list of time points. The second condition limits the time step for a whole range. Observe that, for time points, the computation of the transient is triggered; while for `Range`, this is not the case. `Time` takes the same options as the `Time` keyword in `Plot` in `Solve`. The specification:

```
TurningPoints ( ... (1.e-9 1.e-10) )
```

serves as shorthand for a single time-point condition:

```
TurningPoints ( ... ( Condition ( Time ( 1.e-9 ) ) Value = 1.e-10 ) )
```

> **NOTE**   Turning points related to optical simulations, specified using the unified interface for optical generation computation (see Chapter 21 on page 533), are described in Optical Turning Points on page 552.

Ramping Physical Parameter Values

A `Transient` command allows parameters from the parameter file of Sentaurus Device to be ramped linearly. The `Bias` statement (similar to the subsection `Goal` in a `Quasistationary` command, see Ramping Physical Parameter Values on page 78) has the form:

```
Bias { [ Device = <device> ]
   [ Material = <material> | MaterialInterface = <interface> |
   Region = <region> | RegionInterface = <interface> ]
   Model = <model> Parameter = <parameter> Value = <value_list>
}
```

Specifying the device and location (material, material interface, region, or region interface) is optional. However, the model name and parameter name must always be specified. Example:

```
Transient (
   InitialTime = 0 FinalTime = 1
   Bias( Material = "Silicon"
      Model = DeviceTemperature Parameter = "Temperature"
      Value = (300 at 0.1, 400 at 0.2, 450 at 0.5)
   )
```

```
    Bias( Region = "Channel"
       Model = DeviceTemperature Parameter = "Temperature"
       Value = (550 at 0.6, 400 at 0.8, 300 at 0.9)
    )
) { Coupled { Poisson Electron Hole } }
```

For a list of parameters that can be ramped in a `Transient` command, see Ramping Physical Parameter Values on page 78.

Extrapolation

If the `Extrapolate` option is present in the `Math` section, the `Transient` command uses the linear extrapolation of the last two solutions to predict the next solution. This extrapolation information is preserved between `Transient` commands, and it is also saved and loaded automatically by the `Save` and `Load` commands.

A `Transient` command can use this extrapolation information if the following conditions are met:

1. The previous and current `Transient` commands are contiguous, that is, the final time of the previous `Transient` is equal to the initial time of the current `Transient`.

2. The values of the solution variables have not changed between the two `Transient` commands, for example, by a `Load` command.

If the extrapolation information from a previous `Transient` command can be used successfully, the following message appears in the log file:

```
    Reusing extrapolation from a previous transient
```

The options to control the handling of extrapolation information described in Table 19 on page 83 are available for `Transient` as well.

Transient Ramps

As an alternative, Sentaurus Device provides `Transient` command syntax very similar to the `Quasistationary` command. This `Transient` command simplifies switching from quasistationary simulations to slow transient ones with minimal user effort. Replacing a quasistationary simulation with a slow transient is particularly useful in modeling wide-bandgap semiconductor devices, devices with trap states, breakdown simulations, and in general where convergence can be improved by switching to transient.

The transient ramp is activated by a `Quasistationary`-like command where the `Quasistationary` keyword is replaced by `Transient` and two optional parameters `InitialTime` and `FinalTime` can be used to control the ramp rate:

```
Solve { ...
   Transient (
      InitialTime = 0
      FinalTime = 1
      InitialStep = 0.01
      MaxStep = 0.1
      MinStep = 0.001
      Goal {name="gate" Voltage=5.0}
      Goal {name="drain" Voltage=5.0}
   ) { Coupled {...} }
}
```

The default value for `InitialTime` is 0 or the final simulation time from a previous transient ramp simulation. The `FinalTime` default value is `InitialTime` + 1 second.

When a quasistationary ramp is inserted between two transient ramps, the time for the transient ramp after the quasistationary will be reset to zero if `InitialTime` is not specified.

If the dynamic nonlocal path band-to-band model is activated, the `NonlocalPath` section can be included (see Handling of Derivatives on page 442).

In the following example, the last transient will bias the contact `anode` from 3 V at t = 0 to 0 V at t = 2 s:

```
Solve { ...
   Transient (
      FinalTime = 2
      InitialStep = 0.01
      MaxStep = 0.1
      MinStep = 0.001
      Goal {name="anode" Voltage=2.0}
   ) { Coupled {...} }

   Quasistationary(
      InitialStep = 0.01
      MaxStep = 0.1
      MinStep = 0.001
      Goal {name="anode" Voltage=3.0}
   ) { Coupled {...} }

   Transient (
      FinalTime = 2
      InitialStep = 0.01
      MaxStep = 0.1
```

```
      MinStep = 0.001
      Goal {name="anode" Voltage=0.0}
   ) { Coupled {...} }
}
```

The electrode bias time dependency is computed internally for the electrodes specified in the `Goal` section, so no time-dependent bias specification is allowed in the `Electrode` section for those contacts. `InitialStep`, `MaxStep`, and `MinStep` are like those in the `Quasistationary` case represented on a 0 to 1 scale. Sentaurus Device converts them internally to a scale from `InitialTime` to `FinalTime`.

This feature supports voltage, current, or charge ramps. Therefore, in the `Goal` section, only voltage, current, and charge contacts are allowed.

Large-Signal Cyclic Analysis

For high-speed and high-frequency operations, devices are often evaluated by cyclic biases. After a time, device variables change periodically. This cyclic-bias steady state [3] is a condition that occurs when all parameters of a simulated system return to the initial values after one cycle bias is applied.

In fact, such a cyclic steady state is reached by using standard transient simulation. However, this is not always effective, especially if some processes in the system have very long characteristic times in comparison with the period of the signal.

For example, deep traps usually have relatively long characteristic times. A suggested approach [4] allows for significant acceleration of the process of reaching a cyclic steady state solution. The approach is based on iterative correction of the initial guess at the beginning of each period of transient simulation, using previous initial guesses and focusing on reaching a cyclic steady state. This approach is implemented in Sentaurus Device. An alternative frequency-domain approach is harmonic balance (see Harmonic Balance on page 101).

Description of Method

The original method [4] is summarized. Transient simulation starts from some initial guess. A few periods of transient simulation are performed and, after each period, the change over the period of each independent variable of the simulated system is estimated (that is, the potential at each vertex of all devices, electron and hole concentrations, carrier temperatures, and lattice temperature if hydrodynamic or thermodynamic models are selected, trap occupation probabilities for each trap type and occupation level, and circuit node potentials in the case of mixed-mode simulation).

If x_n^I denotes the value of any variable in the beginning of the n-th period, and x_n^F denotes the same value at the end of the period, the cyclic steady state is reached when:

$$\Delta x_n = x_n^F - x_n^I \tag{16}$$

is equal to zero.

Considering linear extrapolation and that the goal is to achieve $\Delta x_{n+1} = 0$, the next initial guess can be estimated as:

$$x_{n+1}^I = x_n^I - \gamma \frac{x_n^I - x_{n-1}^I}{\Delta x_n - \Delta x_{n-1}} \Delta x_n \tag{17}$$

where γ is a user-defined relaxation factor to stabilize convergence.

As Eq. 17 contains uncertainty such as 0/0, especially when Δx is close to zero (when the solution is close to the steady state), special precautions are necessary to provide robustness of the algorithm.

Consider the derivation of Eq. 17 in a different fashion – near the cyclic steady state. If such a steady state exists, the initial guess $y = x^I$ is expected to behave with time as $y = a\exp(-\alpha t) + b$, where $\alpha > 0$. It is easy to show that Eq. 17 gives $x^I = b$, that is, a desirable cyclic steady-state solution.

It follows that the ratio r:

$$r = -\frac{x_n^I - x_{n-1}^I}{\Delta x_n - \Delta x_{n-1}} \tag{18}$$

can be estimated as $r \approx 1/(1 - \exp(-\alpha t))$. From this, it is clear that because α is positive, the condition $r \geq 1$ must be valid. Moreover, r can be very large if some internal characteristic time (like the trap characteristic time) is much longer than the period of the cycle.

Using the definition of r from Eq. 18, Eq. 17 can be rewritten as:

$$x_{n+1}^I = x_n^I + \gamma r \Delta x_n \tag{19}$$

Although Eq. 18 and Eq. 19 are equivalent to Eq. 17, it is more convenient inside Sentaurus Device to use Eq. 18 and Eq. 19. Sentaurus Device never allows r to be less than 1 because of the above arguments.

To provide convergence and robustness, it is reasonable also not to allow r to become very large. In Sentaurus Device, r cannot exceed a user-specified parameter r_{max}. You can also specify the value of the parameter r_{min}.

An extrapolation procedure, which is described by Eq. 18 and Eq. 19, is performed for every variable of all the devices, in each vertex of the mesh. Instead of densities, which can spatially vary over the device by many orders of magnitude, the extrapolation procedure is applied to the appropriate quasi-Fermi potentials.

For the trap equations, extrapolation can be applied either to the trap occupation probability f_T (the default) or, optionally, to the 'trap quasi-Fermi level,' $\Phi_T = -\ln((1 - f_T)/f_T)$. The cyclic steady state is supposedly reached if the following condition is satisfied:

$$\frac{\Delta x}{x + x_{\text{ref}}} < \varepsilon_{\text{cyc}} \tag{20}$$

Values of x_{ref} are the same as `ErrRef` values of the `Math` section. For every object o of the simulated system (that is, every variable of all devices), an averaged value r_{av}^o of the ratio r is estimated and can be optionally printed. Estimation of r_{av}^o is performed only at such vertices of the object, where the condition:

$$\frac{\Delta x}{x + x_{\text{ref}}} < \frac{\varepsilon_{\text{cyc}}}{f} \tag{21}$$

is fulfilled, that is, the same condition as Eq. 20, but with a possibly different tolerance $\varepsilon 1_{\text{cyc}} = \varepsilon_{\text{cyc}}/f$.

The following extrapolation procedures are allowed:

1. Use of averaged extrapolation factors for every object. This is the default option.

2. Use of the factor r independently for every mesh vertex of all objects. If for some reason, the criterion in Eq. 21 is already reached, the value of factor r is replaced by the user-defined parameter r_{min}. The option is activated by the keyword `-Average` in the `Extrapolate` statement inside the `Cyclic` specification.

3. The same as Step 2, but for the points where Eq. 21 is fulfilled, the value of factor r is replaced by the averaged factor r_{av}^o. The option is activated by the keyword `-Average` in the `Extrapolate` statement inside the `Cyclic` specification, accompanied by the specification of the parameter $r_{\text{min}} = 0$.

Using Cyclic Analysis

Cyclic analysis is activated by specifying the parameter `Cyclic` in the parameter list of the `Transient` statement. `Cyclic` is a complex structure–like parameter and contains cyclic options and parameters in parentheses:

```
Transient( InitialTime=0 FinalTime=2.e-7 InitialStep=2.e-14 MinStep=1.e-16
   Cyclic( <cyclic-parameters> )
) { ... }
```

With sub-options to the optional parameter `Extrapolate` to the `Cyclic` keyword, details of the cyclic extrapolation procedure are defined. Table 190 on page 1388 lists all options for `Cyclic`.

An example of a `Transient` command with `Cyclic` specification is:

```
Transient( InitialTime=0 FinalTime=2.e-7 InitialStep=2.e-14 MinStep=1.e-16
   Cyclic( Period=8.e-10 StartingPeriod=4
      Accuracy=1.e-4 RelFactor=1
      Extrapolate (Average Print MaxVal=50) )
) { ... }
```

NOTE   The value of the parameter `Period` in the `Cyclic` statement must be divisible by the period of the bias signal. A periodic bias signal must be specified elsewhere in the command file.

Small-Signal AC Analysis

An `ACCoupled` solve section is an extension of a `Coupled` section with an extra set of parameters allowing small-signal AC analysis. Table 187 on page 1385 describes these parameters. In general, an `ACCoupled` is used in mixed mode. AC Simulation on page 1024 provides technical background information for the method.

AC Analysis in Mixed-Mode Simulations

AC analysis computes the frequency-dependent admittance matrix Y between circuit nodes of the specified electrical system. For a given excitation frequency ν, it describes the equivalent small-signal model by:

$$\delta I = Y \delta V \tag{22}$$

where δV and δI are the vectors of (complex-valued) voltage and current excitations at selected nodes, respectively. The admittance matrix can be represented as:

$$Y = A + i2\pi\nu\ C \tag{23}$$

by the real-valued conductance matrix A and capacitance matrix C.

Within an `ACCoupled`, you need to specify the frequencies of interest and the circuit nodes considered in the admittance matrix. Furthermore, you may have to exclude some circuit instances from the given electrical system to describe the proper AC system:

- `StartFrequency`, `EndFrequency`, `NumberOfPoints`, `Linear`, and `Decade`: Select the frequencies at which the AC analysis is performed.

- `Node`: Specify the list of AC nodes considered in the admittance matrix. For admittance matrix computations, a nonempty node list must be specified.

- `Exclude`: Specify a list of system instances that should not be part of the AC system.

- `ACExtract`: Specify an `ACCoupled`-specific file-name prefix for the extraction file, where the admittance matrices will be stored. If not specified, the `ACCoupled` writes into the global extraction file (given by `ACExtract` in `File`, which defaults to the extraction file `extraction_ac_des.plt`). The extraction file contains the frequency, the voltages at the nodes, and the entries of the matrices *A* (denoted by `a`) and *C* (denoted by `c`).

- `ACPlot`: Invoke device plots containing AC response functions (solution variables and current densities). Here, you specify a file-name prefix, which generates a corresponding plot file for each AC node voltage excitation and frequency.

The `Exclude` list is used to remove a set of circuit or physical devices from the AC analysis. Typically, the power supply is removed so as not to short-circuit the AC analysis, but the list can also be used to isolate a single device from a whole circuit.

> **NOTE** The system analyzed consists of the equations specified in the body of the `ACCoupled` statement, without the instances removed by the `Exclude` list. The `Exclude` list only specifies instances, therefore, all equations of these instances are removed.

The `ACCompute` option controls AC or noise analysis performances within a `Quasistationary` or `Transient` ramp. The parameters in `ACCompute` are identical to the parameters in the `Plot` and `Save` commands (see), for example:

```
Quasistationary (...) {
   ACCoupled (...
      ACCompute (Time = (0; 0.01; 0.02; 0.03; 0.04; 0.05)
               Time = (Range = (0.9 1.0) Intervals = 4)
               Time = (Range = (0.1 0.2); Range = (0.7 0.8))
               When (Node = in Voltage = 1.5))
      {...}
}
```

In this example, an AC analysis is performed only for the time points:

```
t = 0, 0.01, 0.02, 0.03, 0.04, 0.05
t = 0.9, 0.925, 0.95, 0.975, 1.0
```

and for all time points in the intervals [0.1, 0.2] and [0.7, 0.8]. Additionally, an AC analysis is triggered whenever the voltage at the node `in` reaches the 1.5 V threshold.

If the AC or noise analysis is suppressed by the `ACCompute` option, an `ACCoupled` command behaves like an ordinary `Coupled` command.

The `Quasistationary` or `Transient` ramp that contains the `ACCoupled` also can contain a `CurrentPlot` specification (see When to Write to the Current File on page 107) to select the steps at which current output should occur. The `CurrentPlot` and an `ACCompute` statement that the `ACCoupled` command may contain are completely independent.

Example

This example illustrates AC analysis of a simple device. A 1D resistor is connected to ground (through resistor `to_ground`) and to a voltage source `drive` at reverse bias of –3 V. After calculating the initial voltage point at –3 V, the left voltage is ramped to 1 V in 0.1 V increments. The AC parameters between nodes `left` and `right` are calculated at frequencies $f = 10^3$ Hz, 10^4 Hz, 10^5 Hz, and 10^6 Hz. The circuit element `drive` and `to_ground` are excluded from the AC calculation.

By including circuits, complete Bode plots can be performed:

```
Device "Res" { ...
   Electrode {{Name=anode   Voltage=-3 resist=1}
              {Name=cathode Voltage= 0 resist=1}
   }
   File {Grid = "resist.tdr"}
   Physics {...}
}

System {
   "Res" "1d" (anode="left" cathode="right")
   Vsource_pset drive("left" "right"){dc = -3}
   Resistor_pset to_ground ("right" 0){resistance=1}
}

Math {
   Method=Blocked SubMethod=Super      # 1D, 2D default solvers for Coupled
   ACMethod=Blocked ACSubMethod=Super  # 1D, 2D default solvers for AC analysis
   NoAutomaticCircuitContact
}

Solve { ...
   ACCoupled (
      StartFrequency=1e3 EndFrequency=1e6 NumberOfPoints=4 Decade
      Node("left" "right")
      Exclude(drive to_ground)
      ACMethod=Blocked ACSubMethod("1d")=ParDiSo
```

```
    ) { Poisson Electron Hole Contact Circuit }
    Quasistationary ( ...
       Goal{Parameter=drive.dc Value=1}
    ) {
       ACCoupled(
          StartFrequency=1e3 EndFrequency=1e6 NumberOfPoints=4 Decade
          Node("left" "right")
          Exclude(drive to_ground)
          ACMethod=Blocked ACSubMethod("1d")=ParDiSo
       ) { Poisson Electron Hole Circuit Contact }
    }
  }
}
```

AC Analysis in Single-Device Mode

As previously described, AC analysis requires in general a mixed-mode simulation, that is, a `System` section must be defined. For single-device simulations, a simple AC system is constructed for you if you use `ImplicitACSystem` in the global `Math` section.

This implicit AC system is built internally and is essentially invisible to users. The implicit AC system has the following properties:

- For each voltage-controlled electrode of the device under test (DUT), an electrical circuit node is constructed and connected to the device contact. For other contact types, no nodes are constructed.

- Each implicit node is connected with a system instance describing the stationary and (possibly) transient voltage boundary conditions. Data provided for the device contacts is transferred implicitly to the system instances.

In the case of an implicit AC system generation, the `ACCoupled` provides slightly different default behavior:

- `Node`: If no AC nodes are specified, all implicit system nodes are used as AC nodes. Specified device contact names are interpreted implicitly as the corresponding node name.

- `Exclude`: If no exclude instances are specified, all implicit system instances attached to the AC nodes are excluded. Specified device contact names are interpreted as the corresponding system instance name.

Additional remarks:

- `Goal` statements in `Quasistationary`: `Goal` statements for the electrode-voltage values for the device are interpreted as `Goal` statements for the implicit system instance connected to the corresponding node of the electrode.

- The implicit AC system is extracted before the `Solve` section is executed. Therefore, solve statements that change the mode of the contact type are not supported.

Example

```
Math {
   ImplicitACSystem                * build implicit AC system
}

Electrode { ...
   { Name="c1" Voltage=1 Voltage=(1 at 0. , 2. at 1.e-8) ... }
   { Name="c2" Current=0. }         * contact without implicit node connection
}

Solve { ...
   Quasistat ( ...
      Goal { Name= "c1" Voltage=2"}  * contact goals are mapped onto instances
   ) { Coupled {...} }

   * AC analysis: use all implicit AC nodes
   ACCoupled ( StartFrequency=1.e6 EndFrequency=1.e9 NumberOfPoints=4 Decade
      ACExtract="AC1" ) {...}
   * AC analysis: use only one AC node
   ACCoupled ( StartFrequency=1.e6 EndFrequency=1.e9 NumberOfPoints=4 Decade
      Node ( "c1" )
      ACExtract="AC2" ) {...}
}
```

Optical AC Analysis

Optical AC analysis calculates the quantum efficiency as a function of the frequency of the optical signal. This technique is based on the AC analysis technique, and provides real and imaginary parts of the quantum efficiency versus the frequency.

To start optical AC analysis, add the keyword `Optical` in an `ACCoupled` statement, for example:

```
ACCoupled ( StartFrequency=1.e4 EndFrequency=1.e9
         NumberOfPoints=31 Decade Node(a c)
         Optical Exclude(v1 v2) )
         { poisson electron hole }
```

For more details, see .

Harmonic Balance

Harmonic balance (HB) analysis is a frequency domain method to solve periodic or quasi-periodic, time-dependent problems. Compared to transient analysis (see Transient Command on page 87), HB is computationally more efficient for problems with time constants that differ by many orders of magnitude. Compared to AC analysis (see Small-Signal AC Analysis on page 96), the periodic excitation is not restricted to infinitesimally small amplitudes. An alternative to HB for the periodic case is cyclic analysis (see Large-Signal Cyclic Analysis on page 93).

> **NOTE** Harmonic balance is not supported for traps (see Chapter 17 on page 449) or ferroelectrics (see Chapter 29 on page 797).

The time-dependent simulation problems take the form:

$$\frac{d}{dt}q[r, u(t, r)] + f[r, u(t, r), w(t, r)] = 0 \tag{24}$$

where f and q are nonlinear functions that describe the circuit and the devices, u is the vector of solution variables, and w is a time-dependent excitation.

Assuming w is quasi-periodic with respect to $\underline{f} = (\hat{f}_1, \ldots, \hat{f}_M)^T$, the vector of the positive base frequencies $\hat{f}_m$, and $\underline{H} = (H_1, \ldots, H_M)^T$, the vector of nonnegative maximal numbers of harmonics H_m, the solution u is approximated by a truncated Fourier series:

$$u(t) = U_0 + \sum_{-\underline{H} \le \underline{h} \le \underline{H}} U_{\underline{h}} \exp(i\omega_{\underline{h}} t) \tag{25}$$

where $\omega_{\underline{h}} = 2\pi \underline{h} \cdot \hat{f}$.

In Fourier space, Eq. 24 becomes:

$$L(U) := i\Omega Q(U) + F(U) = 0 \tag{26}$$

where Ω is the frequency matrix, and F and Q are the Fourier series of f and q. The function L depends nonlinearly on U and, therefore, solving Eq. 26 requires a nonlinear (Newton) iteration. For more details on the numerics of harmonic balance, see Harmonic Balance Analysis on page 1027.

Modes of Harmonic Balance Analysis

Sentaurus Device supports two different modes to perform harmonic balance simulations: the MDFT mode and the SDFT mode.

MDFT Mode

The MDFT mode is suitable for multitone analysis and one-tone analysis, and is enabled by the `MDFT` option in the `HB` section of the global `Math` section. It uses the multidimensional Fourier transformation (MDFT) to switch between the frequency and time domain of the system.

This mode requires compact models defined by the compact model interface (CMI), which support assembly routines in the frequency domain, that is, the CMI-HB-MDFT function set as described in Compact Models User Guide, Analytical Description of CMI Models on page 125.

Sentaurus Device provides a basic set of compact models that support this functional behavior (see Compact Models User Guide, CMI Models With Frequency-Domain Assembly on page 167). Standard SPICE models are not supported in this mode.

SDFT Mode

The SDFT mode supports only one-tone HB analysis. The mixed-mode circuit may contain SPICE models and CMI models that do not provide the CMI-HB-MDFT functional set. It is used if the MDFT mode is disabled.

Performing Harmonic Balance Analysis

Harmonic balance simulations are enabled through the keyword `HBCoupled` in the `Solve` section. The syntax of `HBCoupled` is the same as for `Coupled` (see Coupled Command on page 136). In addition, `HBCoupled` supports the options summarized in Table 193 on page 1391.

> **NOTE**   Not all `HBCoupled` options are supported by both modes.

The `Tone` option is mandatory, as no default values are provided.

Specifying several `Tone` options in MDFT mode enables multitone analysis. The base frequencies for the analysis can be given by explicit numeric constants or can refer to the frequencies of time-dependent sources in the `System` section.

An example of a two-tone analysis is:

```
Math {
   HB { MDFT }   * enable MDFT mode
   ...
}
System {
```

```
    ...
    sd_hb_vsource2_pset "va" ( na 0 )        * two-tone voltage source
       { dc = 1.0 freq = 1.e9 mag = 5.e-3 phase = -90.
         freq2 = 1.e3 mag2 = 1.e-3 phase2 = -90.}

    HBPlot "hbplot" ( v(na) i(va na) ... )    * HB circuit output
  }
  Solve {
    * solve the DC problem
    ...
    Coupled { Poisson Electron Hole }

    * solve the HB problem
    HBCoupled ( * two-tone analysis
       Tone ( Frequency = "va"."freq" NumberOfHarmonics = 5 )
       Tone ( Frequency = "va"."freq2" NumberOfHarmonics = 1 )
       Initialize = DCMode
       Method = ILS
       GMRES ( Tolerance = 1.e-2 MaxIterations = 30 Restart = 30 )
    ) { Poisson Electron Hole }
  }
```

The base frequencies $\hat{f}_1$ and $\hat{f}_2$ in this example are taken from the time-dependent voltage source va.

HBCoupled can be used as a top-level Solve statement, or within Plugin, QuasiStationary.

> **NOTE** If a QuasiStationary controls other Solve statements besides a single HBCoupled, step reduction due to convergence problems works correctly only when no HBCoupled in the failing step has converged before the statement that caused the failure is run.

Solve Spectrum

The spectrum to be solved is determined by the specified tones. For different HBCoupled statements, the number of tones and their number of harmonics are allowed to change (where the m-th tone is identified with the m-th tone of the next spectrum, regardless of the value of its frequency, that is, the order of tones is significant).

For some applications, you may be interested only in a few spectrum components or you may want to reduce the computational burden in the Newton process. For such situations, you can reduce the solve spectrum (only for the MDFT mode) by applying spectrum truncation.

This is performed by specifying a list of spectrum (multi-)indices by using `SolveSpectrum` in the `HB` section of the global `Math` section, and referencing to this spectrum in the `HBCoupled` statement, for example:

```
Math { ...
   HB { ... SolveSpectrum ( Name = "sp1" ){ (0 0) (1 0) (0 1) (2 1) (2 -1) } }
}
Solve { ...
   HBCoupled ( ... SolveSpectrum = "sp1" ) { ... }
}
```

where, for example, the multi-index (2 -1) corresponds to the intermodulation frequency $2\hat{f}_1 - 1\hat{f}_2$.

Convergence Parameters

The convergence behavior of `HBCoupled` can be analyzed and influenced independently of specifications for the convergence of `Coupled` solve statements. Some parameters can be set exclusively in the `HB` section of the global `Math` section (see Table 223 on page 1422), others can be set exclusively in the `HBCoupled` statement (see Table 193 on page 1391), and some can be set in both places.

`CNormPrint` is used to print the residuum, the update error, and the number of corrections (the number of grid points where a correction of computed sample points is necessary) in each Newton step for all solved equations of all instances. This information can be used to adjust the numeric convergence parameters.

The `Derivative` flag in `HBCoupled` overwrites the `Derivative` flag of the `Math` section and determines whether all derivatives are included in the HB Newton process.

With `RhsScale` and `UpdateScale`, you can scale the residuum and the update error of individual equations, respectively, which are used as Newton convergence criteria. This is often necessary for the electron and hole continuity equations, and the values differ for different applications and devices.

The parameters `ValueMin` and `ValueVariation` are used for positive solution variables to specify the allowed minimum value in the time domain, and the corresponding ratio of maximum and minimum values, respectively. The number of corrections (given by `CNormPrint`) indicates how many grid points violate the specified bounds.

Harmonic Balance Analysis Output

All frequency-domain output data refers to the one-sided Fourier series representation for real-valued quantities, that is, it refers to $\tilde{U}_{\underline{h}}$ of:

$$
\begin{aligned}
u(t) &= \tilde{U}_0 + \sum_{\underline{h} \in K^+} \mathrm{Re}(\tilde{U}_{\underline{h}} \exp(i\omega_{\underline{h}} t)) \\
&= \tilde{U}_0 + \sum_{\underline{h} \in K^+} \left\{ \mathrm{Re}(\tilde{U}_{\underline{h}}) \cos(\omega_{\underline{h}} t) - \mathrm{Im}(\tilde{U}_{\underline{h}}) \sin(\omega_{\underline{h}} t) \right\}
\end{aligned}
\tag{27}
$$

where the sum is taken over all multi-indices $\underline{h}$, which results in a positive frequency $\omega_{\underline{h}} = \underline{h} \cdot \hat{\underline{\omega}}$.

Device Instance Currents, Voltages, Temperatures, and Heat Components

Each converged HBCoupled plots the results (contact currents and voltages, temperatures, and heat components) both in the time domain and frequency domain into a separate file. The names of the files for the time domain contain a component Tdom; those for the frequency domain contain a component Hdom.

Circuit Currents and Voltages

Additionally, the keyword HBPlot in the System section allows you to plot circuit quantities. The syntax of HBPlot is identical to that of Plot in the System section (see System Plot on page 61). In MDFT mode, each converged HBCoupled plots its results in a Tdom and an Hdom file as for device instances, while in SDFT mode, it will write four files containing all Fourier coefficients (files with the name component Fdomain), the time domain data (Tdomain), the harmonic magnitude (Hmag), and the harmonic phase (Hphase).

Solution Variables

Plotting solution variables is only supported for one-tone HB simulations. This is implicitly done if the HB section in the Math section is present. Sentaurus Device will plot the coefficients $\tilde{U}_i$ of Eq. 27 as a real-valued vector with components $U_0 = \tilde{U}_0$, $U_{2h-1} = \mathrm{Re}(\tilde{U}_h)$, and $U_{2h} = \mathrm{Im}(\tilde{U}_h)$ (for $1 \le h \le 3$), with names composed of a prefix HB, a suffix _C<i> with component <i>, and the names of the solution variables. Additionally, the magnitude and phase of $\tilde{U}_h$ (for $0 \le h \le 3$) are plotted, with the prefixes Mag and Phase to the variable names and suffixes _C<h>.

Application Notes

Note that:

- Convergence: Typically, the nonlinear convergence improves with an increasing number of harmonics H for one-tone HB simulations.

- Linear solvers: Benefiting both memory requirements and simulation time, you can use the iterative linear solver GMRES for most simulations. Only for very small problems, in terms of grid size and number of harmonics, will the direct solver method be sufficient.

References

[1] For information about Perl regular expression syntax, go to http://www.boost.org/doc/libs/1_55_0/libs/regex/doc/html/boost_regex/syntax/perl_syntax.html.

[2] R. J. G. Goossens *et al.*, "An Automatic Biasing Scheme for Tracing Arbitrarily Shaped *I-V* Curves," *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, vol. 13, no. 3, pp. 310–317, 1994.

[3] K. S. Kundert, J. K. White, and A. Sangiovanni-Vincentelli, *Steady-State Methods for Simulating Analog and Microwave Circuits*, Boston: Kluwer Academic Publishers, 1990.

[4] Y. Takahashi, K. Kunihiro, and Y. Ohno, "Two-Dimensional Cyclic Bias Device Simulator and Its Application to GaAs HJFET Pulse Pattern Effect Analysis," *IEICE Transactions on Electronics*, vol. E82-C, no. 6, pp. 917–923, 1999.

CHAPTER 5   Simulation Results

This chapter describes the output of Sentaurus Device, which contains the simulation results.

Sentaurus Device provides several forms of output. Most importantly, the current file contains the terminal characteristics obtained during the numeric experiment. Plot files allow you to visualize device internal quantities, and thereby provide information not available in real experiments. Other output, such as the log file, allows you to investigate the simulation procedure itself and provides an important tool to understand and resolve problems with the simulation itself.

This chapter only describes the most important output that Sentaurus Device provides. Many more specific output files exist. They are described in context in other parts of the user guide.

Current File

When to Write to the Current File

By default, currents are output after each iteration in a `Plugin`, `Quasistationary`, or `Transient` command. This behavior can be modified by a `CurrentPlot` statement in the body of these commands. The `CurrentPlot` statement in the `Solve` section provides full control over the plotting of device currents and circuit currents. If a `CurrentPlot` statement is present, it determines exactly which points are written to the current file. Sentaurus Device can still perform computations for intermediate points, but they are not written to the file.

> **NOTE** Do not confuse the `CurrentPlot` statement in the `Solve` section with the `CurrentPlot` section as described in Tracking Additional Data in the Current File on page 110.

The syntax of the `CurrentPlot` statement is:

```
CurrentPlot (<parameters-opt>) {<system-opt>}
```

Both `<parameters-opt>` and `<system-opt>` are optional and can be omitted. `<parameters-opt>` is a space-separated list, which can consist of the following entries:

`Time = (<entry> ; <entry> ; <entry> ;)`

The list of time entries enumerates the times for which a current plot is requested. The entries are separated by semicolons. A time entry can have these forms:

floating point number
The time value for which a current plot is requested.

`Range = (a b)`
This option specifies a free plot range between a and b. All the time points in this range are plotted.

`Range = (a b) Intervals = n`
This option specifies n intervals in the range between a and b. In other words, these plot points are generated:

$$t = a, t = a + \frac{b-a}{n}, ..., t = b - \frac{b-a}{n}, t = b \tag{28}$$

`Iterations = (<integer>; <integer>; <integer>;)`

The list of integers specifies the iterations for which a plot is required. This option is available for the `Plugin` command.

`IterationStep = <integer>`

This option requests a current plot every n iterations. It is available for the `Plugin` command.

`When (<when condition>)`

A `When` option can be used to request a current plot whenever a condition has been met. This option works in the same way as in a `Plot` or `Save` command (see Table 194 on page 1392).

`<system-opt>` is a space-separated list of devices. If `<system-opt>` is not present, Sentaurus Device plots all device currents and the circuit (in mixed-mode simulations). If `<system-opt>` is present, only the currents of the given devices are plotted. The keyword `Circuit` can be used to request a circuit plot.

Example: CurrentPlot Statements

A `CurrentPlot` statement by itself creates a current plot for each iteration:

```
Quasistationary (InitialStep=0.2 MinStep=0.2 MaxStep=0.2
Goal { Name="drain" Voltage=0.5 })
   { Coupled { Poisson Electron Hole }
   CurrentPlot }
```

If no current plots are required, a current plot for the 'impossible' time $t = -1$ can be specified:

```
Quasistationary (InitialStep=0.2 MinStep=0.2 MaxStep=0.2
Goal { Name ="drain" Voltage=0.5 })
   { Coupled { Poisson Electron Hole }
   CurrentPlot ( Time = (-1)) }
```

In this example, the currents of the device `nmos` are plotted for $t = 0$, $t = 10^{-8}$, and $t = 10^{-7}$:

```
Transient ( MaxStep=1e-8 InitialTime=0 FinalTime=1e-6 )
   { Coupled { Poisson Circuit }
   CurrentPlot ( Time = (0 ; 1e-8; 1e-7)) { nmos } }
```

This `CurrentPlot` statement produces 11 equidistant plot points in the interval 0, 10^{-5}:

```
Transient ( MaxStep = 1e-8 InitialTime=0 FinalTime=1e-5 )
   { Coupled { Poisson Circuit }
   CurrentPlot ( Time = (range = (0 1e-5) intervals = 10)) }
```

In this example, a current plot for iteration 1, 2, 3, and for every tenth iteration is specified:

```
Plugin { Poisson Electron Hole
   CurrentPlot ( Iterations = (1; 2; 3) IterationStep = 10 ) }
```

A `CurrentPlot` statement can also appear at the top level in the `Solve` section. In this case, the currents are plotted when the flow of control reaches the statement.

A `CurrentPlot` statement is also recognized within a `Continuation` command. In this case, the time in the `CurrentPlot` statement corresponds to the arc length in the `Continuation` command. However, only free plot ranges are supported.

NewCurrentPrefix Statement

By default, Sentaurus Device saves all current plots in one file (as defined by the variable `Current` in the `File` section). This behavior can be modified by the `NewCurrentPrefix` statement in the `Solve` section:

```
NewCurrentPrefix = prefix
```

This statement appends the given prefix to the default, current file name, and all subsequent `Plot` statements are directed to the new file. Multiple `NewCurrentPrefix` statements can appear in the `Solve` section, for example:

```
Solve {
   Circuit
   Poisson
   NewCurrentPrefix = "pre1"
   Coupled {Poisson Electron Hole Contact Circuit}
   NewCurrentPrefix = "pre2"
   Transient (
      MaxStep= 2.5e-6 InitialStep=1.0e-6
      InitialTime=0.0 FinalTime=0.0001
      Plot {range=(10e-6,40e-6) Intervals=10}
   )
   {Coupled {Poisson Electron Hole Contact Circuit}}
}
```

In this example, the current files specified in the `File` and `System` sections contain the results of the `Circuit` and `Poisson` solves. The results of the `Coupled` solution are saved in a new current file with the same name but prefixed with `pre1`. The last current file contains the results of the `Transient` solve with the prefix `pre2`.

> **NOTE** The file names for current plots defined in the `System` section, and the plot files of AC analyses are also modified by a `NewCurrentPrefix` statement.

Tracking Additional Data in the Current File

The `CurrentPlot` section on the top level of the command file is used to include selected parameter values and mesh data into the current plot file (`.plt`). Sentaurus Device provides the following options:

■ You can list the desired quantities directly in the `CurrentPlot` section (see CurrentPlot Section on page 111).

■ You can use a current plot PMI (see Current Plot File of Sentaurus Device on page 1239).

- You can use a Tcl formula (see Tcl Formulas on page 115).

- You can use the current plot Tcl interface, which represents an alternative to the current plot PMI (see Current Plot File on page 1317).

CurrentPlot Section

Sentaurus Device can add the scalar data listed in Appendix F on page 1339 to the current plot file.

Data can be plotted according to coordinates. A coordinate is given as one to three (depending on device dimensions) numbers in parentheses. When plotting according to coordinates, the plotted values are interpolated as required.

Furthermore, it is possible to output averages, integrals, maximum, and minimum of quantities over specified domains. To do this, specify the keyword `Average`, `Integrate`, `Maximum`, or `Minimum`, respectively, followed by the specification of the domain in parentheses. A domain specification consists of any number of the following:

- Region specification: `Region=<regionname>`

- Material specification: `Material=<materialname>`

- Region interface specification: `RegionInterface=<regioninterfacename>`

- Material interface specification: `MaterialInterface=<materialinterfacename>`

- Any of the keywords `Semiconductor`, `Insulator`, and `Everywhere`, which match all semiconductor regions, all insulator regions, or the entire device, respectively

- Window specification: `Window[(x1 y1 z1) (x2 y2 z2)]`

- Well specification: `DopingWell(x1 y1 z1)` (for the definition of the doping well boundary, see Initial Guess for Electrostatic Potential and Quasi-Fermi Potentials in Doping Wells on page 178)

The average, integral, maximum, and minimum are applied to all of the specified parts of the device. Multiple specifications of the same part of the device are insignificant. In addition, `Name=<plotname>` is used to specify a name under which the average, integral, maximum, and minimum are written to the `.plt` file. (By default, the name is automatically obtained from a concatenation of the names in the domain specification, which yields impractically long names for complicated specifications.)

For maximum and minimum, Sentaurus Device can write coordinates where the maximum and minimum occur to the `.plt` file.

In the case of average and integral, Sentaurus Device can write the coordinates ($\langle x \rangle$, $\langle y \rangle$, $\langle z \rangle$) of the centroid of a data field f defined:

$$\langle x \rangle = \frac{\int xf(x, y, z)dV}{\int f(x, y, z)dV} \tag{29}$$

where the integration covers the specified domain. The values of $\langle y \rangle$ and $\langle z \rangle$ are defined similarly. Output of coordinates is activated by adding the keyword `Coordinates` in the parentheses where the domain is specified.

The average, integral, maximum, and minimum can be confined to a window by using the window specification. A one-dimensional, 2D, or 3D window is defined by the coordinates (in micrometers) of two opposite corners of the window. In addition, it is possible to confine the domain in a well using the well specification. In this case, the well is defined by the coordinates of a point inside the well. When a list of domains is specified in addition to the window or well, the domains are neglected if the window or well is a valid one.

The length unit for integration and the number of digits used for names in the current plot file can be specified in the `Math` section (see CurrentPlot Options on page 114 for details).

Parameters from the parameter file of Sentaurus Device can also be added to the current plot file. The general specification looks like:

```
[ Material = <material> | MaterialInterface = <interface> |
    Region = <region> | RegionInterface = <interface> ]
Model = <model> Parameter = <parameter>
```

Specifying the location (material, material interface, region, or region interface) is optional. However, the model name and parameter name must always be present.

> **NOTE** The order of specification is fixed. An optional location specification (material, material interface, region, or region interface) must be followed by a model name and a parameter name. Otherwise, Sentaurus Device will report a syntax error.

Ramping Physical Parameter Values on page 78 describes how model names and parameter names can be determined.

Finally, Sentaurus Device also provides a current plot PMI (see Current Plot File of Sentaurus Device on page 1239).

> **NOTE** Do not confuse the `CurrentPlot` section with the `CurrentPlot` statement in the `Solve` section introduced in When to Write to the Current File on page 107.

Example: Mixed Mode

In mixed-mode simulations, the `CurrentPlot` section can appear in the body of a physical device within the `System` section (it is also possible to have a global `CurrentPlot` section), for example:

```
System {
   Set (gnd = 0)
   CAP Cm (Top=node2 Bot=gnd) { CurrentPlot { Potential ((0.7, 0.8, 0.9)) } }
   ...
}
```

Example: Advanced Options

This example is a 2D device that uses the more advanced `CurrentPlot` features:

```
CurrentPlot {
   hDensity((0 1)) * hole density at position (0um, 1um)
   ElectricField/Vector((0 1)) * Electric Field Vector
   Potential (
      (0.1 -0.2)  * coordinates need not be integers
      Average(Region="Channel")  * average over a region
      Average(Everywhere)        * average over entire device
      Maximum(Material="Oxide")  * Maximum in a material
      Maximum(Semiconductor)     * in all semiconductors
      * minimum in a material and a region, output under the name "x":
      Minimum(Name="x" Material="Oxide" Region="Channel")
   )
   eDensity(
      * average and coordinates of centroid
      Average(Semiconductor Coordinates)
      * maximum and coordinates of maximum in well
      Maximum(DopingWell(-0.1 0.3) Coordinates)
      * integral over the semiconductor regions
      Integrate(Semiconductor)
   )
   SpaceCharge(
      * maximum over 2D window
      Maximum(Window[(-0.2 0) (0.2 0.2)])
      * integral over well
      Integrate( DopingWell(-0.1 0.3) )
   )
}
```

Example: Plotting Parameter Values

The following example adds five curves to the current plot file:

```
CurrentPlot {
    Model = DeviceTemperature  Parameter = "Temperature"
    Material = Silicon  Model = Epsilon  Parameter = epsilon
    MaterialInterface = "AlGaAs/InGaAs"
        Model = "SurfaceRecombination"  Parameter = "S0_e"
    Region = "bulk"  Model = LatticeHeatCapacity  Parameter = cv
    RegionInterface = "Region.0/Region.1"
        Model = "SurfaceRecombination"  Parameter = "S0_h"
}
```

This example also shows the fixed order of specification. An optional location (material, material interface, region, or region interface) is followed by a model name and a parameter name. Therefore this example adds the following five parameter values to the current plot file:

1. Global device temperature

2. Dielectric constant ε in silicon

3. Surface recombination parameter s_0 for electrons on AlGaAS–InGaAs material interfaces

4. Lattice heat parameter `cv` for region 'bulk'

5. Surface recombination parameter s_0 for holes on the region interface Region.0–Region.1

CurrentPlot Options

The length unit used during a current plot integration (see Tracking Additional Data in the Current File on page 110) can be selected as follows:

```
Math {
    CurrentPlot (IntegrationUnit = um)
}
```

The possible choices are `cm` (centimeters) and `um` (micrometers). The default is `IntegrationUnit=um`. This option is useful when quantities such as densities (unit of cm^{-3}) are integrated. In a 2D simulation, the unit of the integral is either $\mu m^2 cm^{-3}$ (`IntegrationUnit=um`) or cm^{-1} (`IntegrationUnit=cm`).

The number of digits in the names of quantities in the current plot file can be specified as follows:

```
Math {
    CurrentPlot (Digits = 6)
}
```

The default is `Digits=6`.

This option is useful when the names of two quantities become equal due to rounding. In the following example, you want to monitor the valence band energy in two points:

```
CurrentPlot {
   ValenceBandEnergy ((5.0, 199.011111) (5.0, 199.011112))
}
```

However, with the default setting of `Digits=6`, both quantities are assigned the same name due to rounding:

```
Pos(5,199.011) ValenceBandEnergy
```

By increasing the number of digits, the names in the current plot file become distinct.

Specifying `Digits` affects the names of the following quantities in the current plot file:

- Coordinates
- Well specification
- Window specification

Tcl Formulas

Sentaurus Device can evaluate Tcl formulas and add the results to the current plot file. The Tcl interpreter has access to the data listed in Appendix F on page 1339, and you can provide Tcl commands to compute derived quantities. For example, it is possible to compute the electron conductivity σ_n given by:

$$\sigma_n = qn\mu_n \tag{30}$$

The following operations can be performed with a Tcl formula:

- Evaluation at a given vertex
- Evaluation at a location specified by its coordinates
- Compute the minimum/maximum/average/integral over a domain
- Plot output to a PMI user field

In the case of a minimum/maximum/average/integral operation or plot operation, the domain of the evaluation can be restricted as follows:

- Region
- Material
- Region interface

- Material interface

- Contact

- Semiconductor, insulator, or metal regions

- Entire device

- Doping well

- Window

In the case of a minimum/maximum/average/integral operation, the location of the minimum or maximum, or the centroid of the average or integral operation (see Eq. 29) also will be added to the current plot file.

The following example shows how to compute the average electron conductivity σ_n in the channel region:

```
CurrentPlot {
   Tcl (
      Dataset   = "Ave_channel eConductivity"
      Function  = "Conductivity"
      Formula   = "set q 1.602e-19
                   set n [tcl_cp_ReadScalar eDensity]
                   set mu [tcl_cp_ReadScalar eMobility]
                   set value [expr $q * $n * $mu]"
      Operation = "Average Region = channel"
   )
}
```

The `Tcl` statement supports the following options:

```
CurrentPlot {
   Tcl (
      Dataset   = "..."
      Function  = "..."
      Unit      = "..."
      Init      = "..."
      Formula   = "..."
      Finish    = "..."
      Operation = "..."
   )
}
```

Dataset

Use this option to specify the dataset name that appears in the header section of the current plot file. If this option is not specified, Sentaurus Device generates the name `Tcl_Dataset_<index>` where `<index>` is a unique integer.

Example:

```
Dataset = "channel eConductivity"
```

Function

This is the function name that appears in the header section of the current plot file. If `Function` is not specified, Sentaurus Device generates the name `Tcl_Function_<index>` where `<index>` is a unique integer.

Example:

```
Function = "Conductivity"
```

Unit

This is the unit of the current plot quantity. Currently, the `.plt` file format does not support units. However, a future file format may add this support.

Example:

```
Unit = "cm/s"
```

Init

The Tcl code in this option is executed first for each plot time point. It can be used to initialize quantities that will be referenced in `Formula`.

Example:

```
Init = "set counter 0"
```

Formula

The Tcl code in this option is executed on individual mesh vertices. It must evaluate a formula and assign the result to the Tcl variable `value`.

The following Tcl functions and variables are available:

■ `tcl_cp_dim`: The dimension of the mesh. Possible values are 1, 2, or 3.

■ `tcl_cp_vertex`: The mesh index of the current vertex.

■ `tcl_cp_ContactOuterVoltage`: This Tcl function returns the value of the contact voltage for the local contact vertex (the evaluation domain must be contact).

- `tcl_cp_ContactInnerVoltage`: This Tcl function returns the value of the contact inner voltage for the local contact vertex (the evaluation domain must be contact).

- `proc tcl_cp_ReadScalar {dataname}`: This Tcl function returns the value of a scalar data field for the local vertex. Valid data names can be found in Appendix F on page 1339.

- `proc tcl_cp_ReadVector {dataname index}`: This Tcl function returns a component of a vector data field for the local vertex.

  The parameter `index` must satisfy `0 <= $index < $tcl_cp_dim`. Valid data names can be found in Appendix F on page 1339.

- `proc tcl_cp_WriteScalar {dataname value}`: This Tcl function defines the value of a scalar field for the local vertex. This is a side effect of the Tcl current plot statement, and it is typically used to compute the values of a PMI user field.
  Alternatively, you can use the `Plot` operation (see Operation on page 118).

Example:

```
Formula = "incr counter
           set value [tcl_cp_ReadScalar ElectrostaticPotential]"
```

Finish

The Tcl code in this option is executed last for each plot time point. It can be used for postprocessing purposes. It has access to the Tcl list `result`, which contains the final current plot value.

Example:

```
Finish = "puts \"Used $counter calls\""
```

Operation

This option determines how the current plot formula is evaluated. The recognized operations are:

- `Node = <integer>`: Evaluate formula at specified node.

- `Coordinate = (...)`: Evaluate formula at specified coordinates.

- `Minimum`: Compute minimum over specified domain.

- `Maximum`: Compute maximum over specified domain.

- `Average`: Compute average over specified domain.

- `Integrate`: Compute integral over specified domain.

- `Plot = <name>`: Output formula to PMI user field.

Only one of the above operations must be specified.

To obtain the value of the current plot formula at specified coordinates, Sentaurus Device evaluates the formula at nearby vertices and interpolates these values. The required interpolation scheme can be selected as follows:

- `Interpolation = <method>`: Specify interpolation scheme.

  The available interpolation schemes are: `Arsinh`, `Linear` (default), `Logarithmic`.

A scaling factor for arsinh interpolation also can be specified:

- `ArsinhFactor = <value>`: Specify arsinh scaling factor. The default is 1.

The length unit when computing an integral can be selected as follows:

- `IntegrationUnit = <unit>`: Specify integration unit.

  The possible choices are `cm` (centimeter) and `um` (micrometer). The default is `IntegrationUnit=um`. This option is useful when quantities such as densities (unit of cm^{-3}) are integrated. In a 2D simulation, the unit of the integral is either $\mu m^2 cm^{-3}$ (`IntegrationUnit=um`) or cm^{-1} (`IntegrationUnit=cm`).

In the case of a minimum/maximum/average/integral operation or plot operation, the required domain also can be specified as follows:

- `Region = <regionname>`: Region domain.
- `Material = <materialname>`: Material domain.
- `RegionInterface = <region1/region2>`: Region interface domain.
- `MaterialInterface = <material1/material2>`: Material interface domain.
- `Contact = <contactname>`: Contact domain (for minimum, maximum, average, or integral operation only).
- `Semiconductor`: Use all semiconductor regions as domain.
- `Insulator`: Use all insulator regions as domain.
- `Conductor`: Use all metal regions as domain.
- `Everywhere`: Use entire device as domain (default).
- `DopingWell = (...)`: Doping well domain.
- `Window = [(...) (...)]`: Window domain.

If multiple domains are specified, Sentaurus Device will only evaluate the current plot formula where the domains intersect. For example, it is possible to specify:

```
Operation = "Average Region=drain DopingWell=(1 2)"
```

In this case, the formula is only evaluated for those vertices in the drain region that also lie within the specified doping well.

Region interface, material interface, and contact specifications cannot be combined with other domains.

Example:

```
Operation = "Average Window=[(1 2) (3 4)]"
```

For the contact specification, when the contact is connected to multiple regions, you have the option to select a subset of the contact vertices involved in the operation (the intersection between the contact and a selected region). The selected region is specified by the `RegionName` keyword. For example, to integrate a formula over the intersection of contact `anode` and region `r1`, specify:

```
Operation = "Integrate Contact=\"anode\" RegionName=\"r1\""
```

Examples

Evaluate the electrostatic potential ϕ at $(7.2\ \mu m, 2.1\ \mu m)$:

```
CurrentPlot {
   Tcl (
      Formula   = "set value [tcl_cp_ReadScalar ElectrostaticPotential]"
      Operation = "Coordinate = (7.2 2.1)"
      Dataset   = "7.2_2.1 ElectrostaticPotential"
      Function  = "ElectrostaticPotential"
   )
}
```

Save the electron conductivity $\sigma_n = qn\mu_n$ in semiconductor (see Eq. 30, p. 115) as a PMI user field:

```
CurrentPlot {
   Tcl (
      Formula   = "set q 1.602e-19
                   set n [tcl_cp_ReadScalar eDensity]
                   set mu [tcl_cp_ReadScalar eMobility]
                   set value [expr $q * $n * $mu]"
      Unit      = "Ohm^-1*cm^-1"
      Operation = "Plot = PMIUserField5 Semiconductor"
   )
}
```

Plot the integral of the space charge ρ in the window $[(0\ \mu m, 6\ \mu m) (2.5\ \mu m, 7\ \mu m)]$:

```
CurrentPlot {
   Tcl (
      Formula   = "set value [tcl_cp_ReadScalar SpaceCharge]
      Operation = "Integrate Window = [(0 6) (2.5 7)] IntegrationUnit = cm"
```

```
        Dataset   = "Integral_Window SpaceCharge"
        Function  = "SpaceCharge"
    )
}
```

Compute the integral of the electron Joule heat $\vec{J_n}\vec{E}$ in semiconductor regions:

```
CurrentPlot {
    Tcl (
        Formula   = "set value 0
                     for {set d 0} {$d < $tcl_cp_dim} {incr d} {
                         set j [tcl_cp_ReadVector eCurrentDensity $d]
                         set f [tcl_cp_ReadVector ElectricField $d]
                         set value [expr $value + $j * $f]
                     }"
        Operation = "Integrate Semiconductor IntegrationUnit = cm"
        Dataset   = "Integral_Semiconductor eJouleHeat"
        Function  = "JouleHeat"
    )
}
```

Compute the distributed conductance of the contact `anode`:

```
CurrentPlot {
    Tcl (
        Formula = "set value 0
                   set Vext [tcl_cp_ContactOuterVoltage \"anode\"]
                   set QF [tcl_cp_ReadScalar \"QuasiFermiPotential\"]
                   for {set d 0} {$d < $tcl_cp_dim} {incr d} {
                       set j [tcl_cp_ReadVector eCurrentDensity $d]
                       set N [tcl_cp_ReadVector ContactSurfaceNormal $d]
                       set value [expr $value + $j * $N]
                   }
                   set value [expr $value / ($Vext - $QF + 0.0001)]"
        Operation = "Integrate Contact=\"top1\" RegionName=\"r2\"
                      IntegrationUnit = cm"
        Dataset   = "Conductance"
        Function  = "Conductance"
    )
}
```

Device Plots

Device plots show spatial-dependent datasets in the device and provide a view of the inside of the device.

What to Plot

The `Plot` section specifies the data that is saved at the end of or, optionally, during the simulation to the `Plot` file specified in the `File` section or by the `Plot` command in the `Solve` section. Consecutive plots can be collected in a single file, or written to separate enumerated files, or written to a single file by overwriting the previous plot. To collect consecutive plots in a single file, specify `Plot(collected)=<filename>` in the `File` section. The keywords `Overwrite` and `noOverwrite`, specified as options in the `Plot` command in the `Solve` section (see When to Plot on page 123), control whether plots are written to separate files or to a single file.

> **NOTE** You can control further compression, beyond a basic standard compression of `Plot` files, by specifying `CompressTDR` in the `Math` section. However, further compression might not always lead to a significantly reduced file size and, depending on the content of the file, it might lead to a slightly increased file size.

> **NOTE** Specifying `CompressTDR` in the `Math` section applies to all types of plot commands that generate files containing spatial-dependent datasets.

Vector data can be plotted by appending `/Vector` to the corresponding keyword, for example:

```
Plot {
   ElectricField/Vector
}
```

Element-based scalar data can be plotted by appending `/Element` to the corresponding keyword, for example:

```
Plot {
   eMobility/Element
}
```

Some quantities (such as the carrier densities) are put into the `Plot` file even when they are not listed in the `Plot` section. The keyword `PlotExplicit` in the global `Math` section suppresses this behavior.

By default, the plot file also contains additional information required by `Load` to restart a simulation (see Save and Load on page 157). To suppress writing this additional information, specify `-PlotLoadable` in the global `Math` section.

You can specify the keyword `DatasetsFromGrid` to copy quantities from the TDR grid file directly to the plot file. You can copy all datasets by specifying `DatasetsFromGrid` by itself:

```
Plot {
   DatasetsFromGrid
}
```

Alternatively, you can copy selected quantities by listing their names:

```
Plot {
   DatasetsFromGrid (dataset1 dataset2 dataset3)
}
```

A dataset is only copied from the TDR grid file if it is not computed by Sentaurus Device. Otherwise, the dataset computed by Sentaurus Device takes precedence.

> **NOTE**   The keyword `DatasetsFromGrid` only copies entire datasets from the TDR grid file to the plot file. You cannot copy partial datasets, for example, the components of tensor and vector datasets.

See Table 328 on page 1495 for all possible plot options.

When to Plot

The simplest way to create a device plot is to define `Plot` in the `File` section. By default, the output to the `Plot` file will occur at the end of the simulation only.

The commands for `Quasistationary` and `Transient` analysis support an option `Plot` that allows you to write plots while these commands are executing. The plot file name is derived from the one specified with `Plot` in the `File` section. See Saving and Plotting During a Quasistationary on page 81 and Transient Command on page 87 for the syntax.

The most flexible way to create device plots is through the `Plot` statement in the `Solve` section. It provides full control of when to plot and limited control of the file names. The `Plot` statement can be used at any level of the `Solve` section. The command takes the form:

```
Plot (<parameters-opt>) <system-opt>
```

If `<system-opt>` is not specified, all physical devices and circuits are plotted. Use `<system-opt>` to specify an optional list of devices delimited by braces (see Table 186 on page 1384).

If `<parameters-opt>` is omitted, defaults are used. The keywords `Loadable` and `Explicit` provide plot-specific overrides for `PlotLoadable` and `PlotExplicit` in the global `Math` section (see What to Plot on page 122). For a summary of all options, see Table 194 on page 1392.

Example

```
Solve {
   Plugin {
      Poisson
      Plot ( FilePrefix = "output/poisson")
      Coupled { Poisson Electron Hole }
      Plot (FilePrefix = "output/electric" noOverwrite)
   }
   Transient {
      Coupled { Poisson Electron Hole Temperature }
      Plot ( FilePrefix = "output/trans"
            Time = ( range = (0 1) ;
            range = (0 1) intervals = 4 ; 0.7 ;
            range = (1.e-3 1.e-1) intervals = 2 decade )
            NoOverwrite )
   }
   ...
}
```

The first `Plot` statement in Plugin writes (after the computation of the Poisson equation) to a file named `output/poisson_des.tdr`. The second `Plot` statement in `Plugin` writes to a file called `output/electric_0000_des.tdr` and increases the internal number for each call.

The `Plot` statement in the transient specifies three different types of time entries (separated by semicolons). The first entry indicates all the times within this range when a plot file must be written. The second time entry forces the transient simulation to compute solutions for the given times. In this example, the given times are 0.25, 0.5, 0.75, and 1.0. The third entry is for the single time of 0.7. The fourth entry triggers the plotting at time points given by subdividing the range on the logarithmic scale, resulting for this example in plots at 1.e-3, 1.e-2, and 1.e-1.

Snapshots

Sentaurus Device offers the possibility to save snapshots interactively during a simulation. This can be undertaken by sending a POSIX signal to the Sentaurus Device process. Depending on whether `Plot` or `Save` or both is specified in the `File` section, the signal invokes a request to write a plot (`.tdr`) file or a save (`.sav`) file after the actual time step is finished.

The following signals are supported to save snapshots:

- USR1: The occurrence of the USR1 signal initiates Sentaurus Device to write a plot file or a save file after the simulation has finished its actual time step. The simulation will continue afterwards.

- INT: By default, sending the INT signal causes a process to exit. This behaviour changes if `Interrupt=BreakRequest` or `Interrupt=PlotRequest` is specified in the `Math` section (see). In both cases, the occurrence of the INT signal initiates Sentaurus Device to write a plot file or a save file. `Interrupt=BreakRequest` causes Sentaurus Device to abort the actual solve statement after the snapshot is saved. If `Interrupt=PlotRequest` is specified, the simulation continues.

A signal can be sent to a process by invoking the `kill` command (see the corresponding man page of your operating system). The process ID can be extracted from the `.log` file.

Interface Plots

Data fields defined on interfaces can be plotted by using the modifier `/RegionInterface`:

```
Plot {
   HotElectronInj/RegionInterface
}
```

The following fields are available for interface plots:

```
SurfaceRecombination
HotElectronInj
HotHoleInj
```

> **NOTE** These fields can also be plotted on regions by omitting the qualifier `/RegionInterface`. However, they are zero inside bulk regions, and nonzero values are only produced for vertices along interfaces.

Interface plots are only generated if interface regions appear in the grid file. For TDR files, the following command is available:

```
snmesh -u -AI input.tdr
```

Log File

The name of the log file is specified by `Output` in the `File` section. The log file contains a copy of the messages that Sentaurus Device prints while a simulation runs. The log file contains a variety of information, including:

- Technical information such as the version of Sentaurus Device that is running, the machine where it is running, and the process ID.

- Confirmation as to which structure is simulated, which physical models have been selected, and which parameters are used.

- Detailed information about how the simulation proceeds, including timing and convergence information.

- Warning messages.

The log file is of minor interest as long as your simulations are set up well, and no convergence problems occur. It is an indispensable diagnostic tool during simulation setup, or when convergence problems occur.

A log file annotated with XML tags can be generated by specifying the `--xml` command-line option. This file contains the same information as the regular log file, but features additional XML tags to organize its content. The XML log file uses the same file name as the regular log file, but with the extension `.xml` instead of `.log`.

The XML log file is best displayed with the TCAD Logfile Browser. For more information, see Utilities User Guide, Chapter 2 on page 5.

Extraction File

Sentaurus Device supports a special-purpose file format (extension `.xtr`) for the extraction of MOSFET compact model parameters.

Extraction File Format

The extraction file consists of the following parts:

1. A header identifying the file format.

2. A section containing the process information of the MOSFET such as channel length or channel width.

3. A collection of curves containing the values of a dependent variable as a function of an independent variable, for example, drain current versus gate voltage in an I_d–V_g ramp. In addition, each curve contains the corresponding bias conditions, for example, V_b, V_d, and V_s in an I_d–V_g ramp.

A sample extraction file is:

```
# Synopsys Extraction File Format Version 1.1
# Copyright (C) 2008 Synopsys, Inc.
# All rights reserved.

$ Process
AD 31.50f
AS 31.50f
D NMOS
L 90.00n
NF 1.000
NRD 0.000
NRS 0.000
PD 880.0n
PS 880.0n
SA 500.0n
SB 500.0n
SC 0.000
SCA 0.000
SCB 0.000
SCC 0.000
SD 0.000
W 90.00n

$ Data
Curve: Id_Vg
Bias : Vb = 0 , Vd = 0.5 , Vs = 0
    1.60000000000000E+00    7.95091490486384E-05
    1.63750000000000E+00    8.27433425335473E-05
    1.67500000000000E+00    8.59289596870642E-05
    1.71250000000000E+00    8.90665609661286E-05
    1.75000000000000E+00    9.21567959785304E-05

Curve: Is_Vg
Bias : Vb = 0 , Vd = 0.5 , Vs = 0
    1.60000000000000E+00    -7.95091490484525E-05
    1.63750000000000E+00    -8.27433425333610E-05
    1.67500000000000E+00    -8.59289596868774E-05
    1.71250000000000E+00    -8.90665609659414E-05
    1.75000000000000E+00    -9.21567959783428E-05
```

Analysis Modes

Sentaurus Device supports different analysis modes.

Table 20   Analysis modes

Analysis	Curve[1]	Description
DC	Ii_Vj	The i-th terminal current versus j-th terminal voltage. i,j=b (bulk), d (drain), g (gate), or s (source) Bias conditions: all terminal voltages other than j-th terminal voltage.
AC	Ai_j_Vk	Admittance A_{ij} versus k-th terminal voltage. i,j,k=b (bulk), d (drain), g (gate), or s (source) Bias conditions: all terminal voltages other than k-th terminal voltage and frequency.
	Ai_j_F	Admittance A_{ij} versus frequency. i,j=b (bulk), d (drain), g (gate), or s (source) Bias conditions: V_b, V_d, V_g, V_s.
	Ci_j_Vk	Capacitance C_{ij} versus k-th terminal voltage. where i,j,k=b (bulk), d (drain), g (gate), or s (source) Bias conditions: all terminal voltages other than k-th terminal voltage and frequency.
	Ci_j_F	Capacitance C_{ij} versus frequency. i,j=b (bulk), d (drain), g (gate), or s (source) Bias conditions: V_b, V_d, V_g, V_s.
Noise	noise_Vi_Vj	Autocorrelation noise voltage spectral density (NVSD) for electrode i versus j-th terminal voltage. i,j=b (bulk), d (drain), g (gate), or s (source) Bias conditions: all terminal voltages other than j-th terminal voltage and frequency.
	noise_Vi_F	Autocorrelation noise voltage spectral density (NVSD) for electrode i versus frequency. i=b (bulk), d (drain), g (gate), or s (source) Bias conditions: V_b, V_d, V_g, V_s.
	noise_Ii_Vj	Autocorrelation noise current spectral density (NISD) for electrode i versus j-th terminal voltage. i,j=b (bulk), d (drain), g (gate), or s (source) Bias conditions: all terminal voltages other than j-th terminal voltage and frequency.
	noise_Ii_F	Autocorrelation noise current spectral density (NISD) for electrode i versus frequency. i=b (bulk), d (drain), g (gate), or s (source) Bias conditions: V_b, V_d, V_g, V_s.

1. Underscores are optional and are used to improve legibility.

File Section

The name of the extraction file can be specified in the `File` section of the Sentaurus Device command file:

```
File {
   Extraction = "mosfet_des.xtr"
   ...
}
```

The default file name is `extraction_des.xtr`.

Electrode Section

Sentaurus Device automatically recognizes the four electrodes of a MOSFET if they are called `"bulk"`, `"drain"`, `"gate"`, and `"source"`, or `"b"`, `"d"`, `"g"`, and `"s"` (case insensitive). For other contact names, it is possible to specify the mapping in the `Electrode` section:

```
Electrode {
   { Name = "contact_bulk"   Voltage = 0.0 Extraction {bulk}   }
   { Name = "contact_drain"  Voltage = 0.0 Extraction {drain}  }
   { Name = "contact_gate"   Voltage = 0.0 Extraction {gate}   }
   { Name = "contact_source" Voltage = 0.0 Extraction {source} }
}
```

All four MOSFET electrodes (bulk, drain, gate, and source) must be present. Additional electrodes are allowed, but they will be ignored for extraction purposes.

Extraction Section

The process parameters can be part of the Sentaurus Device grid/doping file. It is also possible to specify the same information in an `Extraction` section:

```
Extraction {
   AD 31.50f
   AS 31.50f
   D NMOS
   L 90.00n
   NF 1.000
   NRD 0.000
   NRS 0.000
   PD 880.0n
   PS 880.0n
```

```
      SA 500.0n
      SB 500.0n
      SC 0.000
      SCA 0.000
      SCB 0.000
      SCC 0.000
      SD 0.000
      W 90.00n
   }
```

Each line in the `Extraction` section consists of a name–value pair. All entries are copied to the extraction file as is.

> **NOTE**   The process parameters in the `Extraction` section of the Sentaurus
>   Device command file take precedence over the information in the grid/
>   doping file.

Solve Section

The `Quasistationary` command in the `Solve` section supports an `Extraction` option to request voltage-dependent extraction curves. Multiple curves can be generated during a single ramp. No extraction curves are produced if the `Extraction` option is missing:

```
Solve {
   # ramp contributes to extraction
   Quasistationary (
      Goal { Name="contact_gate" Voltage=1.5 }
      Extraction { IdVg IsVg ... }
   )
      { Coupled { Poisson Electron }
        CurrentPlot (Time = (Range=(0 1) Intervals=10))
      }

   # ramp does not contribute to extraction
   Quasistationary (
      Goal { Name="contact_base" Voltage=0.5 }
   )
      { Coupled { Poisson Electron } }

   # ramp contributes to extraction
   Quasistationary (
      Goal { Name="contact_drain" Voltage=1.5 }
      Extraction { IdVd IbVd ... }
   )
      { Coupled { Poisson Electron } }
}
```

AC and noise simulations must be performed in mixed mode. Only one physical device is supported in the circuit. Voltage-dependent curves are specified as an option to the `Quasistationary` statement; whereas, frequency-dependent curves appear within the `ACCoupled` statement:

```
Solve {
   Quasistationary (
      ...
      Extraction { Ads_Vg Agg_Vg Cgd_Vg
                   noise_Id_Vg noise_Ig_Vg }
   )
      { ACCoupled (
         ...
         Extraction { Add_F Cgd_F Csd_F
                      noise_Vd_F noise_Vg_F noise_Is_F }
      )
         { Poisson Electron }
   }
}
```

The recognized curves in the `Extraction` option are shown in .

5: Simulation Results
Extraction File
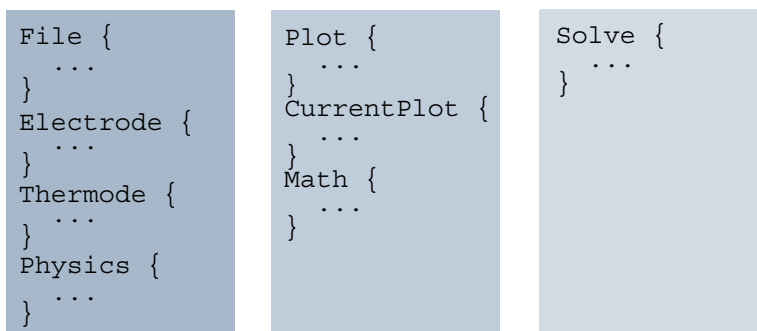
CHAPTER 6   Numeric and Software-Related
            Issues

*This chapter discusses technical issues of simulation that do not
have real-world equivalents.*

To successfully perform an experiment, apart from understanding the device under investigation, the experimenter must understand, control, and skillfully use the measurement equipment. The same holds for numeric *experiments*. This chapter describes the *equipment* available in Sentaurus Device for numeric experiments: linear and nonlinear solvers, control of accuracy, convergence monitors, and other software-related facilities. Additional background information on numerics is available in Chapter 37 on page 1011.

Structure of Command File

The Sentaurus Device command file is divided into sections that are defined by a keyword and braces (see Figure 12). A device is defined by the `File`, `Electrode`, `Thermode`, and `Physics` sections. The solve methods are defined by the `Math` and `Solve` sections. Two sections are used in mixed-mode circuit and device simulation, see Chapter 3 on page 41. This part of the manual concentrates on the input to define single device simulations.

```
File {
  ...
}
Electrode {
  ...
}
Thermode {
  ...
}
Physics {
  ...
}
```

```
Plot {
  ...
}
CurrentPlot {
  ...
}
Math {
  ...
}
```

```
Solve {
  ...
}
```

Figure 12   Different sections of a Sentaurus Device command file

Inserting Files

An insert directive is available in the command file of Sentaurus Device to incorporate other files:

```
Insert = "filename"
```

This directive can appear at the top level in the command file, or inside any of the following sections:

- `CurrentPlot`
- `Device`
- `Electrode`
- `File`
- `Math`
- `MonteCarlo`
- `NoisePlot`
- `NonlocalPlot`
- `Physics`
- `Plot`
- `RayTraceBC`
- `Solve`
- `System`
- `Thermode`

The following search strategy is used to locate a file:

- The current directory is checked first (highest priority).
- If the environment variable `SDEVICEDB` exists, the directory associated with the variable is checked (medium priority).
- Finally, the `$STROOT/tcad/$STRELEASE/lib/sdevice/MaterialDB` directory is checked (lowest priority).

  NOTE   The insert directive is also available for parameter files (see Physical Model Parameters on page 21).

Solve Section: How the Simulation Proceeds

The `Solve` section is the only section in which the order of commands are important. It consists of a series of simulation commands to be performed that are activated sequentially, according to the order of commands in the command file. Many `Solve` commands are high-level commands that have lower level commands as parameters. Figure 13 shows an example of these different command levels:

- The `Coupled` command (the base command) is used to solve a set of equations.

- The `Plugin` command is used to iterate between a number of coupled equations.

- The `Quasistationary` command is used to ramp a solution from one boundary condition to another.

- The `Transient` command is used to run a transient simulation.

Furthermore, small-signal AC analysis can be performed with the `ACCoupled` command. An advanced ramping by continuation method can be performed with the command `Continuation`. (The `ACCoupled` and `Continuation` commands are presented in Small-Signal AC Analysis on page 96 and Continuation Command on page 83, respectively.)
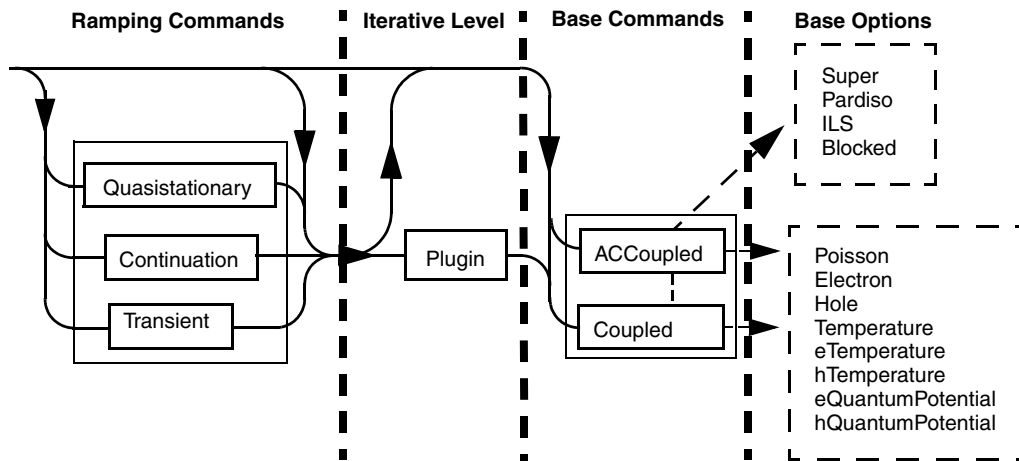
Figure 13   Different levels of Solve commands

Nonlinear Iterations

Coupled Command

The `Coupled` command activates a Newton-like solver over a set of equations. Available equations include the Poisson equation, continuity equations, and the different thermal and energy equations. The syntax of the `Coupled` command is:

```
Coupled ( <optional parameters> ){ <equation> }
```

or:

```
<equation>
```

This last form uses only the keyword `equation`, which is equivalent to a coupled with default parameters and the single equation. For example, if the following command is used:

```
Coupled {Poisson Electron}
```

the electrostatic potential and electron density are computed from the resolution of the Poisson equation and electron continuity equation (using the default parameters).

If the following command is used, only the electrostatic potential is computed using the Poisson equation:

```
Poisson
```

The `Coupled` command is based on a Newton solver. This is an iterative algorithm in which a linear system is solved at each simulation step. Parameters of the command determine:

- The maximum number of iterations allowed.
- The desired precision of the solution.
- The linear solver that must be used.
- Whether the solution is allowed to worsen over a number of iterations.

These parameters and others are summarized in Table 189 on page 1387.

Th e following example limits the previous `Coupled {Poisson Electron}` example to ten iterations and uses the ILS linear solver:

```
Coupled ( Iterations=10 Method=ILS ) {Poisson Electron}
```

> **NOTE** Use a large number of iterations when the coupled iteration is not inside a ramping process. This allows the Newton algorithm to proceed as far as possible. Inside a ramping command (for example, `Quasistationary`, `Transient`), the maximum number of iterations should be limited to approximately ten because if the Newton process does not converge rapidly, it is preferable to try again with a smaller step size than to pursue an iterative process that is not likely to converge.

The best linear method to use in a coupled iteration depends on the type and size of the problem solved. lists the solvers and the size of the problems for which they are designed.

Convergence and Error Control

The `Coupled` command is sensitive to the following `Math` parameters that determine when a coupled solution diverges or converges:

- `Iterations`
- `RhsAndUpdateConvergence`
- `RhsFactor, RhsMin, RhsMax`
- `CheckRhsAfterUpdate`
- `RelErrControl`
- `Digits`
- `ErrRef`
- `Error`
- `UpdateIncrease, UpdateMax`

The parameter `Iterations` in the global `Math` section sets the default for `Iterations` of the `Coupled` command. `Iterations` limits the number of Newton iterations. If the equation being solved is converging quadratically, the number of iterations might increase beyond this limit. For `Iterations=0`, only one iteration is performed.

Convergence of a solution in Sentaurus Device is determined by calculating and examining the following quantities at each Newton iteration:

- *RHS norm* is the norm of the right-hand-side (that is, the residual of the equations).
- *Update error* is a measure of the updates to the equation variables.

These quantities are printed in the log file for each Newton iteration during a solution. By default, a solution is considered converged if the RHS norm < `RhsMin` or if the update error < 1. If `RhsAndUpdateConvergence` is specified, both of these criteria must be satisfied.

During a single Newton step, the solution is considered diverged if the RHS norm increases by more than a factor of `RhsFactor`. For transient simulations, the solution is considered diverged if the RHS norm exceeds `RhsMax`.

Specify `CheckRhsAfterUpdate` to force Sentaurus Device to perform an additional check on the RHS norm after the update error criteria is satisfied. If Sentaurus Device assesses that the RHS norm can be made smaller, additional iterations will be performed. This can sometimes improve the quality of a solution and may result in better overall convergence.

> **NOTE** `CheckRhsAfterUpdate` usually adds no more than one or two extra iterations. However, when convergence is slow or when using extended-precision accuracy, this option can result in several additional iterations if the RHS norm continues to be reduced. In such cases, a larger value for `Iterations` might be needed. In all cases, however, Sentaurus Device will accept a converged solution when the maximum number of iterations is reached, even if the RHS norm is still improving.

There are two formulations of the update error calculations used in Sentaurus Device, depending on whether `RelErrControl` (the default) or `-RelErrControl` is specified. For both formulations, Sentaurus Device tries to determine the value of an equation variable x, such that the computed update Δx is small enough to satisfy an error criterion:

$$
\begin{aligned}
\frac{|\Delta x|}{|x| + x_{\text{ref}}} &< \varepsilon_R \quad , \text{ RelErrControl} \\
\frac{|\Delta x / x^*|}{\varepsilon_R |x/x^*| + \varepsilon_A} &< 1 \,, \text{ -RelErrControl}
\end{aligned}
\tag{31}
$$

where:

- $\varepsilon_R = 10^{-\text{Digits}}$ is the relative error.
- $x_{\text{ref}} = $ `ErrRef(<equation>)` is the reference error parameter.
- $\varepsilon_A = $ `Error(<equation>)` is the absolute error parameter.
- x^* is a scaling constant for the equation variable.

For large values of x ($|x| \rightarrow \infty$), the conditions in Eq. 31 become relative error criteria:

$$
\frac{|\Delta x|}{|x|} < \varepsilon_R
\tag{32}
$$

Conversely, for small values of x ($|x| \rightarrow 0$), they become absolute error criteria:

$$
|\Delta x| < x_{\text{ref}} \cdot \varepsilon_R \quad \text{or} \quad |\Delta x / x^*| < \varepsilon_A
\tag{33}
$$

Therefore, Eq. 31 ensures a smooth transition between absolute and relative error control.

To account for all coupled equations i at all vertices j, Sentaurus Device extends the conditions in Eq. 31 and defines the update error as:

$$\text{update error} = \begin{cases} \sqrt{\left(\sum_{i=1}^{N_i}\sum_{j=1}^{N_{vi}}\left(\dfrac{|\Delta x_{i,j}|}{\varepsilon_R(|x_{i,j}|+x_{\text{ref},i})}\right)^2\right)\Big/\left(\sum_{i=1}^{N_i}N_{vi}\right)} & , \texttt{RelErrControl} \\[3em] \sqrt{\left(\sum_{i=1}^{N_i}\sum_{j=1}^{N_{vi}}\left(\dfrac{|\Delta x_{i,j}/x_i^*|}{\varepsilon_R|x_{i,j}/x_i^*|+\varepsilon_{A,i}}\right)^2\right)\Big/\left(\sum_{i=1}^{N_i}N_{vi}\right)} & , \texttt{-RelErrControl} \end{cases} \tag{34}$$

where:

- N_i is the number of coupled equations.

- N_{vi} is the number of vertices being solved for equation i.

The value of ε_R is defined by specifying the keyword `Digits`.

The values of x_{ref} and ε_A can be defined commonly or independently for each equation with the keywords `ErrRef` and `Error`, respectively. Default values are listed in Table 191 on page 1388.

The parameters `UpdateMax` and `UpdateIncrease` are used to detect divergence of the Newton algorithm. If the update error is larger than `UpdateMax`, or its increase from Newton step to Newton step exceeds `UpdateIncrease`, the Newton is regarded as diverged.

Damped Newton Iterations

Line search damping and Bank–Rose damping are two different damping methods. These approaches try to achieve convergence of the coupled iteration far from the final solution by changing the solution by smaller amounts than a normal Newton iteration would. Damping is useful to find an initial solution, but during `Quasistationary` or `Transient` ramps, using smaller time steps is usually preferable.

Line search damping is switched off by default. It is activated when the value of `LineSearchDamping` is set to a value smaller than one. This value determines the minimum factor by which the normal Newton update Δx can be damped. The damping method determines the actual damping factor automatically in each Newton step. If the actual factor falls below the minimum specified by `LineSearchDamping`, line search damping is considered to fail and is disabled for the following Newton iterations.

Bank–Rose damping is a method that automatically adjusts the size of the update based on how the RHS changes [1]. It can be used sometimes to improve convergence when large bias steps

are taken. Bank–Rose damping becomes activated when the number of iterations exceeds the value specified with `NotDamped` in the `Math` section (default is 1000).

`LineSearchDamping` and `NotDamped` are set in the global `Math` section and by parameters of the `Coupled` command. The former specification sets the defaults for the latter.

Derivatives

For most problems, Newton iterations converge best with full derivatives. Furthermore, for small-signal analysis, and noise and fluctuation analysis, using full derivatives is mandatory. Therefore, by default, Sentaurus Device takes full derivatives into account. For rare occasions where omission of derivatives improves convergence or performance significantly, use the keywords `-AvalDerivatives` and `-Derivatives` in the global `Math` section to switch off mobility and avalanche derivatives.

The derivatives are usually computed analytically, but a numeric computation can be used by specifying `Numerically`. This does not work with the method `Blocked` and, generally, is discouraged.

Incomplete Newton Algorithm

Certain simple simulations, such as I_d–V_g ramps, can be accelerated by using a modified Newton algorithm (see Fully Coupled Solution on page 1036 for a description of the standard Newton algorithm). The incomplete Newton algorithm, also known as the Newton–Richardson method, tries to reuse the Jacobian matrix to avoid the expense of evaluating derivatives and computing matrix factorizations.

It can be switched on either in the global `Math` section:

```
Math {
    IncompleteNewton
    ...
}
```

or it can be used as an option in a `Coupled` command:

```
Coupled (IncompleteNewton) {poisson electron hole}
```

The Jacobian matrix is reused if the following two conditions are satisfied:

$$\left\| \text{Rhs}_k \right\| < \text{RhsFactor} \cdot \left\| \text{Rhs}_{k-1} \right\| \tag{35}$$

$$\left\| \text{Update}_k \right\| < \text{UpdateFactor} \cdot \left\| \text{Update}_{k-1} \right\| \tag{36}$$

where k denotes the iteration index, `Rhs` denotes the right-hand side of the nonlinear equations, and `Update` denotes the Newton step. The values of $\|\mathrm{Rhs}_k\|$ and $\|\mathrm{Update}_k\|$ are displayed in the log file of Sentaurus Device during Newton iterations in the columns `|Rhs|` and `|step|`.

The parameters `RhsFactor` and `UpdateFactor` can be specified as arguments to the `IncompleteNewton` keyword:

```
IncompleteNewton (UpdateFactor=0.1 RhsFactor=10)
```

The default values are `UpdateFactor=0.1` and `RhsFactor=10`.

Additional Equations Available in Mixed Mode

The `Contact`, `Circuit`, `TContact` and `TCircuit` equations are introduced for mixed-mode problems. The keyword `Circuit` activates the solution of the electrical circuit models and nodes. `Contact` activates the solution of the electrical interface condition at the contacts. Similarly, `TContact` and `TCircuit` activate the solution of the thermal interface condition and thermal circuit, respectively.

By default, the keywords `Contact` and `Circuit` are not required because the Poisson equation also covers the contact and circuit domains. If only the Poisson equation is solved, no additional equations are added. Only if additional equations to `Poisson` appear in a `Coupled` statement, the circuit and contact equations are also added. Therefore:

```
Coupled { Poisson Electron Hole }
```

is equivalent to:

```
Coupled { Poisson Electron Hole Circuit Contact }
```

> **NOTE**   Sentaurus Device does not add the circuit and contact equations if
> `Poisson` is restricted to instances, for example:
>
> ```
> Coupled {device1.Poisson device1.Electron
>   device1.Hole
>   device2.Poisson device2.Electron
>   device2.Hole}
> ```

If the keyword `NoAutomaticCircuitContact` appears in the `Math` section, Sentaurus Device does not add the circuit and contact equations automatically (see Figure 14).
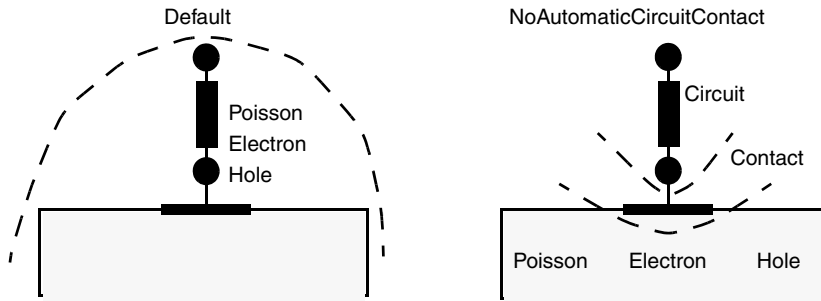
Figure 14   Range of equation keywords Circuit, Contact, Poisson, Electron, and Hole

Selecting Individual Devices in Mixed Mode

The default usage of an equation keyword such as `Poisson` activates the given equations for all devices. With complex multiple-device systems, such an action is not always desirable especially when a fully consistent solution has not yet been found. Sentaurus Device allows each equation to be restricted to a specific device by adding the name of the device instance to the equation keyword separated with a period. The syntax is:

```
<identifier>.<equation>
```

Device-specific solutions are used to obtain the initial solution for the whole system. For example, with two or more devices, it is often better to solve each device individually before coupling them all. Such a scheme can be written as:

```
System {
   ... device1 ...
   ... device2 ...
}
Solve {
   # Solve Circuit equation  Circuit

   # Solve poisson and full coupled for each device
   Coupled { device1.Poisson device1.Contact }
   Coupled { device1.Poisson device1.Contact
             device1.Electron device1.Hole }
   Coupled { device2.Poisson device2.Contact }
   Coupled { device2.Poisson device2.Contact
             device2.Electron device2.Hole }

   # Solve full coupled over all devices
   Coupled { Circuit Poisson Contact Electron Hole }
}
```

Relaxed Newton Method

The relaxed Newton method allows Sentaurus Device to consider whether a solution that has neither converged nor diverged by the final Newton iteration should be accepted as a converged solution based on relaxed convergence criteria. This method applies to `Quasistationary`, `Transient`, and `Continuation` ramps.

Relaxed convergence criteria are established from relaxed Newton parameters that are specified by users in the `AcceptNewtonParameter` (ANP) statement of the global `Math` section. These parameters are used to calculate an *ANP RhsMin* and an *ANP error* that will be used to test for relaxd convergence:

```
Math { ...
   AcceptNewtonParameter (
      [RhsAndUpdateConvergence]    * Use -RhsAndUpdateConvergence to relax
                                   * convergence
      [RhsMin=<float>]             * The ANP RhsMin that is used for relaxed
                                   * convergence
      [UpdateScale=<float>]        * This multiplies update error to give
                                   * a relaxed ANP error
      [RelErrControl]              * Specifies the error control method for
                                   * calculating the ANP error
      [Digits=<integer>]           * The number of relative error digits in the
                                   * ANP error calculation
      [ErrRef (                    * Reference error parameters to use in the ANP
                                   * error calculation
         [Poisson=<float>] [Electron=<float>] [Hole=<float>]
         [Temperature=<float>] [eTemperature=<float>] [hTemperature=<float>]
         [eQuantumPotential=<float>] [hQuantumPotential=<float>]
       )]
      [Error (                     * Absolute error parameters to use in the ANP
                                   * error calculation
         [Poisson=<float>] [Electron=<float>] [Hole=<float>]
         [Temperature=<float>] [eTemperature=<float>] [hTemperature=<float>]
         [eQuantumPotential=<float>] [hQuantumPotential=<float>]
       )]
      [InvokeAtDivergence]         * Allows relaxed convergence for diverging
                                   * solutions
   )
}
```

To activate the relaxed Newton method, specify `AcceptNewtonParameter` in the `Quasistationary`, `Transient`, or `Continuation` statements of the `Solve` section, along with a `ReferenceStep` (except for `Continuation`). For example:

```
Solve { ...
   Quasistationary ( ...
      AcceptNewtonParameter ( ReferenceStep = 1.e-3 )
   ) { Coupled { ... } }
}
```

or:

```
Solve { ...
   Transient ( ...
      AcceptNewtonParameter ( ReferenceStep = 1.e-9 )
   ) { Coupled { ... } }
}
```

or:

```
Solve { ...
   Continuation ( ...
      AcceptNewtonParameter
   ) { Coupled { ... } }
}
```

During the simulation, if the `Quasistationary` or `Transient` step size is reduced below the value specified with `ReferenceStep`, Sentaurus Device will begin to calculate an ANP error in addition to the standard update error for each Newton iteration during a solution. This will be used to determine whether relaxed convergence has been achieved if the solution fails to converge using the standard error criteria. For `Continuation`, the check for relaxed convergence is activated for all step sizes.

Relaxed convergence is considered achieved if the calculated ANP error < 1 or the RHS norm < ANP `RhsMin`, for any iteration. If relaxed convergence is achieved, Sentaurus Device will store the solution obtained from the iteration with the smallest standard update error occurring after relaxed convergence is triggered. In most cases, this is a reasonable choice for the "best" solution.

Note the following:

- The relaxed Newton parameters are passed only to the next-level `Coupled` statements, that is, `Coupled` statements in `Plugin` statements do not use the relaxed Newton parameters.

- Only specified parameter values are passed to the `Coupled` statement, that is, no default values are used.

Plugin Command

The `Plugin` command controls an iterative loop over two or more `Coupled` commands. It is used when a fully coupled method would use too many resources of a given machine, or when the problem is not yet solved and a full coupling of the equations would diverge.

The `Plugin` syntax is defined as:

```
Plugin ( <options> ) ( <list-of-coupled-commands> )
```

`Plugin` commands can have any complexity but, usually, only a few combinations are effective. One standard form is the Gummel iteration in which each basic semiconductor equation is solved consecutively.

With the `Plugin` command, this is written as:

```
Plugin { Poisson Electron Hole }
```

summarizes the options of `Plugin`.

`Plugin` commands can be used with other `Plugin` commands, such as:

```
Plugin{ Plugin{ ... } Plugin { ... } }
```

illustrates the corresponding loop structure. A hierarchy of `Plugin` commands allows more complex iterative solve patterns to be created.
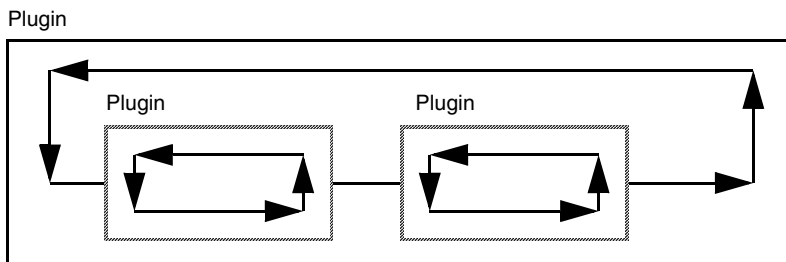
Figure 15   Example of hierarchy of Plugin commands

Linear Solvers

The `Math` parameters to the solution algorithms are device independent and must only appear in the base `Math` section. These can be grouped by solver type. The control parameters for the linear solvers are `Method` and `SubMethod`. The keyword `Method` selects the linear solver to be used, and the keyword `SubMethod` selects the inner method for block-decomposition methods (see for available linear solvers).

The keywords `ACMethod` and `ACSubMethod` determine the linear solver used for AC analysis.

> **NOTE** `ACMethod=Blocked` is the only valid choice for `ACMethod`. However, any of the available linear solvers can be selected for `ACSubMethod`.

Table 224 on page 1423 lists the options that are available for the linear solver PARDISO. The options are specified in parentheses after the solver specification:

```
Method = ParDiSo (NonsymmetricPermutation IterativeRefinement)
```

The default options `NonsymmetricPermutation`, `-IterativeRefinement`, and `-RecomputeNonsymmetricPermutation` provide the best compromise between speed and accuracy. To improve speed, select `-NonsymmetricPermutation`.

To improve accuracy, at the expense of speed, activate `IterativeRefinement`, or `RecomputeNonsymmetricPermutation`, or both.

All ILS options can be specified within an `ILSrc` statement in the global `Math` section:

```
Math {
   ILSrc = "
      set (...) {
         iterative (...);
         preconditioning (...);
         ordering (...);
         options (...);
      };
      ...
   "
   ...
}
```

Additional ILS options can be found in Table 224 on page 1423.

The two linear solvers PARDISO and ILS support the option `MultipleRHS` to solve linear systems with multiple right-hand sides. This option is only appropriate for AC analysis. ILS may produce a small parallel speedup or slightly more accurate results if this option is selected.

Use the `Math` option `PrintLinearSolver` to obtain additional information regarding the linear solver being used.

Nonlocal Meshes

Nonlocal meshes are one-dimensional, special-purpose meshes that Sentaurus Device needs to implement one-dimensional, nonlocal physical models. A nonlocal mesh consists of nonlocal

lines. Each nonlocal line is subdivided by nonlocal mesh points, to allow for the discretization of the equations that constitute the physical models. Sentaurus Device performs this subdivision automatically to obtain optimal interpolation between the nonlocal mesh and the normal mesh.

The 1D Schrödinger equation (see 1D Schrödinger Solver on page 285), the nonlocal tunneling model (see Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722), and the trap tunneling model (see Tunneling and Traps on page 463) use nonlocal meshes. The documentation of the former two models introduces the use of nonlocal meshes in the context of the particular model and is restricted to typical cases. This section describes the construction of nonlocal meshes in detail.

Specifying Nonlocal Meshes

Nonlocal meshes are specified by the keyword `Nonlocal` in the global `Math` section. `Nonlocal` is followed by a string that gives the name of the nonlocal mesh and a list of options that control the construction of the nonlocal mesh. You can specify any number of nonlocal meshes; individual specifications are independent. For example, with:

```
Math {
   Nonlocal "GateNonLocalMesh" (
      Electrode="Gate"
      Length=5e-7
   )
}
```

Sentaurus Device constructs a nonlocal mesh named `GateNonLocalMesh` that consists of nonlocal lines for semiconductor vertices up to a distance of 5 nm from the `Gate` electrode, and:

```
Math {
   Nonlocal "for_tunneling" (
      Barrier(Region="gateoxide")
   )
}
```

constructs a nonlocal mesh named `for_tunneling` that consists of lines that connect the different sides of the region `gateoxide`.

For a summary of available options, see Table 228 on page 1424. For a comprehensive description of the construction of a nonlocal mesh, see Constructing Nonlocal Meshes on page 149.

Visualizing Nonlocal Meshes

Sentaurus Device can visualize the nonlocal meshes it constructs. This feature is used to verify that the nonlocal mesh constructed is the one actually intended. For visualizing data defined on nonlocal meshes, see Visualizing Data Defined on Nonlocal Meshes on page 148.

To visualize nonlocal meshes, use the keyword `NonLocal` in the `Plot` section (see Device Plots on page 122). The keyword causes Sentaurus Device to write two vector fields to the plot file that represent the nonlocal meshes constructed in the device.

For each vertex (of the normal mesh) for which a nonlocal line exists, the first vector field `NonLocalDirection` contains a vector that points from the vertex to the end of the nonlocal line in the direction of the reference surface for which the nonlocal line was constructed. The vector in the second field `NonLocalBackDirection` points from the vertex to the other end of the nonlocal line. The unit of both vectors is μm.

For vertices for which no nonlocal line exists, both vectors are zero. For vertices for which more than one nonlocal line exists, Sentaurus Device plots the vectors for one of these lines.

Visualizing Data Defined on Nonlocal Meshes

To visualize data defined on nonlocal meshes:

■ In the `File` section, specify a file name using the `NonLocalPlot` keyword.

■ On the top level of the command file, specify a `NonLocalPlot` section. There, `NonLocalPlot` is followed by a list of coordinates in parentheses and a list of datasets in braces.

Sentaurus Device writes nonlocal plots at the same time it writes normal plots. Nonlocal plot files have the extension `.plt` or `.tdr`.

Sentaurus Device picks nonlocal lines close to the coordinates specified in the `NonLocalPlot` section for output. The datasets given in the `NonLocalPlot` section are the datasets that can be used in the `Plot` section (see Device Plots on page 122). `NonLocalPlot` does not support the `/Vector` option. Additionally, the Schrödinger equation provides special-purpose datasets available only for `NonLocalPlot` (see Visualizing Schrödinger Solutions on page 290).

In addition to the datasets explicitly specified, Sentaurus Device automatically includes the `Distance` dataset in the output. It provides the coordinate along the nonlocal line. The values in the `Distance` dataset are measured in μm. The interface or contact for which a nonlocal mesh line was constructed is located at zero, and its mesh vertex is located at positive

coordinates. The following example plots electron and hole densities for the nonlocal lines close to the coordinates $(0, 0, 0)$ and $(0, 1, 0)$ in the device:

```
NonLocalPlot(
    (0 0) (0 1)
){
    eDensity hDensity
}
```

Constructing Nonlocal Meshes

Nonlocal meshes are specified in the global `Math` section:

```
Math {
    NonLocal <string> (
        Barrier(...)
        RegionInterface=<string>
        MaterialInterface=<string>
        Electrode=<string>
        ...
    )
}
```

The string following `NonLocal` is the name of the nonlocal mesh. The name relates the nonlocal mesh to the physical models defined on it.

Sentaurus Device supports two ways to specify nonlocal meshes:

- By specifying the regions and materials that form the tunneling barrier (keyword `Barrier`).
- By specifying a reference surface (keywords `RegionInterface`, `MaterialInterface`, and `Electrode`).

The `Barrier` specification is simpler but less general, and it is only suitable for nonlocal meshes used for direct tunneling through insulator barriers.

Specification Using Barrier

As an option to `Barrier`, specify all regions that belong to the tunneling barrier, using any number of `Region=<string>` or `Material=<string>` specifications. Sentaurus Device connects each side of the barrier to any other with nonlocal lines. Here, *side* means a conductively connected part of the surface of the barrier.

By default, semiconductor regions, metal regions, and electrodes are considered to be conductive. To enforce that a particular region (such as a wide-bandgap semiconductor region)

is treated as not conductive, use the option `-Endpoint`, which accepts as an option a list of regions and materials, using the same syntax as for `Barrier`. For example:

```
Nonlocal "NLM" (
    ...
    -Endpoint(Material="GaN" Region="buffer1" Region="buffer2")
)
```

will cause regions `buffer1` and `buffer2`, and all GaN regions to be considered nonconductive when constructing the nonlocal mesh `NLM`.

Use `Length=<float>` (in centimeters) to restrict the length on nonlocal lines (to suppress very long tunneling paths).

Specification Using a Reference Surface

`RegionInterface`, `MaterialInterface`, and `Electrode` specify a region interface name, material interface name, or electrode name. All interfaces and electrodes together form the reference surface that determines where in the device the nonlocal mesh is constructed.

The nonlocal lines link vertices of the normal mesh to the reference surface on the geometrically shortest path. The parameter `Length` of `NonLocal` determines the maximum distance of the vertex to the reference surface (in centimeters). Sentaurus Device provides no default value for `Length`; all nonlocal meshes must specify `Length` explicitly.

`Length` and `Permeation` are limited to the value of the parameter `NonLocalLengthLimit`, which is specified in centimeters in the global `Math` section and defaults to 10^{-4}. This parameter is used to capture cases where users accidentally specify lengths in micrometers rather than centimeters.

The property that nonlocal lines connect a vertex to the reference surface on the geometrically shortest path is fundamental. If any of the other rules described in this section inhibits the construction of a nonlocal line for this path, but a longer connection obeys all these restrictions, Sentaurus Device still does not use this connection to construct an alternative nonlocal line.

The parameter `Permeation` specifies a length by which Sentaurus Device extends the nonlocal lines, across the reference surface, towards the opposite of the side for which the line is constructed. `Permeation` defaults to zero. Sentaurus Device never extends the lines outside the device or into regions flagged with `-Permeable` (see below). The extension is not affected by the `Transparent` and `Endpoint` options (see below).

The `Direction` parameter specifies a direction that the nonlocal lines approximately should have. Nonlocal lines with directions that deviate from the specified direction by an angle greater than `MaxAngle` are suppressed. If `Direction` is the zero vector or `MaxAngle`

exceeds 90 (this is the default), nonlocal lines can have any direction. The length and sign of the direction vector are otherwise insignificant.

`Discretization` specifies the maximum spacing of the nonlocal mesh vertices. When necessary, Sentaurus Device further refines the mesh created on a nonlocal line according to the built-in rules to yield a spacing no bigger than `Discretization` demands.

The flags `Transparent`, `Permeable`, `Endpoint`, and `Refined`, as well as their negation, specify flags for regions or materials that control nonlocal mesh construction. Each of the flags can be specified in two different ways:

■ As an option to the main specification in the global `Math` section.

■ As an option to `NonLocal` in a region-specific or material-specific `Math` section.

In the former case, the flag is followed by a list of region or material specifications that determine where the flag applies. In the latter case, the region or material of applicability is the location of the `Math` specification. Specifications of the latter style provide defaults that can be overwritten by specifications of the former style.

The part of a nonlocal line between the mesh vertex for which the line is constructed and the reference surface must not pass through regions flagged with `-Transparent`. By default, all regions are `Transparent`. For the exterior of the device, the flag `Outside` has the same meaning; this flag is an option to the main `NonLocal` specification.

The `-Permeable` flag limits extension on nonlocal lines across the reference surface. By default, all regions are `Permeable`.

For regions flagged with `-Endpoint`, Sentaurus Device does not construct nonlocal lines that end in this region. The default is `-Endpoint` for insulator regions, and `Endpoint` for other regions.

Inside regions flagged as `-Refined`, the generation of nonlocal mesh points at element boundaries is suppressed. By default, all regions are `Refined`.

Special Handling of 1D Schrödinger Equation

For performance reasons, Sentaurus Device solves the 1D Schrödinger equation (see) only on a reduced subset of nonlocal lines that still cover all vertices of the normal mesh for which nonlocal lines are constructed according to the rules outlined above.

To avoid artificial geometric quantization, Sentaurus Device extends nonlocal lines used for the 1D Schrödinger equation that are shorter than `Length` to reach full length. Sentaurus Device

never extends the lines outside the device or into regions flagged by the `-Permeable` option. The extension is not affected by the `Transparent` and `Endpoint` options.

For nonlocal line segments in regions not marked by `-Refined` and `-Endpoint`, Sentaurus Device computes the intersections with the boxes of the normal mesh. Sentaurus Device needs this information to interpolate results from the 1D Schrödinger equation back to the normal mesh. Therefore, in regions where `-Refined` or `-Endpoint` is specified, 1D Schrödinger density corrections are not available, even when the regions are covered by nonlocal lines.

Special Handling of Nonlocal Tunneling Model

Sentaurus Device computes the intersections of the nonlocal lines with the boxes (see Discretization on page 1011); to this end, some lines may become longer than `Length`. The nonlocal tunneling model (see Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722) uses the intersection points to limit the spatial range of the integrations Sentaurus Device must perform to compute the contribution to tunneling that comes from the particular vertex. For mesh points that border regions flagged with `-Endpoint`, the integration range is extended into that region, to pick up the Fowler–Nordheim current that enters it.

For nonlocal meshes used only for nonlocal tunneling, when `Permeation` is zero, Sentaurus Device assumes that the nonlocal lines cross the reference plane by an infinitesimal length. Therefore, if `-Endpoint` is specified for one of the regions that border the reference plane, Sentaurus Device suppresses nonlocal lines that point into that region.

If `Permeation` is positive, for nonlocal lines at nonmetal interfaces, Sentaurus Device switches to a nonlocal mesh construction mode similar to the one used for the Schrödinger equation: Sentaurus Device constructs only as many lines as needed to cover all vertices that must be covered, and extends all those lines to their maximum length. Furthermore, for nonlocal meshes not used for tunneling to traps, the integration range for tunneling covers the entire line. Tunneling to and from segments of the line marked by `–Endpoint` or `–Refined` will be assigned to the vertices for boxes crossed immediately outside those segments, to pick up Fowler–Nordheim currents in a similar manner as for the line construction mode with `Permeation=0`.

Unnamed Meshes

For backward compatibility, Sentaurus Device also allows you to specify nonlocal meshes in interface-specific or electrode-specific `Math` sections. For this kind of specification, the location of the mesh is the location of the `Math` section and, therefore, no interface or electrode specification must appear as an option to `NonLocal`.

Furthermore, the name of the nonlocal mesh must be omitted; physical models are associated with the nonlocal mesh by activating them in a `Physics` section specific to the same interface or electrode for which the nonlocal mesh was constructed.

For unnamed nonlocal meshes, vertices in regions with the trap tunneling model (see Tunneling and Traps on page 463) are connected irrespective of the material of the region or the `Endpoint` specification.

Performance Suggestions

To limit the negative performance impact of the nonlocal tunneling model, it is important to limit the number of nonlocal lines. To this end, most importantly, select `Length` and `Permeation` to be only as long as necessary. The option `-Endpoint` can be used to suppress the construction of lines to regions for which you know, in advance, that will not receive much tunneling current. The option `-Transparent` allows you to neglect tunneling through materials with comparatively high tunneling barrier, for example, oxides near a Schottky contact or heterointerface for which nonlocal tunneling has been activated.

Another use of the option `-Transparent` is at heterointerfaces, where there is no tunneling to the side of the material with the lower band edge (as there is no barrier to tunnel through). To restrict the construction of nonlocal lines to lines that go through the larger band-edge material, declare the lower band-edge material as not transparent by using `-Transparent`.

The option `-Refined` does not reduce the number of nonlocal lines, but it can reduce the size of the Jacobian matrix. The option `-Refined` is most useful for insulator regions, where the band-edge profile is approximately linear.

Monitoring Convergence Behavior

When Sentaurus Device has convergence problems, it can be helpful to know in which parts of the device and for which equations the errors are particularly large. With this information, it is easier to make adjustments to the mesh or the models used, to improve convergence.

Sentaurus Device can print the locations in the device where the largest errors occur (see CNormPrint on page 154). This provides limited information and has negligible performance impact. Sentaurus Device can also plot solution error information for the entire device after each Newton step (see NewtonPlot on page 154). This information is comprehensive, but can generate many files and can take significant time to write.

Both approaches provide access to the internal data of Sentaurus Device. Therefore, in both cases, the output is implementation dependent. Its proper interpretation can change between different Sentaurus Device releases.

CNormPrint

To obtain basic error information, specify the `CNormPrint` keyword in the global `Math` section. Then, after each Newton step and for each equation solved, Sentaurus Device prints to the standard output:

- The largest error according to Eq. 33, p. 138 that occurs anywhere in the device for the equation.
- The vertex where the largest error occurs.
- The coordinates of the vertex.
- The current value of the solution variable for that vertex.

NewtonPlot

Sentaurus Device can write the spatial values of solution variables, the errors, the right-hand sides, and the solution updates to a `NewtonPlot` file after each Newton step. `NewtonPlot` files then can be read into Sentaurus Visual for examination. To use this feature:

- Use the `NewtonPlot` keyword in the `File` section to specify a file name for the plot. This name can contain up to two C-style integer format specifiers (for example, `%d`). If present, for the file name generation, the first one is replaced by the iteration number in the current Newton step and the second, by the number of Newton steps in the simulation so far. Sentaurus Device does not enforce any particular file name extension, but prepends the device instance name to the file name in mixed mode.

- Sentaurus Device writes Newton information to a `NewtonPlot` file during execution of a `Quasistationary` or `Transient` command when the step size decreases below a certain value. By default, the criterion is step size $< 2 \times$ `MinStep`, where `MinStep` is the lower limit for the step size that is set in a `Quasistationary` or `Transient` command. This condition usually occurs immediately before a simulation is about to fail.

- Alternatively, use the `NewtonPlotStep` parameter to specify the step-size criterion. `NewtonPlotStep` can be specified as an option to the `NewtonPlot` keyword in the `Math` section of the command file, in which case, it applies to all `Quasistationary` and `Transient` commands. It also can be specified as an option to a particular `Quasistationary` or `Transient` command, in which case, it only applies to that particular command.

- By default, when the step-size criterion is met, Sentaurus Device writes the current values of the solution variables only to the `NewtonPlot` file. Additional data can be included in the output by specifying options to `NewtonPlot` in the `Math` section. See Table 211 on page 1403 for a list of available options.

- In addition, `MinError` can be specified as an option to `NewtonPlot`. If present, Sentaurus Device writes the `NewtonPlot` file only if the error of the actual iteration is smaller than all previous errors within the current Newton step. In this case, the first `%d` format specifier in the `NewtonPlot` file name will be replaced with `min` instead of the iteration number.

Automatic Activation of CNormPrint and NewtonPlot

By default, `CNormPrint` and `NewtonPlot` are activated automatically when certain criteria are met:

- For `CNormPrint`: step size < `AutoCNPMinStepFactor` × `MinStep`

- For `NewtonPlot`: step size < `AutoNPMinStepFactor` × `MinStep`

where the step size is calculated during the execution of a `Quasistationary` or `Transient` command, and `AutoCNPMinStepFactor` and `AutoNPMinStepFactor` are parameters that can be specified in the `Math` section of the command file:

```
Math {
    AutoCNPMinStepFactor = <float>   #default = 2.0
    AutoNPMinStepFactor = <float>    #default = 2.0
}
```

You can disable the automatic activation of `CNormPrint` and `NewtonPlot` by specifying values of zero for the above parameters.

When `NewtonPlot` files are created as a result of automatic activation, the `Error`, `Residual`, `Update`, and `MinError` options for `NewtonPlot` will be used by default. However, any user-specified options for `NewtonPlot` in the `Math` section of the command file will override the default behavior.

In addition, `NewtonPlot` will be activated automatically for solutions that are not part of a `Quasistationary` or `Transient` when the maximum-allowed iterations for the solution have been reached. The same output options described in the previous paragraph will be used in this case as well (except for `MinError`), and the iteration number will replace the `%d` format specifier in the file name.

Simulation Statistics for Plotting and Output

Simulation Statistics in Current Plot Files

To include various simulation statistics in current plot files for visualization, specify the `SimStats` option in the `Math` section of the command file:

```
Math {SimStats}
```

When this option is specified, Sentaurus Device will write a `SimStats` group of datasets to the current plot file (`*.plt` file) after each successful solution. The following datasets are included in the `SimStats` group:

`Restarts`	Number of consecutive restarts before the solution converged
`CumulativeRestarts`	Total number of restarts so far
`Stepsize`	Step size used for quasistationary or transient solution
`Rhs`	Final RHS norm for the solution
`error`	Final error for the solution
`Iterations`	Number of iterations required for solution
`CumulativeIterations`	Total number of iterations so far
`AssemblyTime`	CPU time spent building RHS and Jacobian for the solution
`SolveTime`	CPU time used by solver for the solution
`TotalTime`	Total CPU time for the solution (includes overhead time)
`CumulativeAssemblyTime`	Total assembly time so far
`CumulativeSolveTime`	Total solve time so far
`CumulativeTotalTime`	Total CPU time so far
`AssemblyTime_wall`	Wallclock time spent building RHS and Jacobian for the solution
`SolveTime_wall`	Wallclock time used by solver for the solution
`TotalTime_wall`	Total wallclock time for the solution (includes overhead time)
`CumulativeAssemblyTime_wall`	Total wallclock assembly time so far
`CumulativeSolveTime_wall`	Total wallclock solve time so far
`CumulativeTotalTime_wall`	Total wallclock time so far
`PeakMemory`	Peak memory (watermark) so far
`AverageMemory`	Average memory for the time step

Simulation Statistics in DOE Variables

Cumulative simulation statistics can be written to the end of a Sentaurus Device output file
(`*.log` file) as DOE variables by specifying the `WriteDOE` option to `SimStats` in the `Math`
section:

```
Math {
    SimStats ( WriteDOE [DOE_prefix = <string>] )
}
```

When `WriteDOE` is specified, the following DOE variables will be written:

```
DOE: Restarts            <value>
DOE: Iterations          <value>
DOE: AssemblyTime        <value>
DOE: SolveTime           <value>
DOE: TotalTime           <value>
DOE: AssemblyTime_wall   <value>
DOE: SolveTime_wall      <value>
DOE: TotalTime_wall      <value>
```

The option `DOE_prefix` allows a string to be prepended to the DOE variable names. For
example, specifying `DOE_prefix = "test_"` writes the DOE variable `test_Restarts`
instead of `Restarts`.

Save and Load

The `Save` and `Load` statements allow you to store the current simulation state of a device in a
file and later (often, from another simulation run) to reload it, and to resume from where you
stopped. By default, `Plot` files can be reloaded as well (see Device Plots on page 122). The
`Save` statement generates files of type .sav, which only contain the information required to
restart a simulation:

- Contact biases and currents

- The values of solution variables

- Occupation probability of traps

- Ferroelectric history (electric field and polarization) if the ferroelectric model is switched
  on

Loading traps is supported only if the specifications of traps for the saving and loading
simulation are identical, that is, the set of traps and their order in the command file must be
identical, as well as their types. A mismatch of trap specifications is silently ignored and could
lead to partially correctly, incorrectly, or not loaded trap occupations. In this case, you must
verify if the traps are initialized as intended.

When the file is loaded, all this information is restored.

> **NOTE**   Contact voltages stored in the loaded file overwrite the bias conditions
> that are specified in the command file.

When you specify a `Save` file in the `File` section, the simulation state is saved automatically to that file at the end of the simulation. When you specify a `Load` file in the `File` section, the state stored in that file is loaded at the beginning of the simulation. The geometry of a loaded file must match the geometry specified in the `Grid` file.

> **NOTE**   Interfaces regions are required in the grid file to save and load data on
> interfaces (see Interface Plots on page 125).

More control is possible with `Save` and `Load` commands in the `Solve` section. The commands are defined as:

```
Save(<parameters-opt>) <system-opt>
Load(<parameters-opt>) <system-opt>
```

The options are as for `Plot`, see When to Plot on page 123. `Save` statements can be used at any level of the `Solve` section, the `Load` statement can only be used as a base level of the `Solve` statement.

For example, in the case of a transient simulation, `Load` can only be used before or after the transient, not during it. Multiple `Load` and `Save` commands are allowed in a `Solve` statement. For example:

```
Solve {
  ...
  # Ramp the gate and save structures
    # First gate voltage
    Quasistationary (InitialStep=0.1 MaxStep=0.1 MinStep=0.01
                     Goal {Name="gate" Voltage=1})
                     {Coupled {Poisson Electron Hole}}
                     Save(FilePrefix="vg1")
    # Second gate voltage
    Quasistationary (InitialStep=0.1 Maxstep=0.1 MinStep=0.01
                     Goal {Name="gate" Voltage=3})
                     {Coupled {Poisson Electron Hole}}
                     Save(FilePrefix="vg2")
  # Load the saved structures and ramp the drain
    # First curve
    Load(FilePrefix="vg1")
    NewCurrentPrefix="Curve1"
    Quasistationary (InitialStep=0.1 MaxStep=0.5 MinStep=0.01
                     Goal {Name="drain" Voltage=2.0})
                     {Coupled {Poisson Electron Hole}}
```

```
      # Second curve
      Load(FilePrefix="vg2")
      NewCurrentPrefix="Curve2"
      Quasistationary (InitialStep=0.1 MaxStep=0.5 MinStep=0.01
                       Goal {Name="drain" Voltage=2.0})
                       {Coupled {Poisson Electron Hole}}
}
```

Tcl Command File

The Sentaurus Device command-line option `--tcl` invokes the Tcl interpreter to execute the command file. Tcl provides valuable extensions to the standard command file of Sentaurus Device, including:

- Variables
- Expressions
- Control structures

In addition, all of the Inspect Tcl commands are available (refer to the *Inspect User Guide* for more information). These commands are useful for the purpose of parameter extraction (see Extraction on page 163). However, the graphical functionality of the Inspect commands has been disabled.

Overview

An entire device simulation can be performed by the Tcl command `sdevice`. The following example shows a quasistationary ramp to computed contact values:

```
set vd 0.2
set vg [expr {10*$vd}]

sdevice "
   Electrode{
      { Name = \"source\" Voltage = 0.0 }
      { Name = \"gate\" Voltage = 0.0 }
      { Name = \"drain\" Voltage = $vd }
      { Name = \"bulk\" Voltage = 0.0 }
   }

   File{
      Grid    = \"mosfet.tdr\"
      Plot    = \"mosfet_des.tdr\"
      Current = \"mosfet_des.plt\"
      Output  = \"mosfet_des.log\"
```

```
      }

      Physics {
         Mobility (DopingDependence)
         Recombination (SRH (DopingDependence))
      }

      Solve{
         Poisson
         QuasiStationary (Goal {Name=\"gate\" Voltage=$vg})
         { Coupled {Poisson Electron Hole} }
      }
   "
```

Sometimes, it is more useful to perform a device simulation in stages. In this case, the `sdevice_init` command is used for initialization, and multiple `sdevice_solve` commands are used to drive the simulation.

In the following example, an I_d–V_g sweep is performed, and the threshold voltage is extracted from the current plot file:

```
# initialize Sentaurus Device simulation
sdevice_init {
   Electrode{
      { Name = "source" Voltage = 0.0 }
      { Name = "gate" Voltage = 0.0 }
      { Name = "drain" Voltage = 0.2 }
      { Name = "bulk" Voltage = 0.0 }
   }

   File{
      Grid    = "mosfet.tdr"
      Plot    = "extract_VT_des.tdr"
      Current = "extract_VT_des.plt"
      Output  = "extract_VT_des.log"
   }

   Physics{
      EffectiveIntrinsicDensity (Slotboom)
      Mobility (DopingDependence)
      Recombination (SRH (DopingDependence))
   }
}

# compute idvgs curve
sdevice_solve {
   Solve{
      NewCurrentPrefix = "initial_"
```

```
      Poisson
      Coupled {Poisson Electron Hole}

      Save (FilePrefix = "extract_VT_inital_save")

      NewCurrentPrefix = ""
      QuasiStationary (
         InitialStep=0.05 Increment=1.3
         MaxStep=0.05 MinStep=1e-4
         Goal {Name="gate" Voltage=2}
      )
      { Coupled {Poisson Electron Hole} }
   }
}

# extract threshold voltage
set VT [extract_VT extract_VT_des.plt gate drain]

# ramp gate voltage to threshold voltage
sdevice_solve "
   Solve{
      NewCurrentPrefix = \"ignore_\"

      Load (FilePrefix = \"extract_VT_inital_save\")

      QuasiStationary (
         InitialStep=0.25 Increment=1.3
         MaxStep=0.25 MinStep=1e-4
         Goal {Name=\"gate\" Voltage=$VT}
      )
      { Coupled {Poisson Electron Hole} }
   }
"

# save final plot file
sdevice_finish
```

The final command `sdevice_finish` signals the end of a sequence of `sdevice_solve` statements, and Sentaurus Device saves the final plot files.

sdevice Command

The Tcl `sdevice` command expects a single argument. This argument describes an entire device simulation, that is, it includes a `File` section, `Physics` section, and `Solve` section.

The `sdevice` command returns 1 if the device simulation converges. Otherwise, the value 0 is returned.

sdevice_init Command

The Tcl `sdevice_init` command expects a single argument. This argument initializes a device simulation, that is, it can contain all of the sections of a standard command file of Sentaurus Device (except a `Solve` section).

No return value is computed by `sdevice_init`. If an error is encountered, Sentaurus Device will abort.

sdevice_solve Command

The Tcl `sdevice_solve` command expects a single argument. It can only be used after an `sdevice_init` command. The argument must contain a single `Solve` section. All the commands in the `Solve` section are executed.

The `sdevice_solve` command returns 1 if the device simulation converges. Otherwise, the value 0 is returned.

sdevice_finish Command

The Tcl `sdevice_finish` command expects no arguments, and it can be called after a series of `sdevice_solve` commands. It indicates that the device simulation performed by the `sdevice_solve` commands is finished, and the final plot file is generated. All open current plot files are closed.

sdevice_parameters Command

The Tcl `sdevice_parameters` command expects two arguments: a file name and the contents of a Sentaurus Device parameter file. It is an auxiliary function, which writes the parameter file to the given file name.

The following example generates the file `models.par` containing a permittivity parameter:

```
sdevice_parameters models.par {
   Epsilon {
      epsilon = 11.7
   }
}
```

Flowchart

Figure 16 shows the sequence in which the various Tcl sdevice commands can be invoked.
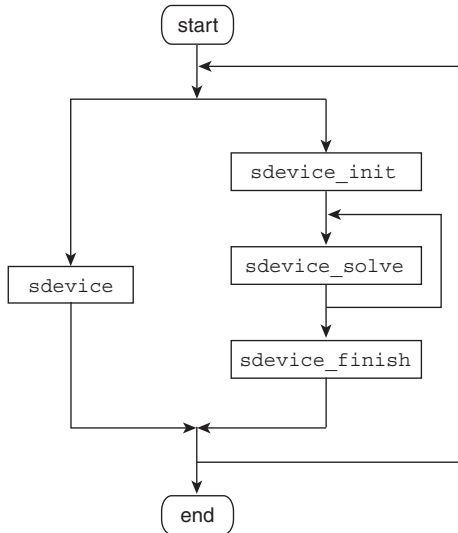
Figure 16   Flowchart of sequence for Tcl commands

Extraction

The Tcl interpreter in Sentaurus Device provides access to all of the Inspect commands. In this way, you can easily analyze .plt files generated by Sentaurus Device and extract parameters. The following example shows a gate ramp followed by the extraction of the threshold voltage:

```
sdevice {
   Electrode {
      { Name = "source" Voltage = 0.0 }
      { Name = "gate"   Voltage = 0.0 }
      { Name = "drain"  Voltage = 0.2 }
      { Name = "bulk"   Voltage = 0.0 }
   }

   File {
      Grid    = "mosfet.tdr"
      Plot    = "extract_VT_des.tdr"
      Current = "extract_VT_des.plt"
      Output  = "extract_VT_des.log"
   }

   Physics { ... }
```

```
Solve {
   QuasiStationary (
      InitialStep=0.05 MaxStep=0.05
   Goal {Name="gate" Voltage=2}
   )
   { Coupled {Poisson Electron Hole} }
}
}

proj_load extract_VT_des.plt proj
cv_create idvgs "proj gate OuterVoltage" "proj drain TotalCurrent"
set VT [f_VT idvgs]
puts stdout "threshold voltage VT = ${VT}V"
```

Available Inspect Tcl Commands

Inspect Tcl commands can be used in Sentaurus Device.

Table 21   Inspect Tcl commands available for use in Sentaurus Device

Command functions	Tcl commands
Reading and writing files	graph_load, graph_write, load_library, param_load, param_write, proj_getDataSet, proj_getList, proj_getNodeList, proj_load, proj_unload, proj_write
Curve commands	cv_abs, cv_compute, cv_create, cv_createFromScript, cv_createWithFormula, cv_delete, cv_delPts, cv_getVals, cv_getValsX, cv_getValsY, cv_getXaxis, cv_getYaxis, cv_getZero, cv_inv, cv_log10Scale, cv_logScale, cv_printVals, cv_rename, cv_renameCurve, cv_reset, cv_scaleCurve, cv_set_interpol, cv_split, cv_split_disc, cv_write, macro_define
Parameter extraction	f_Gamma, f_gm, f_IDSS, f_KP, f_Ron, f_Rout, f_TetaG, f_VT, f_VT1, f_VT2, ft_scalar
Curve comparison library (load_library curvecomp)	cvcmp_CompareTwoCurves, cvcmp_DeltaTwoCurves
Extraction library (load_library EXTRACT)	cv_linTransCurve, cv_scaleCurve, ExtractBVi, ExtractBVv, ExtractEarlyV, ExtractGm, ExtractGmb, ExtractIoff, ExtractMax, ExtractRon, ExtractSS, ExtractValue, ExtractVtgm, ExtractVtgmb, ExtractVti

Table 21   Inspect Tcl commands available for use in Sentaurus Device (Continued)

Command functions	Tcl commands
RF extraction library (`load_library RFX`)	`rfx_abs_c`, `rfx_abs2_c`, `rfx_add_c`, `rfx_con_c`, `rfx_div_c`, `rfx_Export2csv`, `rfx_ExtractVal`, `rfx_GetFK1`, `rfx_GetFmax`, `rfx_GetFt`, `rfx_GetK_MSG_MAG`, `rfx_GetMUG`, `rfx_GetNearestIndex`, `rfx_GetRFCList`, `rfx_im_c`, `rfx_load`, `rfx_mag_phase`, `rfx_mul_c`, `rfx_PolarBackdrop`, `rfx_re_c`, `rfx_ReIm2Abs`, `rfx_ReIm2Phase`, `rfx_S2K`, `rfx_sign`, `rfx_SmithBackdrop`, `rfx_sub_c`, `rfx_Y2H`, `rfx_Y2K`, `rfx_Y2S`, `rfx_Y2U`, `rfx_Y2Z`, `rfx_Z2U`
IC-CAP model parameter extraction library (`load_library ise2iccap`)	`iccap_Write`

Output Redirection

The Tcl commands `sdevice`, `sdevice_init`, `sdevice_solve`, and `sdevice_finish` allow you to redirect standard output and standard errors.

Table 22   Syntax for output redirection

Syntax	Description
`> filename`	Writes standard output to `filename`.
`2> filename`	Writes standard error to `filename`.
`>& filename`	Writes both standard output and standard error to `filename`.
`>> filename`	Appends standard output to `filename`.
`2>> filename`	Appends standard error to `filename`.
`>>& filename`	Appends both standard output and standard error to `filename`.

Known Restrictions

The following solve commands only apply to the subsequent statements within a single `Solve` section. They do not apply beyond an `sdevice_solve` command:

■   `NewCurrentPrefix` (see NewCurrentPrefix Statement on page 110)

■   `Set (TrapFilling=...)` (see Explicit Trap Occupation on page 468)

If a transient simulation is performed using several `sdevice_solve` commands, the correct initial time must be specified. Sentaurus Device does not remember the last transient time from the previous `sdevice_solve` command.

Parallelization

Sentaurus Device uses thread parallelism to accelerate simulations on shared memory computers. Table 23 gives an overview of the components of Sentaurus Device that have been parallelized.

Table 23   Areas of parallelization

Area	Description
Matrix assembly	Computation of mobility, avalanche, current density, energy flux; assembly of Poisson, continuity, lattice, and temperature equations; modified local-density approximation (MLDA); computation of box method coefficients.
Linear solver	Direct solver PARDISO; iterative solver ILS.

The number of threads can be specified in the global `Math` section of the Sentaurus Device command file:

```
Math {
   NumberOfThreads = number of threads
}
```

You can specify a constant for the number of threads, such as:

```
NumberOfThreads = 2
```

or:

```
NumberOfThreads = maximum
```

where `maximum` is equivalent to the number of processors available on the execution platform.

If required, the number of threads also can be specified separately for both the assembly and the linear solvers:

```
Math {
   NumberOfAssemblyThreads = number of assembly threads
   NumberOfSolverThreads = number of solver threads
}
```

In addition, the values of the following environment variables are checked:

```
SDEVICE_NUMBER_OF_THREADS, SNPS_NUMBER_OF_THREADS
SDEVICE_NUMBER_OF_ASSEMBLY_THREADS
SDEVICE_NUMBER_OF_SOLVER_THREADS
OMP_NUM_THREADS
```

Table 24 summarizes the priority of the various methods for specifying the number of threads.

Table 24   Specification of number of threads

Priority	Matrix assembly	Linear solver
Highest	NumberOfAssemblyThreads	NumberOfSolverThreads
	NumberOfThreads	NumberOfThreads
	SDEVICE_NUMBER_OF_ASSEMBLY_THREADS	SDEVICE_NUMBER_OF_SOLVER_THREADS
	SDEVICE_NUMBER_OF_THREADS	SDEVICE_NUMBER_OF_THREADS
	SNPS_NUMBER_OF_THREADS	SNPS_NUMBER_OF_THREADS
Lowest		OMP_NUM_THREADS

The stack size per assembly thread can be specified in the global `Math` section of the Sentaurus Device command file:

```
Math {
   StackSize = stacksize in bytes
}
```

Alternatively, the following UNIX environment variables are recognized:

```
SDEVICE_STACKSIZE, SNPS_STACKSIZE
```

By default, Sentaurus Device uses only one thread and the stack size is 1 MB. For most simulations, the default stack size is adequate.

Sentaurus Device requires one parallel license for every four threads. For example, a parallel simulation with 2–4 threads requires one parallel license, 5–8 threads require two licenses, 9–12 threads require three licenses, and so on. In the `Math` section, you can specify the behavior if there are not enough parallel licenses available:

```
Math {
   ParallelLicense (option)
}
```

Table 25   Available options if insufficient parallel licenses are available

Option	Description
Abort	Abort the simulation.
Serial	(Default) Continue the simulation in serial mode.
Wait	Wait until enough parallel licenses become available.

NOTE   These options apply only to the initial checkout of parallel licenses. Under certain circumstances, Sentaurus Device may later check in and check out parallel licenses as well. This might occur when another required license is temporarily unavailable. In this case, Sentaurus Device checks in all the licenses that have been checked out so far (including parallel licenses), waits until all the required licenses become available, and checks them out again.

Observe the following recommendations to obtain the best results from a parallel Sentaurus Device run:

- Speedups are only obtained for sufficiently large problems. In general, the device grid should have at least 5000 vertices. Three-dimensional problems are good candidates for parallelization.

- It is sensible to run a parallel Sentaurus Device job on an empty computer. As soon as multiple jobs compete for processors, performance decreases significantly.

- Use the keyword `Wallclock` in the `Math` section of the Sentaurus Device command file to display wallclock times rather than CPU times.

- The parallel execution produces different rounding errors. Therefore, the number of Newton iterations might change.

Extended Precision

Sentaurus Device allows you to perform simulations using extended precision floating-point arithmetic. This option is switched on in the global `Math` section by the keyword `ExtendedPrecision`. Table 26 lists the available options, the size of a floating-point number, and the precision.

Table 26   Extended precision floating-point arithmetic

Option	Description	Size	Precision
`-ExtendedPrecision`	double (default)	64 bits	$2.22{\times}10^{-16}$
`ExtendedPrecision`	long double	80 bits (Linux)	$1.08{\times}10^{-19}$
`ExtendedPrecision(128)`	double-double	128 bits	$4.93{\times}10^{-32}$
`ExtendedPrecision(256)`	quad-double	256 bits	$1.22{\times}10^{-63}$
`ExtendedPrecision(Digits=<digits>)`	arbitrary	320 + 4.5<digits> bits	$10^{-<digits>}$

On Linux, 80-bit extended precision arithmetic is supported in hardware with no noticeable degradation in performance. However, the gain in accuracy compared to normal precision (19 decimal digits versus 16 decimal digits) is limited.

The data types double-double and quad-double are implemented in software on all platforms. They provide significant improvements in accuracy (32 and 63 decimal digits, respectively). However, the runtimes increase by a factor of 10 and 100, respectively.

Arbitrary precision supports floating-point arithmetic with an arbitrary number of digits. It can be used for small research problems where even quad-double may not provide sufficient accuracy, for example, ultrawide-bandgap semiconductors.

The storage requirements of arbitrary precision increase linearly with the number of digits. The runtimes, however, increase quadratically with the number of digits.

Extended precision can be a powerful tool to simulate wide-bandgap semiconductors, where it is necessary to resolve accurately small currents and very low carrier concentrations. It may or may not be beneficial for general convergence problems.

When using extended precision, the following points should be observed for the best results:

- In general, the direct linear solver SUPER provides the best accuracy. Additional choices include the direct linear solver PARDISO and the iterative linear solver ILS. Other linear solvers do not support extended precision.

- In the `Math` section:

  - Increase the value of `Digits`. Possible values are `Digits=15` for `ExtendedPrecision(128)` and `Digits=25` for `ExtendedPrecision(256)`. The value of `Digits` can be increased even further with arbitrary precision.

  - Decrease the value of `RhsMin`. Possible values are `RhsMin=1e-15` for `ExtendedPrecision(128)` and `RhsMin=1e-25` for `ExtendedPrecision(256)`. The value of `RhsMin` can be decreased even further with arbitrary precision.

  - Slightly increase `Iterations`, for example, from 15 to 20.

  - In the case of arbitrary precision, you may need to increase the maximum-allowed error (`UpdateMax` parameter) as well as to increase `Digits`. For example, `UpdateMax=1e220` is recommended for `Digits=200`.

Some features of Sentaurus Device do not take advantage of extended precision, including:

- Input and output to files
- Compact circuit models (refer to the *Compact Models User Guide*)
- CMI and the standard C++ interface in the PMI (see Part V of this user guide)
- Monte Carlo (refer to the *Sentaurus™ Device Monte Carlo User Guide*)
- Optical simulations
- Integration of beam distribution for optical generation (see the keyword `RecBoxIntegr` in Transfer Matrix Method on page 625)

System Command

The `System` command allows UNIX commands to be executed during a Sentaurus Device simulation:

```
System ("UNIX command")
```

The `System` command can appear as an independent command in the `Solve` section, as well as within a `Transient`, `Plugin`, or `Quasistationary` command. The string argument of the `System` command is passed to a UNIX shell for evaluation.

By default, the return status of the UNIX command is ignored. If the variant:

```
+System ("UNIX command")
```

is used, Sentaurus Device examines the return status. The `System` command is considered to have converged if the return status is zero. Otherwise, it has not converged.

References

[1]   R. E. Bank and D. J. Rose, "Global Approximate Newton Methods," *Numerische Mathematik*, vol. 37, no. 2, pp. 279–295, 1981.

Part II Physics in Sentaurus Device

This part of the *Sentaurus™ Device User Guide* contains the following chapters:

CHAPTER 7   Electrostatic Potential and Quasi-Fermi Potentials

This chapter discusses electrostatic potential and the quasi-Fermi potentials.

In all semiconductor devices, mobile charges (electrons and holes) and immobile charges (ionized dopants or traps) play a central role. The charges determine the electrostatic potential and, in turn, are themselves affected by the electrostatic potential. Therefore, each electrical device simulation at the very least must compute the electrostatic potential.

When all contacts of a device are biased to the same voltage, the device is in equilibrium, and the electron and hole densities are described by a constant quasi-Fermi potential. Therefore, together with the electrostatic potential, the relation between the quasi-Fermi potentials and the electron and hole densitìes is sufficient to perform the simplest possible device simulation.

Maxwell–Boltzmann statistics is the default in Sentaurus Device, and you can choose to use Fermi–Dirac statistics as described in Fermi Statistics on page 176.

Electrostatic Potential

The electrostatic potential is the solution of the Poisson equation, which is:

$$\nabla \cdot (\varepsilon \nabla \phi + \vec{P}) = -q(p - n + N_{\mathrm{D}} - N_{\mathrm{A}}) - \rho_{\mathrm{trap}} \tag{37}$$

where:
- ε is the electrical permittivity.
- $\vec{P}$ is the ferroelectric polarization (see Chapter 29 on page 797).
- q is the elementary electronic charge.
- n and p are the electron and hole densities.
- N_{D} is the concentration of ionized donors.
- N_{A} is the concentration of ionized acceptors.
- ρ_{trap} is the charge density contributed by traps and fixed charges (see Chapter 17 on page 449).

The dataset name for the electrostatic potential is `ElectrostaticPotential`. The right-hand side of Eq. 37 (divided by $-q$) is stored in the `SpaceCharge` dataset. The keyword for the Poisson equation in the `Solve` section is `Poisson`.

The dimensionless relative permittivity (that is, the permittivity in units of the vacuum permittivity ε_0) is given by the parameter `epsilon` in the `Epsilon` parameter set. The boundary conditions for the Poisson equation are discussed in Chapter 10 on page 201.

Dipole Layer

At material interfaces, dipole layers of immobile charges can occur, leading to a potential jump across the interface. They are modeled by:

$$\phi_2 - \phi_1 = \frac{q\sigma_D}{\varepsilon_r\varepsilon_0} \tag{38}$$

where:

- ϕ_1 and ϕ_2 refer to the electrostatic potential at both sides of the interface (index 1 is the reference side).
- σ_D is the dipole surface density.
- ε_0 is the free space permittivity.
- ε_r is the relative interface permittivity.
- q is the elementary electronic charge.

The dipole interface model can be invoked for insulator–insulator interfaces by specifying:

```
Dipole ( Reference = "R1" )
```

in the `Physics` section of the interface. `Reference` denotes the reference side of the interface, and it can be either a region name or the material name.

The parameters of the model are given in the `Dipole` parameter set of the region or material interface section in the parameter file, and are listed in Table 27.

Table 27   Dipole model parameters

Symbol	Parameter name	Default value	Unit
σ_D	sigma_D	0.	cm^{-1}
ε_r	epsilon	3.9	1

NOTE   At critical points, where heterointerfaces and dipole interfaces intersect, the semiconductor regions must be interface connected. Interface traps with tunneling cannot be located on dipole interfaces.

Equilibrium Solution

For some models (see Conductive Insulators on page 244 or Modified Ohmic Contacts on page 202), the equilibrium electrostatic potential is required internally. In this case, the Poisson equation is solved with equilibrium boundary conditions before any other `Coupled` statement and the solution is saved for use during the simulation.

Sentaurus Device allows you to control the parameters of the nonlinear solver for the equilibrium Poisson equation. The parameters `Iterations`, `Digits`, `NotDamped`, `LineSearchDamping`, and `RelErrControl` described in Table 189 on page 1387 can be specified as options to the keyword `EquilibriumSolution` in the `Math` section (see Table 220 on page 1421) to control the Newton solver behavior. The following example forces the Newton solver to solve for an equilibrium solution with 7 digits as the target accuracy and a maximum number of 100 iterations:

```
Math {
   ...
   EquilibriumSolution(Iterations=100 Digits=7)
   ...
}
```

Quasi-Fermi Potential With Boltzmann Statistics

Electron and hole densities can be computed from the electron and hole quasi-Fermi potentials, and vice versa. If Boltzmann statistics is assumed, the formulas read:

$$n \ = \ N_{\mathrm{C}}\exp\!\left(\frac{E_{\mathrm{F},n}-E_{\mathrm{C}}}{kT}\right) \tag{39}$$

$$p \ = \ N_{\mathrm{V}}\exp\!\left(\frac{E_{\mathrm{V}}-E_{\mathrm{F},p}}{kT}\right) \tag{40}$$

where:

- N_{C} and N_{V} are the effective density-of-states.
- $E_{\mathrm{F},n} \ = \ -q\Phi_n$ and $E_{\mathrm{F},p} \ = \ -q\Phi_p$ are the quasi-Fermi energies for electrons and holes.
- Φ_n and Φ_p are electron and hole quasi-Fermi potentials, respectively.

- E_C and E_V are conduction and valence band edges, defined as:

$$E_C = -\chi - q(\phi - \phi_{ref}) \tag{41}$$

$$E_V = -\chi - E_{g,eff} - q(\phi - \phi_{ref}) \tag{42}$$

where χ denotes the electron affinity, $E_{g,eff}$ is the effective band gap, and ϕ_{ref} is a constant reference potential, see below. The zero level for the quasi-Fermi potential agrees with the zero level for the voltages applied at the contacts.

In unipolar devices, such as MOSFETs, it is sometimes possible to assume that the value of quasi-Fermi potential for the minority carrier is constant in certain regions. In this case, the concentration of the minority carrier can be directly computed from Eq. 39 or Eq. 40. This strategy is applied in Sentaurus Device if one of the carriers (electron or hole) is not specified inside the `Coupled` statement of the `Solve` section. Sentaurus Device uses an approximation scheme to determine the constant value of the quasi-Fermi potential.

> **NOTE**   In many cases if avalanche generation is important, the one carrier approximation cannot be applied even for unipolar devices.

The datasets for $E_{F,n}$. Φ_n, $E_{F,p}$, and Φ_p are named `eQuasiFermiEnergy`, `eQuasiFermiPotential`, `hQuasiFermiEnergy`, and `hQuasiFermiPotential`, respectively.

The `ConstRefPot` parameter allows you to specify ϕ_{ref} explicitly. Otherwise, Sentaurus Device computes ϕ_{ref} from the vacuum level, using the following rules:

- If there is silicon in any simulated semiconductor structure, the intrinsic Fermi level of silicon is selected as reference, $\phi_{ref} = \Phi_{intr}(Si)$.
- Otherwise, if any simulated device structure contains GaAs, $\phi_{ref} = \Phi_{intr}(GaAs)$.
- In all other cases, Sentaurus Device selects the material with the smallest band gap (assuming a mole fraction of 0) and takes the value of its intrinsic Fermi level as ϕ_{ref}.

Fermi Statistics

For the equations presented in the previous section, Boltzmann statistics was assumed for electrons and holes. Physically more correct, Fermi (also called Fermi–Dirac) statistics can be used. Fermi statistics becomes important for high values of carrier densities, for example, $n > 1 \times 10^{19}\,\mathrm{cm}^{-3}$ in the active regions of a silicon device.

For Fermi statistics, Eq. 39 and for Eq. 40 are replaced by:

$$n = N_C F_{1/2}\left(\frac{E_{F,n} - E_C}{kT}\right) \tag{43}$$

$$p = N_V F_{1/2}\left(\frac{E_V - E_{F,p}}{kT}\right) \tag{44}$$

where $F_{1/2}$ is the Fermi integral of order 1/2.

Alternatively, you can write these expressions as:

$$n = \gamma_n N_C \exp\left(\frac{E_{F,n} - E_C}{kT}\right) \tag{45}$$

$$p = \gamma_p N_V \exp\left(\frac{E_V - E_{F,p}}{kT}\right) \tag{46}$$

where γ_n and γ_p are the functions of η_n and η_p:

$$\gamma_n = \frac{n}{N_C} \exp(-\eta_n) \tag{47}$$

$$\gamma_p = \frac{p}{N_V} \exp(-\eta_p) \tag{48}$$

$$\eta_n = \frac{E_{F,n} - E_C}{kT} \tag{49}$$

$$\eta_p = \frac{E_V - E_{F,p}}{kT} \tag{50}$$

Using Fermi Statistics

To activate Fermi statistics, the keyword `Fermi` must be specified in the global `Physics` section:

```
Physics {
   ...
   Fermi
}
```

> **NOTE** Fermi statistics can be activated only for the whole device. Region-specific or material-specific activation is not possible, and the keyword `Fermi` is ignored in any `Physics` section other than the global one.

Initial Guess for Electrostatic Potential and Quasi-Fermi Potentials in Doping Wells

To determine an initial guess for the electrostatic potential and quasi-Fermi potentials, the device is divided into doping well regions, where a doping well region is a semiconductor region consisting of a set of connected semiconductor elements bounded by nonsemiconductor elements or by vacuum (a doping well region may contain several mesh semiconductor regions). Then, each doping well region is further subdivided into wells of n-type and p-type doping, such that p-n junctions (`DopingConcentration=0`) serve as dividers between wells. For doping wells with more than one contact, the wells are further subdivided, such that no well is associated with more than one contact. Every well is connected uniquely to a contact or it has no contact (floating well).

> **NOTE** Sentaurus Device uses integers to enumerate all doping wells. You can visualize the indices of the doping wells by plotting the `DopingWells` field.

In wells with contacts, the quasi-Fermi potential of the majority carrier is set to the voltage on the contact associated with the well. For wells that have no contacts, the following equations define the quasi-Fermi potential for the majority carriers:

$$\Phi_p = k_{\text{float}} V_{\max} + (1 - k_{\text{float}}) V_{\min} \tag{51}$$

$$\Phi_n = (1 - k_{\text{float}}) V_{\max} + k_{\text{float}} V_{\min} \tag{52}$$

where $V_{\min}$ and $V_{\max}$ are the minimum and maximum of the contact voltages of the semiconductor wells with contacts in the doping well region, where the contactless well under consideration is located. The coefficient k_{float} is an adjustable parameter with a default value of 0. To change the value of k_{float}, use the keyword `FloatCoef` in the `Physics` section.

If a well has a contact and it is the only well in the doping well region to which it belongs, then the quasi-Fermi potential of the minority carrier is set equal to the quasi-Fermi potential of the majority carrier. For all other wells, the quasi-Fermi potential of the minority carrier is set to $V_{\min}$ or $V_{\max}$ if the well is n-type or p-type, respectively, with $V_{\min}$ and $V_{\max}$ described above.

The electrostatic potential in a well is set to the value of the quasi-Fermi potential of the majority carrier adjusted by the built-in potential, that is, the initial solution will obey charge neutrality in all semiconductor regions.

Regionwise Specification of Initial Quasi-Fermi Potentials

You can set initial quasi-Fermi potentials regionwise. This is especially useful in CCD simulations, where a CCD cell or region must be initially in a certain state (usually, deep depletion). By specifying an initial quasi-Fermi potential, the region or set of regions can be brought to the proper state or states at the start of the simulation.

The initial quasi-Fermi potentials for electrons and holes can be specified regionwise in the `Physics` section using `eQuasiFermi` for electrons and `hQuasiFermi` for holes, followed by the value in volts:

```
Physics(Region="region_1") {
   eQuasiFermi = 10
}
```

The initial quasi-Fermi potential is recomputed when the continuity equation for the respective carrier is solved. If the continuity equation for the carrier whose quasi-Fermi potential has been specified is not solved, then the quasi-Fermi potential does not change. In this case, the device can be biased to an initial state through a quasistationary or transient simulation, while keeping the initial specified quasi-Fermi potential.

Electrode Charge Calculation

Sentaurus Device outputs the electrode charge to the current plot file (`*.plt` file) after each bias or time point.

For an electrode that contacts an insulator region only, the charge is computed from Gauss's law and represents the charge that would sit on the surface of a real contact to the device.

For an electrode that contacts a semiconductor region, the charge also is computed from Gauss's law; however, the Gaussian surface used for the integration includes the doping well associated with the electrode. In this case, the electrode charge represents the charge that sits on the electrode plus the space charge in the doping well.

CHAPTER 8 Carrier Transport in Semiconductors

This chapter discusses carrier transport models for electrons and holes in inorganic semiconductors.

Introduction to Carrier Transport Models

Sentaurus Device supports several carrier transport models for semiconductors. They all can be written in the form of continuity equations, which describe charge conservation:

$$\nabla \cdot \vec{J}_n \;=\; q(R_{\text{net},n} - G_{\text{net},n}) + q\frac{\partial n}{\partial t} \qquad -\nabla \cdot \vec{J}_p \;=\; q(R_{\text{net},p} - G_{\text{net},p}) + q\frac{\partial p}{\partial t} \tag{53}$$

where:

- $R_{\text{net},n}$ and $R_{\text{net},p}$ are the electron and hole net recombination rate, respectively.
- $G_{\text{net},n}$ and $G_{\text{net},p}$ are the electron and hole net generation rate, respectively.
- $\vec{J}_n$ is the electron current density.
- $\vec{J}_p$ is the hole current density.
- n and p are the electron and hole density, respectively.

The transport models differ in the expressions used to compute $\vec{J}_n$ and $\vec{J}_p$. These expressions are the topic of this chapter. Additional equations to compute temperatures are usually also considered part of a transport model but are deferred to Chapter 9 on page 189. Models for $R_{\text{net,n}}$ and $R_{\text{net,p}}$ are discussed in Chapter 16 on page 391, Chapter 17 on page 449, and Chapter 24 on page 715. The boundary conditions for Eq. 53 are discussed in Chapter 10 on page 201.

Depending on the device under investigation and the level of modeling accuracy required, you can select different transport models:

- Drift-diffusion

  Isothermal simulation, suitable for low-power density devices with long active regions.

- Thermodynamic

  Accounts for self-heating. Suitable for devices with low thermal exchange, particularly, high-power density devices with long active regions.

- Hydrodynamic

  Accounts for energy transport of the carriers. Suitable for devices with small active regions.

- Monte Carlo

  Solves the Boltzmann equation for a full band structure.

The numeric approach for the Monte Carlo method (and the physical models usable with it) differs significantly from the other transport models. Therefore, the Monte Carlo method is described in a separate manual (see Sentaurus™ Device Monte Carlo User Guide).

For all other transport models, the solution of Eq. 53 is requested by the keywords `Electron` and `Hole` in the `Solve` section. When the equation for a density is not solved in a `Solve` statement, the quasi-Fermi potential for the respective carrier type remains fixed, unless the keyword `RecomputeQFP` is present in the `Math` section and the equation for the other density is solved.

The solutions of the densities n and p are stored in the datasets `eDensity` and `hDensity`, respectively. The current densities $\vec{J}_n$ and $\vec{J}_p$ are stored in the vector datasets `eCurrentDensity` and `hCurrentDensity`, their sum is stored in `ConductionCurrentDensity`, and the total current density (including displacement current) is stored in `TotalCurrentDensity`. An alternative representation of the total current density is described in Current Potential on page 185.

> **NOTE** Maxwell–Boltzmann statistics is the default for transport models in Sentaurus Device, and you can choose to use Fermi–Dirac statistics as described in Fermi Statistics on page 176.

Drift-Diffusion Model

The drift-diffusion model is the default carrier transport model in Sentaurus Device. For the drift-diffusion model, the current densities for electrons and holes are given by:

$$\vec{J}_n = \mu_n(n\nabla E_\mathrm{C} - 1.5nkT\nabla\ln m_n) + D_n(\nabla n - n\nabla\ln\gamma_n) \tag{54}$$

$$\vec{J}_p = \mu_p(p\nabla E_\mathrm{V} + 1.5pkT\nabla\ln m_p) - D_p(\nabla p - p\nabla\ln\gamma_p) \tag{55}$$

The first term takes into account the contribution due to the spatial variations of the electrostatic potential, the electron affinity, and the band gap. The remaining terms take into account the contribution due to the gradient of concentration, and the spatial variation of the effective masses m_n and m_p. For Fermi statistics, γ_n and γ_p are given by Eq. 47 and Eq. 48, p. 177. For Boltzmann statistics, $\gamma_n = \gamma_p = 1$.

By default, the diffusivities D_n and D_p are given through the mobilities by the Einstein relation, $D_n = kT\mu_n$ and $D_p = kT\mu_p$. However, it is possible to compute them independently (see Non-Einstein Diffusivity on page 376).

When the Einstein relation holds, the current equations can be simplified to:

$$\vec{J}_n = -nq\mu_n\nabla\Phi_n \tag{56}$$

$$\vec{J}_p = -pq\mu_p\nabla\Phi_p \tag{57}$$

where Φ_n and Φ_p are the electron and hole quasi-Fermi potentials, respectively (see Quasi-Fermi Potential With Boltzmann Statistics on page 175).

It is possible to use the drift-diffusion model together with a lattice temperature equation, but it is not mandatory. It is not possible to use the drift-diffusion model for a particular carrier type and to solve the carrier temperature for the same carrier type; the hydrodynamic model is required for that (see Hydrodynamic Model for Current Densities on page 184).

Thermodynamic Model for Current Densities

In the thermodynamic model [1], the relations Eq. 56 and Eq. 57 are generalized to include the temperature gradient as a driving term:

$$\vec{J}_n = -nq\mu_n(\nabla\Phi_n + P_n\nabla T) \tag{58}$$

$$\vec{J}_p = -pq\mu_p(\nabla\Phi_p + P_p\nabla T) \tag{59}$$

where P_n and P_p are the absolute thermoelectric powers [2] (see Thermoelectric Power (TEP) on page 913), and T is the lattice temperature.

The model differs from drift-diffusion when the lattice temperature equation is solved (see Thermodynamic Model for Lattice Temperature on page 193). However, it is possible to solve the lattice temperature equation even when using the drift-diffusion model.

To activate the thermodynamic model, specify the `Thermodynamic` keyword in the global `Physics` section.

Hydrodynamic Model for Current Densities

In the hydrodynamic model, current densities are defined as:

$$\vec{J}_n = \mu_n \left(n\nabla E_C + kT_n\nabla n - nkT_n\nabla\ln\gamma_n + \lambda_n f_n^{\mathrm{td}} kn\nabla T_n - 1.5nkT_n\nabla\ln m_n \right) \tag{60}$$

$$\vec{J}_p = \mu_p (p\nabla E_V - kT_p\nabla p + pkT_p\nabla\ln\gamma_p - \lambda_p f_p^{\mathrm{td}} kp\nabla T_p + 1.5pkT_p\nabla\ln m_p) \tag{61}$$

The first term takes into account the contribution due to the spatial variations of electrostatic potential, electron affinity, and the band gap. The remaining terms in Eq. 60 and Eq. 61 take into account the contribution due to the gradient of concentration, the carrier temperature gradients, and the spatial variation of the effective masses m_n and m_p. For Fermi statistics, γ_n and γ_p are given by Eq. 47 and Eq. 48, p. 177, and $\lambda_n = F_{1/2}(\eta_n)/F_{-1/2}(\eta_n)$ and $\lambda_p = F_{1/2}(\eta_p)/F_{-1/2}(\eta_p)$ (with η_n and η_p from Eq. 49 and Eq. 50, p. 177); for Boltzmann statistics, $\gamma_n = \gamma_p = \lambda_n = \lambda_p = 1$.

The thermal diffusion constants f_n^{td} and f_p^{td} are available in the `ThermalDiffusion` parameter set. They default to zero, which corresponds to the Stratton model [3][4].

Eq. 60 and Eq. 61 assume that the Einstein relation $D = \mu kT$ holds (D is the diffusion constant), which is true only near the equilibrium. Therefore, Sentaurus Device provides the option to replace the carrier temperatures in Eq. 60 and Eq. 61 by $gT_c + (1-g)T$, an average of the carrier temperature (T_n or T_p) and the lattice temperature. This can be useful in devices where the carrier diffusion is important. The coefficient g for electrons and holes can be specified in the `ThermalDiffusion` parameter set. It defaults to one.

To activate the hydrodynamic model, the keyword `Hydrodynamic` must be specified in the global `Physics` section. If only one carrier temperature equation is to be solved, `Hydrodynamic` must be specified with an option, either `Hydrodynamic(eTemperature)` or `Hydrodynamic(hTemperature)`.

Numeric Parameters for Continuity Equation

Carrier concentrations must never be negative. If during a Newton iteration a concentration erroneously becomes negative, Sentaurus Device applies damping procedures to make it positive. The concentration that finally results from a Newton iteration is limited to a value that can be specified (in cm^{-3}) by `DensLowLimit=<float>` in the global `Math` section; the default is $10^{-100}\,\mathrm{cm}^{-3}$.

Numeric Approaches for Contact Current Computation

By default, Sentaurus Device computes the contact current as the sum of the integral of the current density over the surface of the doping well associated with the contact and the integral of the charge generation rate over the volume of the doping well. The following alternative, mutually exclusive approaches can be selected in the global `Math` section:

■ `CurrentWeighting` activates a domain-integration method that uses a solution-dependent weighting function to minimize numeric errors (see [5] for details).

■ `DirectCurrent` activates computation of the current as the surface integral of the current density over the contact area.

> **NOTE** The current that flows into nodes in mixed-mode simulations is always computed with the `DirectCurrent` approach, regardless of the specification in the `Math` section.

Current Potential

The total current density:

$$\vec{J} = \vec{J}_n + \vec{J}_p + \vec{J}_{\mathrm{D}} \tag{62}$$

satisfies the conservation law:

$$\nabla \cdot \vec{J} = 0 \tag{63}$$

Consequently, $\vec{J}$ can be written as the curl of a vector potential $\vec{W}$:

$$\vec{J} = \nabla \times \vec{W} \tag{64}$$

In a 2D simulation, $\vec{W}$ only has a nonzero component along the z-axis, which is written simply as $W_z = W$. The total current density is then given by:

$$\vec{J} = \begin{bmatrix} \dfrac{\partial W}{\partial y} \\ -\dfrac{\partial W}{\partial x} \end{bmatrix} \tag{65}$$

The function W has the following important properties:

- The contour lines of W are the current lines of $\vec{J}$.

- The difference between the values of W at any two points equals the total current flowing across any line linking these points.

Sentaurus Device computes the 2D current potential according to the approach proposed by Palm and Van de Wiele [6].

To visualize the results, add the keyword `CurrentPotential` to the `Plot` section:

```
Plot {
   CurrentPotential
}
```

Figure 17 displays plots of the total current density and current potential for a simple square device.
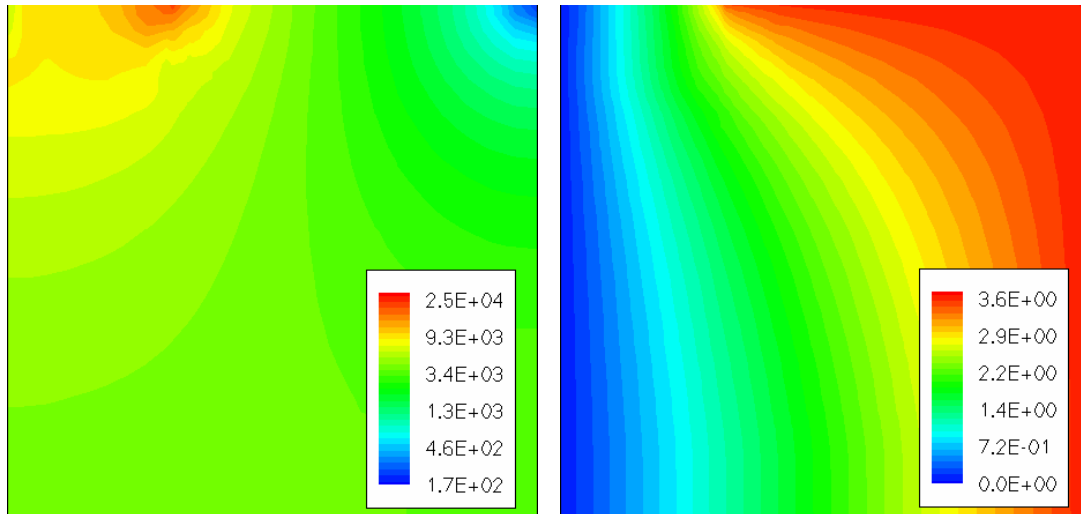
Figure 17   (*Left*) Total current density [Acm^{-1}] and (*right*) current potential [Acm^{-1}]

References

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CHAPTER 9　Temperature Equations

This chapter describes the equations for lattice and carrier temperatures.

Introduction to Temperature Equations

Sentaurus Device can compute up to three different temperatures: lattice temperature, electron temperature, and hole temperature. Lattice temperature describes self-heating of devices. The electron and hole temperatures are required to model nonequilibrium effects in deep-submicron devices (in particular, velocity overshoot and impact ionization).

The following options are available:

- The lattice temperature can be computed from the total dissipated heat, assuming the temperature is constant throughout the device.

- The lattice temperature can be computed nonuniformly using the default model, or the thermodynamic model, or the hydrodynamic model.

- One or both carrier temperatures can be computed using the hydrodynamic model.

Irrespective of the model used, the lattice temperature is stored in the dataset `Temperature`, and the electron and hole temperatures are stored as `eTemperature` and `hTemperature`, respectively.

To solve the lattice temperature, it is necessary to specify a thermal boundary condition (see Thermal Boundary Conditions on page 226). To solve the carrier temperatures, no thermal boundary conditions are required.

By default (and as an initial guess), the lattice temperature is set to $300\,\mathrm{K}$ throughout the device, or to the value of `Temperature` set in the `Physics` section. If the device has one or more defined thermodes, an average temperature is calculated from the temperatures at the thermodes and is set throughout the device. As an initial guess, electron and hole temperatures are set to the lattice temperature. Carrier temperatures that are not solved are assumed to equal the lattice temperature throughout the simulation.

Uniform Self-Heating

A simple self-heating model is available to account for self-heating effects without solving the lattice heat flow equation. The self-heating effect can be captured with a uniform temperature, which is bias dependent or current dependent. The global temperature is computed from a global heat balance equation where the dissipated power P_{diss} is equal to the sum of the boundary heat fluxes (on thermodes with finite thermal resistance):

$$P_{\mathrm{diss}} = \sum_i \frac{T - T_{\mathrm{thermode}}^{(i)}}{R_{\mathrm{th}}^{(i)}} + \sum_k \frac{T - T_{\mathrm{circ}}^{(k)}}{R_{\mathrm{th}}^{(k)}} \tag{66}$$

where:

- T is the device global temperature.
- $T_{\mathrm{thermode}}^{(i)}$ and $R_{\mathrm{th}}^{(i)}$ are the temperature and thermal resistivity of thermode i not connected in a thermal circuit.
- $T_{\mathrm{circ}}^{(k)}$ and $R_{\mathrm{th}}^{(k)}$ are the temperature and thermal resistivity of thermode k connected in a thermal circuit.

The second sum in Eq. 66 becomes zero when the device is not connected to any thermal circuit.

For a thermode k connected in a thermal circuit, an additional thermal circuit equation is solved for the temperature at the respective thermode $T_{\mathrm{circ}}^{(k)}$. The thermal circuit equation solved is derived from the condition that the heat flux through the connected thermode is equal to the flux flowing through the thermal circuit element to which the thermode is connected.

In the case of thermode k connected to a thermal resistor, the thermal circuit equation becomes:

$$(T - T_{\mathrm{circ}}^{(k)})/R_{\mathrm{th}}^{(k)} = \nabla T^{\mathrm{resistor}}/R_{\mathrm{th}} \tag{67}$$

where:

- The left-hand side represents the thermal flux at thermode k.
- The right-hand side represents the heat flux flowing through the thermal resistor with thermal resistivity R_{th}.
- $\nabla T^{\mathrm{resistor}} = T_{\mathrm{resistor}} - T_{\mathrm{circ}}^{(k)}$ is the temperature drop across the thermal resistor.

For a thermal capacitor, the thermal equation becomes $(T - T_{\mathrm{circ}}^{(k)})/R_{\mathrm{th}}^{(k)} = C_{\mathrm{th}} \frac{d}{dt} \nabla T^{\mathrm{capacitor}}$ where $\nabla T^{\mathrm{capacitor}} = T_{\mathrm{capacitor}} - T_{\mathrm{circ}}^{(k)}$ is the voltage drop across the thermal capacitor in a transient simulation.

If a thermode does not specify a thermal resistance or a thermal conductance, then by default, a zero surface conductance is assumed. In this case, the thermode is not accounted for in the sum on the right-hand side of Eq. 66 because the respective heat flux is zero. When none of the thermodes specifies any thermal resistance or conductance, Eq. 66 cannot be solved.

The dissipated power P_{diss} can be calculated as either the sum of all terminal currents multiplied by their respective terminal voltages ($\sum IV$), the sum of IVs from the user-specified node, or the total Joule heat $\int_V (\vec{J} \cdot \vec{F}) dv$.

The global temperature T_i for the point t_i (in transient or quasistationary simulations) is computed based on the estimation of T_i at the previous point t_{i-1} and the solution temperature T_{i-1} at the same point t_{i-1}.

> **NOTE** For uniform self-heating, the temperature is obtained by postprocessing, rather than computed self-consistently with all other solution variables. Therefore, the simulation results may depend on the simulation time step used in quasistationary or transient simulations. In addition, uniform self-heating must not be used for AC, noise, or harmonic balance (HB) simulations.

Using Uniform Self-Heating

The uniform self-heating equation is activated in the global `Physics` section using the `PostTemperature` keyword:

```
Physics {
   PostTemperature
   ...
}
```

The heat fluxes at thermodes are defined in the `Thermode` sections by specifying `Temperature` and `SurfaceResistance` or `SurfaceConductance`:

```
Thermode {
   {Name= "top" Temperature=300 SurfaceConductance=0.1}
   ...
   {Name= "bottom" Temperature=300 SurfaceResistance=0.01}
}
```

The way P_{diss} is computed can be chosen by options to `PostTemperature` in the command file:

- As $\sum IV$ over all electrodes:

```
Physics {
   PostTemperature(IV_diss)
   ...
}
```

- As $\sum IV$ at user-selected electrodes:

```
Physics {
   PostTemperature(IV_diss("contact1" "contact2"))
   ...
}
```

- As the integral of Joule heat over the device volume:

```
Physics {
   PostTemperature
   ...
}
```

Uniform self-heating can be used during a quasistationary or transient simulation. As the feature replaces the lattice heat flow equation (Eq. 68, Eq. 69, and Eq. 75, p. 196), it cannot be used with the lattice temperature equation activated in the `Coupled` section.

Default Model for Lattice Temperature

Sentaurus Device can compute a spatially dependent lattice temperature even when neither the thermodynamic nor the hydrodynamic model is activated. The equation for the temperature is:

$$\frac{\partial W_{\text{L}}}{\partial t} + \nabla \cdot \vec{S}_{\text{L}} = \left.\frac{dW_{\text{L}}}{dt}\right|_{\text{coll}} + \frac{1}{q}\vec{J}_n \cdot \nabla E_{\text{C}} + \left.\frac{dW_n}{dt}\right|_{\text{coll}} + \frac{1}{q}\vec{J}_p \cdot \nabla E_{\text{V}} + \left.\frac{dW_p}{dt}\right|_{\text{coll}} \qquad (68)$$

(See Hydrodynamic Model for Current Densities on page 184 for an explanation of the symbols.) That is, the model is similar to the hydrodynamic model, but all temperatures merge into the lattice temperature, and all heating terms are accounted for in the lattice temperature equation.

To use this model, specify the keyword `Temperature` in the `Solve` section. You do not have to specify a model in the `Physics` section.

To account for Peltier heat at a contact, or a metal–semiconductor interface, or a conductive insulator–semiconductor interface, switch on the Peltier heating model explicitly. See Heating at Contacts, Metal–Semiconductor and Conductive Insulator–Semiconductor Interfaces on page 916 for more details.

Thermodynamic Model for Lattice Temperature

With the thermodynamic model, the lattice temperature T is computed from:

$$
\begin{aligned}
\frac{\partial}{\partial t}(c_L T) - \nabla \cdot (\kappa \nabla T) &= -\nabla \cdot [(P_n T + \Phi_n)\vec{J_n} + (P_p T + \Phi_p)\vec{J_p}] \\
&\quad -\frac{1}{q}\left(E_C + \frac{3}{2}kT\right)(\nabla \cdot \vec{J_n} - qR_{\text{net},n}) \\
&\quad -\frac{1}{q}\left(-E_V + \frac{3}{2}kT\right)(-\nabla \cdot \vec{J_p} - qR_{\text{net},p}) + \hbar\omega G^{\text{opt}}
\end{aligned}
\tag{69}
$$

where:

- κ is the thermal conductivity (see Thermal Conductivity on page 901).
- c_L is the lattice heat capacity (see Heat Capacity on page 899).
- E_C and E_V are the conduction and valence band energies, respectively.
- G^{opt} is the optical generation rate from photons with frequency ω (see Chapter 21 on page 533).
- $R_{\text{net},n}$ and $R_{\text{net},p}$ are the electron and hole net recombination rates, respectively.
- The current densities J_n and J_p are computed as described in Thermodynamic Model for Current Densities on page 183.

In metals, Eq. 69 degenerates into:

$$
\frac{\partial}{\partial t}(c_L T) - \nabla \cdot (\kappa \nabla T) = -\nabla \cdot [(PT + \Phi_M)\vec{J_M}]
\tag{70}
$$

where:

- P is the metal thermoelectric power.
- Φ_M is the Fermi potential in the metal.
- $\vec{J_M}$ is the metal current density as defined in Eq. 148, p. 239.

Total Heat and Its Contributions

The RHS of Eq. 69 is the total heat H. In the stationary case, the second term and the third term disappear, that is, the total heat is then given by:

$$H = -\nabla \cdot [(P_n T + \Phi_n)\vec{J_n} + (P_p T + \Phi_p)\vec{J_p}] + \hbar\omega G^{\text{opt}} \tag{71}$$

The electron part can be rewritten as:

$$-\nabla \cdot [(P_n T + \Phi_n)\vec{J_n}] = \frac{1}{qn\mu_n}\left|\vec{J_n}\right|^2 - qT\nabla P_n \cdot \vec{J_n} + [(P_n T + \Phi_n)\vec{J_n} \cdot n_S]_S \delta_S - q(P_n T + \Phi_n)R_{\text{net},n} \tag{72}$$

where:

- n_S is the surface normal at region interface S.

- δ_S denotes the surface delta function at region interface S.

- $[\alpha]_S$ denotes the jump of a function α across the region interface S.

The resulting four terms are often denoted as the electron part of the Joule heat, Thomson heat, Peltier heat, and recombination heat, respectively.

Using the Thermodynamic Model

To use the thermodynamic model, the keyword `Temperature` must be specified inside the `Coupled` command of the `Solve` section. Use the keyword `Thermodynamic` in the `Physics` section to activate extra terms in the current density equations (due to the gradient of the temperature).

To account for Peltier heat at a contact, or a metal–semiconductor interface, or a conductive insulator–semiconductor interface, switch on the Peltier heating model explicitly. See Heating at Contacts, Metal–Semiconductor and Conductive Insulator–Semiconductor Interfaces on page 916 for more details.

Sentaurus Device allows the total heat generation rate to be plotted and the separate components of the total heat to be estimated and plotted. The total heat generation rate is the term on the right-hand side of Eq. 69. It is plotted using the `TotalHeat` keyword in the `Plot` section. The total heat is calculated only when Sentaurus Device solves the temperature equation. Table 28 on page 195 shows the formulas to estimate individual heating mechanisms and the appropriate keywords for use in the `Plot` section of the command file (see Device Plots on page 122). The individual heat terms that are used for plotting and that are written to the `.log` file are less accurate than those Sentaurus Device uses to solve the transport equations. They serve as illustrations only.

Table 28   Terms and keywords used in Plot section of command file

Heat name	Keyword	Formula
Electron Joule heat	`eJouleHeat`	$\dfrac{\left|\vec{J}_n\right|^2}{qn\mu_n}$
Hole Joule heat	`hJouleHeat`	$\dfrac{\left|\vec{J}_p\right|^2}{qp\mu_p}$
Joule heat in conductive insulators	`JouleHeat`	$\dfrac{\left|\vec{J}_{CI}\right|^2}{\sigma}$
Recombination heat	`RecombinationHeat`	$qR_{\text{total}}((\Phi_p + TP_p) - (\Phi_n + TP_n))$
Net recombination heat	`netRecombinationHeat`	$qR_{\text{net},p}(\Phi_p + TP_p) - qR_{\text{net},n}(\Phi_n + TP_n)$
Thomson plus Peltier heat [1]	`ThomsonHeat`	$-\vec{J}_n \cdot T\nabla P_n - \vec{J}_p \cdot T\nabla P_p$
Peltier heat	`PeltierHeat`	$-T\left(\dfrac{\partial P_n}{\partial n}\vec{J}_n \cdot \nabla n + \dfrac{\partial P_p}{\partial p}\vec{J}_p \cdot \nabla p\right)$

Here $R_{\text{total}} = 0.5(R_{\text{net,p}} + R_{\text{net,n}})$. To plot the lattice heat flux vector $\kappa\nabla T$, specify the keyword `lHeatFlux` in the `Plot` section (see Device Plots on page 122).

Hydrodynamic Model for Temperatures

Deep-submicron devices cannot be described properly using the conventional drift-diffusion transport model. In particular, the drift-diffusion approach cannot reproduce velocity overshoot and often overestimates the impact ionization generation rates. In this case, the hydrodynamic (or energy balance) model provides a good compromise between physical accuracy and computation time.

Since the work of Stratton [2] and Bløtekjær [3], there have been many variations of this model. The full formulation includes the so-called convective terms [4]. Sentaurus Device implements a simpler formulation without convective terms. In addition to the Poisson equation (Eq. 37, p. 173) and continuity equations (Eq. 53, p. 181), up to three additional equations for the lattice temperature T and the carrier temperatures T_n and T_p can be solved. The energy balance equations read:

$$\frac{\partial W_n}{\partial t} + \nabla \cdot \vec{S}_n = \vec{J}_n \cdot \nabla E_C / q + \left.\frac{dW_n}{dt}\right|_{\text{coll}} \tag{73}$$

$$\frac{\partial W_p}{\partial t} + \nabla \cdot \vec{S}_p = \vec{J}_p \cdot \nabla E_{\mathrm{V}}/q + \frac{dW_p}{dt}\bigg|_{\mathrm{coll}} \tag{74}$$

$$\frac{\partial W_{\mathrm{L}}}{\partial t} + \nabla \cdot \vec{S}_{\mathrm{L}} = \frac{dW_{\mathrm{L}}}{dt}\bigg|_{\mathrm{coll}} \tag{75}$$

where the energy fluxes are:

$$\vec{S}_n = -\frac{5 r_n \lambda_n}{2}\left(\frac{kT_n}{q}\vec{J}_n + f_n^{\mathrm{hf}}\hat{\kappa}_n \nabla T_n\right) \tag{76}$$

$$\vec{S}_p = -\frac{5 r_p \lambda_p}{2}\left(\frac{-kT_p}{q}\vec{J}_p + f_p^{\mathrm{hf}}\hat{\kappa}_p \nabla T_p\right) \tag{77}$$

$$\vec{S}_{\mathrm{L}} = -\kappa_{\mathrm{L:}}\nabla T_{\mathrm{L}} \tag{78}$$

$$\hat{\kappa}_n = \frac{k^2}{q}n\mu_n T_n \tag{79}$$

$$\hat{\kappa}_p = \frac{k^2}{q}p\mu_p T_p \tag{80}$$

and λ_n and λ_p are defined as for Eq. 60 and Eq. 61, p. 184. The parameters r_n, r_p, f_n^{hf}, and f_p^{hf} are accessible in the parameter file of Sentaurus Device. Different values of these parameters can significantly influence the physical results, such as velocity distribution and possible spurious velocity peaks. By changing these parameters, Sentaurus Device can be tuned to a very wide set of hydrodynamic/energy balance models as described in the literature. The default parameter values of Sentaurus Device are:

$$r_n = r_p = 0.6 \tag{81}$$

$$f_n^{\mathrm{hf}} = f_p^{\mathrm{hf}} = 1 \tag{82}$$

By changing the constants f_n^{hf} and r_{n}, the convective contribution and the diffusive contributions can be changed independently. With the default set of transport parameters of Sentaurus Device, the prefactor of the diffusive term has the form:

$$\kappa_n = \frac{3}{2}\cdot\frac{k^2\lambda_n}{q}n\mu_n T_n \tag{83}$$

The collision terms are expressed by this set of equations:

$$\frac{\partial W_n}{\partial t}\bigg|_{\text{coll}} = -H_n - \xi_n \frac{W_n - W_{n0}}{\tau_{en}} \tag{84}$$

$$\frac{\partial W_p}{\partial t}\bigg|_{\text{coll}} = -H_p - \xi_p \frac{W_p - W_{p0}}{\tau_{ep}} \tag{85}$$

$$\frac{\partial W_L}{\partial t}\bigg|_{\text{coll}} = H_L + \xi_n \frac{W_n - W_{n0}}{\tau_{en}} + \xi_p \frac{W_p - W_{p0}}{\tau_{ep}} \tag{86}$$

Here, H_n, H_p, and H_L are the energy gain/loss terms due to generation–recombination processes. The expressions used for these terms are based on approximations [5] and have the following form for the major generation–recombination phenomena:

$$H_n = 1.5kT_n(R_{\text{net}}^{\text{SRH}} + R_{\text{net}}^{\text{rad}} + R_{n,\,\text{net}}^{\text{trap}}) - E_{\text{g,eff}}(R_n^{\text{A}} - G_n^{\text{ii}}) - \alpha(\hbar\omega - E_{\text{g,eff}})G^{\text{opt}} \tag{87}$$

$$H_p = 1.5kT_p(R_{\text{net}}^{\text{SRH}} + R_{\text{net}}^{\text{rad}} + R_{p,\,\text{net}}^{\text{trap}}) - E_{\text{g,eff}}(R_p^{\text{A}} - G_p^{\text{ii}}) - (1-\alpha)(\hbar\omega - E_{\text{g,eff}})G^{\text{opt}} \tag{88}$$

$$H_L = [R_{\text{net}}^{\text{SRH}} + 0.5(R_{n,\,\text{net}}^{\text{trap}} + R_{p,\,\text{net}}^{\text{trap}})](E_{\text{g,eff}} + 1.5kT_n + 1.5kT_p) \tag{89}$$

where:

- $R_{\text{net}}^{\text{SRH}}$ is the Shockley–Read–Hall (SRH) recombination rate (see Shockley–Read–Hall Recombination on page 391).

- $R_{\text{net}}^{\text{rad}}$ is the radiative recombination rate (see Radiative Recombination on page 407).

- R_n^{A} and R_p^{A} are Auger recombination rates related to electrons and holes (see Auger Recombination on page 408).

- $\hbar\omega$ is the photon energy (see Hydrodynamic Model Parameters on page 198).

- α is a dimensionless parameter that describes how the surplus energy of the photon splits between the bands (see Hydrodynamic Model Parameters on page 198).

- G_n^{ii} and G_p^{ii} are impact ionization rates (see Avalanche Generation on page 413).

- $R_{n,\,\text{net}}^{\text{trap}}$ and $R_{p,\,\text{net}}^{\text{trap}}$ are the recombination rates through trap levels (see Chapter 17 on page 449).

- G^{opt} is the optical generation rate (see Chapter 21 on page 533).

Surface recombination is taken into account in a way similar to bulk SRH recombination. Usually, the influence of H_n, H_p, and H_L is small, so they are not activated by default. To take these energy sources into account, the keyword `RecGenHeat` must be specified in the `Physics` section.

The energy densities W_n, W_p, and W_L are given by:

$$W_n = nw_n = n\left(\frac{3kT_n}{2}\right) \tag{90}$$

$$W_p = pw_p = p\left(\frac{3kT_p}{2}\right) \tag{91}$$

$$W_L = c_L T \tag{92}$$

The corresponding equilibrium energy densities are:

$$W_{n0} = nw_0 = n\frac{3kT}{2} \tag{93}$$

$$W_{p0} = pw_0 = p\frac{3kT}{2} \tag{94}$$

The parameters ξ_n and ξ_p in Eq. 84 to Eq. 86 improve numeric stability.

They speed up relaxation for small densities and they approach 1 for large densities:

$$\xi_n = 1 + \frac{n_{min}}{n}\left(\frac{n_0}{n_{min}}\right)^{\max[0, (T - T_n)/100\,\text{K}]} \tag{95}$$

and likewise for ξ_p. Here, n_{min} and n_0 are adjustable small density parameters.

Hydrodynamic Model Parameters

The default set of transport coefficients (Eq. 81 and Eq. 82, p. 196) can be changed in the parameter file. The coefficients r and f^{hf} are specified in the `EnergyFlux` and `HeatFlux` parameter sets, respectively. Energy relaxation times τ_{en} and τ_{ep} can be modified in the `EnergyRelaxationTime` parameter set.

α in Eq. 87 and Eq. 88 divides the contribution of the optical generation rate into the energy gain or loss terms H_n and H_p. `OptGenOffset` specifies α, which can take values between 0 and 1 (default is 0.5). The angular frequency ω in Eq. 87 and Eq. 88 corresponds to the wavelength specified to compute the optical generation rate. This wavelength is defined by `OptGenWavelength` if the optical generation is loaded from a file (see Optical AC Analysis on page 661). `OptGenOffset` and `OptGenWavelength` are both options to `RecGenHeat` (see Table 233 on page 1427).

The parameters $n_{\min}$ and n_0 in Eq. 95 are set with `RelTermMinDensity` and `RelTermMinZeroDensity`, respectively, in the global `Math` section. The default values for $n_{\min}$ and n_0 are $10^3 \, \text{cm}^{-3}$ and $2 \times 10^8 \, \text{cm}^{-3}$, respectively.

Using the Hydrodynamic Model

To activate the hydrodynamic model, the keyword `Hydrodynamic` must be specified in the `Physics` section. If only one carrier temperature equation is to be solved, `Hydrodynamic` must be specified with the appropriate parameter, either `Hydrodynamic(eTemperature)` or `Hydrodynamic(hTemperature)`. If the hydrodynamic model is not activated for a particular carrier type, Sentaurus Device merges the temperature for this carrier with the lattice temperature. That is, these temperatures are equal, and their heating terms (see the right-hand sides of Eq. 73, Eq. 74, and Eq. 75) are added.

In addition, the keywords `eTemperature`, `hTemperature`, and `Temperature` must be specified inside the `Coupled` command of the `Solve` section (see Coupled Command on page 136) to actually solve a carrier temperature equation or the lattice temperature equation. Temperatures remain fixed during `Solve` statements in which their equation is not solved.

By default, the energy conservation equations of Sentaurus Device do not include generation–recombination heat sources. To activate them, the keyword `RecGenHeat` must be specified in the `Physics` section.

To plot the electron, hole, and lattice heat flux vectors $\vec{S}_n, \vec{S}_p, \vec{S}_L$ (see Eq. 76, Eq. 77, and Eq. 78), specify the corresponding keywords `eHeatFlux`, `hHeatFlux`, and `lHeatFlux` in the `Plot` section (see Device Plots on page 122).

Numeric Parameters for Temperature Equations

Validity Ranges for Lattice and Carrier Temperatures

Lower and upper limits for the lattice temperature and the carrier temperatures exist. The allowed temperature ranges are specified (in K) by `lT_Range=(<float> <float>)` (with defaults $50 \, \text{K}$ and $5000 \, \text{K}$) and `cT_Range=(<float> <float>)` (with defaults $10 \, \text{K}$ and $80000 \, \text{K}$). These ranges apply both to the temperatures during the Newton iterations and to the final results.

Scaling of Lattice Heat Generation

For the lattice heat equation, you have the possibility to disable the heat term by using:

```
Physics ( Region="Bulk" ) { ... HeatPreFactor = 0. }
```

This reduces or even eliminates the strong coupling, given by the Joule heat, of the lattice heat equation with the carrier continuity equations, and leads in general to smooth temperature profiles. This simplified coupled system of carrier transport and lattice temperature might converge easier than the fully coupled system including the heat term. Instead of ramping the fully coupled system to a required bias condition, it might be easier to ramp first the simplified coupled system to the required bias condition, and ramp subsequently the `HeatPreFactor` from zero to one. In the command file, this second ramp could be:

```
Quasistationary (
   Goal { Region="Bulk" ModelParameter="Physics/HeatPreFactor" Value=1 }
) { Coupled { Poisson Electron Hole Temperature } }
```

> **NOTE** The `Goal` statement requires the specification of a `Region`, and a `Physics` section for the corresponding region must be specified in the command file.

References

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Boundary Conditions

This chapter describes the boundary conditions available in Sentaurus Device.

This chapter describe the properties of electrical contacts, thermal contacts, floating contacts, as well as boundary conditions at other borders of a domain where an equation is solved. Continuity conditions (how the solutions of one equation on two neighboring regions are matched at the region interface) are discussed elsewhere (see, for example, Dipole Layer on page 174). This chapter is restricted to the boundary conditions for the equations presented in Chapter 7 on page 173, Chapter 8 on page 181, and Chapter 9 on page 189. Boundary conditions for less important equations are discussed with the equations themselves (see, for example, Chapter 11 on page 235).

Electrical Boundary Conditions

Ohmic Contacts

By default, contacts on semiconductors are Ohmic, with a resistance of $0.001\,\Omega$ when connected to a circuit node, and no resistance otherwise.

Charge neutrality and equilibrium are assumed at Ohmic contacts:

$$n_0 - p_0 = N_D - N_A \tag{96}$$

$$n_0 p_0 = n_{i,eff}^2 \tag{97}$$

For Boltzmann statistics, these conditions can be expressed analytically:

$$\phi = \phi_F + \frac{kT}{q} \operatorname{asinh}\left(\frac{N_D - N_A}{2n_{i,eff}}\right) \tag{98}$$

$$n_0 = \sqrt{\frac{(N_D - N_A)^2}{4} + n_{i,eff}^2} + \frac{N_D - N_A}{2} \;,\;\; p_0 = \sqrt{\frac{(N_D - N_A)^2}{4} + n_{i,eff}^2} - \frac{N_D - N_A}{2} \tag{99}$$

where n_0, p_0 are the electron and hole equilibrium concentrations, and ϕ_F is the Fermi potential at the contact (which equals the applied voltage if it is not a resistive contact; see

Resistive Contacts on page 213). For Fermi statistics, Sentaurus Device computes the equilibrium solution numerically.

By default, $n = n_0, p = p_0$ are applied for concentrations at the Ohmic contacts. If the electron or hole recombination velocity is specified, Sentaurus Device uses the following current boundary conditions:

$$\vec{J}_n \cdot \hat{n} = qv_n(n - n_0) \qquad \vec{J}_p \cdot \hat{n} = -qv_p(p - p_0) \tag{100}$$

where v_n, v_p are the electron and hole recombination velocities. In the command file, the recombination velocities can be specified as:

```
Electrode { ...
   { Name="Emitter" Voltage=0 eRecVelocity = $v_n$ hRecVelocity = $v_p$ }
}
```

NOTE If the values of the electron and hole recombination velocities equal zero ($v_n = 0, v_p = 0$), then $\vec{J}_n \cdot \hat{n} = 0, \vec{J}_p \cdot \hat{n} = 0$. That is, the electrode only defines the electrostatic potential (which is useful for SOI devices).

By specifying `Poisson=Neumann` for an electrode, the boundary condition for the Poisson equation at a contact can be switched to a homogeneous Neumann boundary condition, that is, Eq. 98 is not applied.

Modified Ohmic Contacts

Ohmic contacts, as described in Ohmic Contacts on page 201, can often lead to incorrect results around p-n junctions and heterointerfaces. The main cause is the charge neutrality condition imposed at the contact vertices located within the charged depletion region of the p-n junction or heterointerface. Ideally, the carrier densities at such contacts should be an extension of bulk densities with no sharp jump along the contact.

Sentaurus Device supports an alternative for Ohmic contacts that does not impose the charge neutrality condition. In this approach, the equilibrium nonlinear Poisson equation is solved at the beginning of the simulation with the Ohmic contacts under consideration removed. The equilibrium electrostatic potential ϕ_{eq} obtained in this way is used instead of the built-in potential $\phi_{bi} = kT \, \text{asinh}[(N_D - N_A)/2n_{i,\text{eff}}]/q$ on the vertices of the Ohmic contacts under consideration. The boundary conditions for the continuity equations remain formally the same as in the case of Ohmic contacts but with the built-in potential ϕ_{bi} replaced by ϕ_{eq}.

The modified Ohmic contacts can be set in the `Electrode` section with the keyword `EqOhmic`:

```
Electrode {
   ...
   {Name="drain" Voltage=0 EqOhmic}
}
```

NOTE   Currently, the feature is only supported for isothermal simulations.

Contacts on Insulators

For contacts on insulators (for example, gate contacts), the electrostatic potential is:

$$\phi = \phi_F - \Phi_{MS} \tag{101}$$

where ϕ_F is the Fermi potential at the contact (which equals the applied voltage if it is not a resistive contact, see Resistive Contacts on page 213), and Φ_{MS} is the workfunction difference between the metal and an intrinsic reference semiconductor.

NOTE   If an Ohmic contact touches both an insulator and a semiconductor, the electrostatic potential along the contact can be discontinuous because the boundary conditions (Eq. 98 and Eq. 101) usually contradict. Eq. 98 takes precedence over Eq. 101.

Φ_{MS} can be specified in the `Electrode` section, either directly with `Barrier`, by specifying the metal workfunction with `WorkFunction`, or by specifying the electrode material:

```
Electrode { ...
   { Name="Gate" Voltage=0 Barrier = 0.55 }
}
Electrode { ...
   { Name="Gate" Voltage=0 WorkFunction = 5 }
}
Electrode { ...
   { Name="Gate" Voltage=0 Material="Gold" }
}
```

In the last case, the value for the workfunction is obtained from the parameter file:

```
Material = "Gold" {
   Bandgap { WorkFunction = 5 }
}
```

To emulate a poly gate, a semiconductor material and doping concentration can be specified in the `Electrode` section:

```
Electrode { ...
    { Name="Gate" Voltage=0 Material="Silicon" (N = 5e19) }
}
```

where `N` is used to specify the doping in an n-type semiconductor material. The built-in potential is approximated by $(kT/q)\ln(N/n_i)$. A p-type doping can be selected, similarly, by the letter `P`. If the value of the doping concentration is not specified (only `N` or `P`), the Fermi potential of the electrode is assumed to equal the conduction or valence band edge.

> **NOTE** If the keyword `-MetalConductivity` is used in the `Math` section, the electrostatic potential ϕ in Eq. 101 is computed as $\phi = \phi_F$. In this case, Φ_{MS} specified in the `Electrode` section as previously described is neglected.

Schottky Contacts

The physics of Schottky contacts is considered in detail in [1] and [2]. In this section, a typical model for Schottky contacts [3] is considered. The following boundary conditions hold:

$$\phi = \phi_F - \Phi_B + \frac{kT}{q}\ln\left(\frac{N_C}{n_{i,\text{eff}}}\right) \tag{102}$$

$$\vec{J_n} \cdot \hat{n} = qv_n(n - n_0^B) \qquad \vec{J_p} \cdot \hat{n} = -qv_p(p - p_0^B) \tag{103}$$

$$n_0^B = N_C\exp\left(\frac{-q\Phi_B}{kT}\right) \qquad p_0^B = N_V\exp\left(\frac{-E_{g,\text{eff}} + q\Phi_B}{kT}\right) \tag{104}$$

where:

- ϕ_F is the Fermi potential at the contact that is equal to an applied voltage V_{applied} if it is not a resistive contact (see Resistive Contacts on page 213).
- Φ_B is the barrier height (the difference between the contact workfunction and the electron affinity of the semiconductor in n-type semiconductors, or the difference between the band gap and the barrier as defined for n-type semiconductors in the case of p-type semiconductors).
- v_n and v_p are the thermionic emission velocities.
- n_0^B and p_0^B are the equilibrium densities.

The default values for the thermionic emission velocities v_n and v_p are 2.573×10^6 cm/s and 1.93×10^6 cm/s, respectively.

The recombination velocities can be set in the `Electrode` section, for example:

```
Electrode { ...
   { Name="Gate" Voltage=0 Schottky Barrier = Φ_B eRecVelocity = v_n
      hRecVelocity = v_p }
}
```

> **NOTE**   The `Barrier` specification can produce wrong results if the Schottky contact is connected to several different semiconductors. In such cases, use `WorkFunction` instead of `Barrier`. See Contacts on Insulators on page 203 for more details.

Sentaurus Device also allows thermionic emission velocities v_n and v_p to be defined as functions of lattice temperature:

$$v_n(T) = v_n(300 \text{ K}) \sqrt{\frac{m_n(300 \text{ K})}{m_n(T)}} \sqrt{\frac{T}{300 \text{ K}}} \qquad v_p(T) = v_p(300 \text{ K}) \sqrt{\frac{m_p(300 \text{ K})}{m_p(T)}} \sqrt{\frac{T}{300 \text{ K}}} \qquad (105)$$

where:

- m_n and m_p are the temperature-dependent electron and hole DOS effective masses.
- $v_n(300 \text{ K})$ and $v_p(300 \text{ K})$ are the recombination velocities at 300 K specified in the `Electrode` section by `eRecVelocity` and `hRecVelocity`.

The default values for the thermionic emission velocities $v_n(300 \text{ K})$ and $v_p(300 \text{ K})$ are 2.573×10^6 cm/s and 1.93×10^6 cm/s, respectively.

To activate the temperature-dependent recombination velocity, specify `eRecVel(TempDep)`, or `hRecVel(TempDep)`, or `RecVel(TempDep)` in the electrode-specific `Physics` section:

```
Physics (Electrode = "cathode") { RecVel(TempDep) }
```

Fermi-Level Pinning at Schottky Contacts

At a metal semiconductor contact or interface, there is a charge transfer between the metal and the interface states located inside the semiconductor bandgap. The charge transfer creates an interfacial dipole, which can change the Schottky barrier. This phenomenon, known as Fermi-level pinning, can be modeled by a Schottky pinning parameter S.

The Schottky potential barrier accounting for the correction due to the charge transfer between the metal and the interface states in the semiconductor bandgap (pinning effect) is modeled as:

$$\Phi_B = S\left(\Phi_M - \frac{E_{CNL}}{q}\right) + \left(\frac{E_{CNL}}{q} - \frac{\chi}{q}\right) \tag{106}$$

where:

- Φ_M is the metal workfunction in V.
- E_{CNL} is the charge neutrality level with respect to the vacuum level in eV.
- S is the Schottky pinning parameter. For $S = 1$ (no pinning), there is no charge transfer, and the Schottky barrier becomes the classical Schottky limit. For $S = 0$ (strong pinning), you obtain the Bardeen limit where the metal Fermi level is pinned by the interface states at E_{CNL}.

The models available in Sentaurus Device for the Schottky pinning parameter S are the Sze model and the Mönch model.

The Sze model is defined as [4]:

$$S = \frac{1}{1 + \dfrac{q^2(N_I d)}{\varepsilon\varepsilon_0}} \tag{107}$$

where ε is the semiconductor permittivity, N_I is the density of interface states per unit energy, and d is their extent into the semiconductor. The parameters N_I and d are mole fraction dependent and can be modified in the Schottky section of the parameter file.

The Mönch model, which is the default, is an empirical formula and is defined as [5]:

$$S = \frac{1}{1 + A(\varepsilon_\infty - 1)^B} \tag{108}$$

where ε_∞ is the high-frequency limit of the permittivity (set to 12 for most materials), and A and B are mole fraction–adjustable parameters that you can modify in the Schottky section of the parameter file. You can set ε_∞ in the Epsilon_Inf section of the parameter file:

```
Epsilon_Inf {
    epsilon_inf = 12
}
```

The charge neutrality level E_{CNL} is also a mole fraction–dependent parameter adjustable in the parameter file.

NOTE   In general, ε_∞ is tabulated for standard materials, so S can be reliably determined from Eq. 108 for those materials. Using the S equivalency between Eq. 107 and Eq. 108 values for $N_I d$ can be inferred.

To activate the pinning effect at the Schottky contacts, specify the `Pinning` keyword in the `Electrode` section, with the model defined as an option for the keyword `Model`:

```
Electrode { ...
   { name = "cnt1" voltage = 0 Schottky(Pinning(Model="Sze"))
      Workfunction=4.75 }
}
```

If the keyword `Model` is omitted, the Mönch model is used. The pinning model specification in the `Electrode` section has a higher priority. If the pinning model is specified in both the `Electrode` section and the electrode `Physics` section, the specification in the `Electrode` section is chosen.

The pinning model parameters in Eq. 107 and Eq. 108 are accessible in the `Schottky` subsection in the `Electrode` section of the parameter file.

Table 29   Parameters and their default values for Schottky pinning

Symbol	Parameter name	Default value	Unit
A	`Pinning_A`	0.1	1
B	`Pinning_B`	2	1
N_I	`Pinning_Nint`	10^{10}	$\mathrm{cm}^{-2}\mathrm{eV}^{-1}$
d	`Pinning_d`	2×10^{-7}	cm
E_{CNL}	`Pinning_CNL`	5.01964	eV

For example, to specify a mole fraction–dependent `CNL` on the contact `drain`, which is on the top of a mole fraction–dependent SiGe region `r3` defined as:

```
Physics(Region = "r3") {   # Ge(x)Si(1-x)
* Mole-dependent material: SiGe(x=0) = Silicon
* Mole-dependent material: SiGe(x=1) = Germanium
   MoleFraction(
      xFraction=0.35
   )
}
```

specify in the parameter file something like:

```
Region = "r3" {
   Schottky {
      Xmax(0)=0.0
      Xmax(1)=0.8
      Xmax(2)=1.0

      Electrode = "drain" {
         Pinning_CNL(0) = 3.5
         Pinning_CNL(1) = 3.7
         Pinning_CNL(2) = 3.8
      }
   }
}
```

See Resistive Contacts on page 213 for a detailed description on how to specify mole-fraction parameters on contacts and interfaces.

Barrier Lowering at Schottky Contacts

The barrier-lowering model for Schottky contacts can account for different physical mechanisms. The most important one is the image force [3], but it can also model tunneling and dipole effects.

The barrier lowering seen by the electron being emitted from metal into the conduction band and for the hole being emitted into the valence are given by:

$$
\Delta\Phi_{\mathrm{B,e}}(\vec{F}) = \begin{cases} aa_{1,\mathrm{e}}\left(\dfrac{|\vec{F}\cdot\hat{n}|}{F_0}\right)^{pp_{1,\mathrm{e}}} + aa_{2,\mathrm{e}}\left(\dfrac{|\vec{F}\cdot\hat{n}|}{F_0}\right)^{pp_{2,\mathrm{e}}} & \text{if } \vec{F}\cdot\hat{n} > 0 \\ \\ 0 & \text{if } \vec{F}\cdot\hat{n} \le 0 \end{cases}
\tag{109}
$$

$$
\Delta\Phi_{\mathrm{B,h}}(\vec{F}) = \begin{cases} aa_{1,\mathrm{h}}\left(\dfrac{|\vec{F}\cdot\hat{n}|}{F_0}\right)^{pp_{1,\mathrm{h}}} + aa_{2,\mathrm{h}}\left(\dfrac{|\vec{F}\cdot\hat{n}|}{F_0}\right)^{pp_{2,\mathrm{h}}} & \text{if } \vec{F}\cdot\hat{n} \le 0 \\ \\ 0 & \text{if } \vec{F}\cdot\hat{n} > 0 \end{cases}
\tag{110}
$$

where:

- $\vec{F}\cdot\hat{n}$ is the normal component of the electric field on the local exterior normal pointing from semiconductor region to metal contact, $F_0 = 1\,\mathrm{Vcm}^{-1}$.

- $aa_{1,\mathrm{e}}, aa_{2,\mathrm{e}}, pp_{1,\mathrm{e}}, pp_{2,\mathrm{e}}, aa_{1,\mathrm{h}}, aa_{2,\mathrm{h}}, pp_{1,\mathrm{h}}, pp_{2,\mathrm{h}}$ are the model coefficients that can be specified in the parameter file of Sentaurus Device. Their default values are

$$aa_{1,e} = aa_{1,h} = 2.6 \times 10^{-4} \text{eV}, \quad pp_{1,e} = pp_{1,h} = 0.5, \quad aa_{2,e} = aa_{2,h} = 0 \text{eV}, \quad \text{and}$$
$$pp_{2,e} = pp_{2,h} = 1.$$

The final value of the Schottky barrier is computed as $\Phi_B - \Delta\Phi_{B,e}(\vec{F})$ for the electrons in the conduction band and as $\Phi_B + \Delta\Phi_{B,h}(\vec{F})$ for the holes in the valence band. The barrier lowering also affects the equilibrium concentration of electrons n_0^B and holes p_0^B corresponding to its formula (Eq. 104), through the correction in barrier Φ_B described above.

In addition, Sentaurus Device implements a simplified model for barrier lowering. In this case, the barrier lowering is:

$$\Delta\Phi_B(F) = \begin{cases} a_1\left[\left(\frac{F}{F_0}\right)^{p_1} - \left(\frac{F_{eq}}{F_0}\right)^{p_{1,eq}}\right] + a_2\left[\left(\frac{F}{F_0}\right)^{p_2} - \left(\frac{F_{eq}}{F_0}\right)^{p_{2,eq}}\right] & \text{if } F > \eta F_{eq} \\ 0 & \text{if } F \leq \eta F_{eq} \end{cases} \tag{111}$$

where $F_0 = 1 \text{Vcm}^{-1}$, and $a_1, a_2, p_1, p_{1,eq}, p_2$, and $p_{2,eq}$ are the model coefficients that can be specified in the parameter file of Sentaurus Device. Their default values are $a_1 = 2.6 \times 10^{-4} \text{eV}$, $p_1 = p_{1,eq} = 0.5$, $a_2 = 0 \text{eV}$, and $p_2 = p_{2,eq} = 1$. For fields smaller than ηF_{eq} (where η is one by default), barrier lowering is zero. The final value of the Schottky barrier is computed as $\Phi_B - \Delta\Phi_B(F)$ for n-doped contacts and $\Phi_B + \Delta\Phi_B(F)$ for p-doped contacts, because a difference between the metal workfunction and the valence band must be considered if holes are majority carriers. This model does not account for the direction of the electric field that determines in which band the barrier forms. For example, assume a Schottky contact on an n-type semiconductor with Schottky barrier 0.8V. The flat band condition is at a forward bias of approximately 0.8V. For a reverse bias and forward bias less than 0.8V, the barrier is in the conduction band, so the barrier lowering is applied correctly for electrons. On the other hand, for a forward bias greater than 0.8V, the barrier is now in the valence band, so the barrier lowering should be applied to holes, not to electrons as the model does. In this case, this simplified model fails. This model is tuned to work properly for reverse biases, where the barrier lowering produces a sizable change in I–V characteristics of the Schottky device.

You can use the `weight` parameter to combine one of the barrier models with the barrier lowering with interfacial insulator layer model described by Eq. 112. If the barrier-lowering model is the only model specified (no interfacial insulator layer model), the value of `weight` is 1 regardless of the value specified in the parameter file by `c_weight`.

Table 30   Parameters and their default values for the barrier-lowering models

Symbol	Parameter name	Default value	Unit
$aa_{1,e}$	aa1	$a_1 = 2.6 \times 10^{-4}$	eV
$aa_{1,h}$	aa1	$a_1 = 2.6 \times 10^{-4}$	eV
$aa_{2,e}$	aa2	0	eV

Table 30   Parameters and their default values for the barrier-lowering models (Continued)

Symbol	Parameter name	Default value	Unit
$aa_{2,h}$	aa2	0	eV
$pp_{1,e}$	pp1	0.5	1
$pp_{1,h}$	pp1	0.5	1
$pp_{2,e}$	pp2	1	1
$pp_{2,h}$	pp2	1	1
a_1	a1	$a_1 = 2.6 \times 10^{-4}$	eV
a_2	a2	0	eV
p_1	p1	0.5	1
p_2	p2	1	1
$p_{1,eq}$	p1_eq	0.5	1
$p_{2,eq}$	p2_eq	1	1
η	eta	1	1
weight	c_weight	1	1

To activate the barrier-lowering model, specify `BarrierLowering` in the electrode-specific `Physics` section for the simplified model:

```
Physics(Electrode = "Gate") { BarrierLowering }
```

and for the complete model, specify:

```
Physics(Electrode = "Gate") { BarrierLowering(Full) }
```

To specify parameters of the model, create the following parameter set:

```
Electrode = "Gate"{
   BarrierLowering {
      a1 = a₁              * [eV]
      p1 = p₁              * [1]
      p1_eq = p₁,eq        * [1]
      a2 = a₂              * [eV]
      p2 = p₂              * [1]
      p2_eq = p₂,eq
      eta = η              * [1]
      aa1 = aa₁,e , aa₁,h   * [eV]
      pp1 = pp₁,e , pp₁,h   * [1]
```

```
        aa2 = aa₂,ₑ , aa₂,ₕ      * [eV]
        pp2 = pp₂,ₑ , pp₂,ₕ      * [1]
    }
  }
```

To emulate the barrier-lowering effect at a metal-semiconductor contact, with a thin virtual interfacial layer between the metal and the semiconductor, Sentaurus Device supports another barrier-lowering model that takes into account such an insulating interface layer. The model [6] assumes that a finite insulator layer is present between the metal and the semiconductor, and it includes both images with respect to the metal–insulator and insulator–semiconductor interfaces.

Sentaurus Device implements the barrier lowering with interfacial insulating layer model described in detail in [6] as:

$$
\Delta\Phi_B(d_0) = \begin{cases}
\dfrac{q}{16\pi\varepsilon_{ins}}\left(\dfrac{1}{d_\varepsilon} + \dfrac{\beta}{t_{ox} - d_\varepsilon}\right) & 0 \le d_0 \le d_\varepsilon \\[3mm]
\dfrac{q}{16\pi\varepsilon_{ins}}\left(\dfrac{1}{d_0} + \dfrac{\beta}{t_{ox} - d_0}\right) & d_\varepsilon < d_0 \le t_{ox} - d_\varepsilon \\[3mm]
\dfrac{q}{16\pi\varepsilon_{ins}}\left(\dfrac{1}{t_{ox} - d_\varepsilon} + \dfrac{\beta}{d_\varepsilon}\right) - A\dfrac{t_{ox} - d_\varepsilon}{2d_\varepsilon} + \dfrac{A}{2d_\varepsilon}d_0 & t_{ox} - d_\varepsilon < d_0 \le t_{ox} + d_\varepsilon \\[3mm]
\dfrac{q}{16\pi\varepsilon_{sem}}\left(\dfrac{1}{d_0} + \dfrac{\beta}{t_{ox} - d_0}\right) & d_0 > t_{ox} + d_\varepsilon
\end{cases}
\tag{112}
$$

where:

- $\beta = \dfrac{\varepsilon_{sem} - \varepsilon_{ins}}{\varepsilon_{sem} + \varepsilon_{ins}}$.

- $A = \dfrac{q}{16\pi\varepsilon_{sem}}\left(\dfrac{1}{t_{ox} + d_\varepsilon} - \dfrac{\beta}{d_\varepsilon}\right) - \dfrac{q}{16\pi\varepsilon_{ins}}\left(\dfrac{1}{t_{ox} - d_\varepsilon} + \dfrac{\beta}{d_\varepsilon}\right)$.

- ε_{sem} is the semiconductor layer permittivity.

- ε_{ins} is the insulator layer permittivity.

- t_{ox} is the conforming insulator layer thickness.

- d_o is the distance from the metal surface (contact) to the point where the barrier lowering is evaluated.

- d_ε is a computational-adjustable parameter used to handle critical points in the model.

The second branch in Eq. 112 represents the barrier lowering due to the image-force potential of the electron in the insulator layer, where a numeric adjustment is applied to the edges of the layer to avoid infinite values. The first branch is introduced to saturate the value of the image-force potential close to the metal surface (contact), which otherwise would become infinite for $d_o \to 0$. The last branch represents the barrier lowering due to the image-force potential of the

electron in the semiconductor layer. To avoid discontinuity and infinite values at the insulator–semiconductor interface, a linear transitional region is introduced (the third branch).

The d_ε parameter, which should be smaller than t_{ox} for geometric reasons, allows you to adjust the functional shape of the model around the model critical points).

For consistency, when $t_{ox} = 0$, the model reverts to $\Delta\Phi_B(d_0, d_0 > 0) = \dfrac{q}{16\pi\varepsilon_{sem}d_0}$, which is the typical image-force barrier lowering for a metal–semiconductor interface.

As an option, you can select to compute a barrier-lowering average based on Eq. 112 over the distance d_o from the contact or an average around d_o.

The barrier lowering with interfacial insulator layer model can be combined as a weighted sum with any of the barrier-lowering models described by Eq. 109 (or Eq. 110) or Eq. 111, but not with both.

To activate the barrier lowering with interfacial insulator layer model, specify `InsBarrierLowering` in the `Schottky` subsection of the `Electrode` or the electrode-specific `Physics` section:

```
Electrode { ...
   { name = "cnt1" voltage = 0 Schottky(InsBarrierLowering))
     Workfunction=4.75 }
}

Physics(Electrode = "cnt1") { ...
   Schottky(InsBarrierLowering)
}
```

To compute an average based on Eq. 112 over the distance d_o, specify also the keyword `Average`:

```
Physics(Electrode = "Gate") { InsBarrierLowering(Average) }
```

To compute an average based on Eq. 112 over a symmetric interval `delta`, centered around d_o, specify the keyword `DeltaAverage` in the `InsBarrierLowering` section of the command file:

```
Physics(Electrode = "Gate") { InsBarrierLowering(DeltaAverage) }
```

The parameter `InsBL_delta` can be adjusted in the `Schottky` section of the parameter file:

```
Electrode = "anode" {
   Schottky {
      InsBL_delta = 1.0000e-08    * [cm]
   }
}
```

The model parameters t_{ox}, ε_{ins}, d_ε, d_0, and nn can be specified in the Schottky section of the parameter file (see Table 31). The parameter nn controls the number of equidistant intervals over which the integration is performed using the trapezoidal rule in the case of averaging. The t_{ox}, ε_{ins}, and d_ε parameters are mole fraction dependent.

You can use the weight parameter to combine the barrier lowering with the interfacial insulator layer model with either the barrier model described by Eq. 109 (or Eq. 110) or Eq. 111. If only the barrier lowering with interfacial insulator layer model is specified (by InsBarrierLowering in the electrode-specific Physics section), the value of weight is 1 regardless of the value specified in the parameter file by InsBL_c_weight. If the model is used together with other barrier-lowering models, the weight parameters in both models can be adjusted individually such that their sum is 1. The overall barrier-lowering effect would be a weighted sum of the models.

Table 31   Parameters of barrier lowering with interfacial insulator layer model

Symbol	Parameter name	Default value	Unit
t_{ox}	InsBL_tox	2×10^{-7}	cm
ε_{ins}	InsBL_epsins	3.9	1
d_0	InsBL_d0	1×10^{-7}	cm
d_ε	InsBL_d_eps	1×10^{-8}	cm
nn	InsBL_nn	20	1
weight	InsBL_c_weight	1	1
delta	InsBL_delta	1×10^{-8}	cm

Resistive Contacts

By default, contacts have a resistance of $1\,\text{m}\Omega$ when they are connected to a circuit node, and no resistance otherwise. The resistance can be changed with Resist or DistResist or both in the Electrode section.

The following example defines an emitter as a contact with resistance $1\,\Omega$ (assuming that AreaFactor is one):

```
Electrode { ...
   { name = "emitter" voltage = 2 Resist=1 }
}
```

The following example defines an emitter as a contact with a distributed resistance of $0.0002\ \Omega\text{cm}^2$ in series with a $100\ \Omega$ lump resistor, with the $2\ \text{V}$ external voltage applied to the lump resistor:

```
Electrode { ...
   { name = "emitter" voltage = 2 Resist=100 DistResist=2e-4 }
}
```

If V_{applied} is applied to the contact through a resistor R (Resist in the Electrode section) or distributed resistance R_{d} (DistResist in the Electrode section), there is an additional equation to compute ϕ_F in Eq. 98, Eq. 101, and Eq. 102.

For a distributed resistance, ϕ_F is different for each mesh vertex of the contact and is computed as a solution of the following equation for each contact vertex, self-consistently with the system of all equations:

$$\hat{n} \cdot [\vec{J}_p(\phi_F) + \vec{J}_n(\phi_F) + \vec{J}_D(\phi_F)] = \frac{(V_{\text{applied}} - \phi_F)}{R_{\text{d}}} \tag{113}$$

For a resistor, ϕ_F is a constant over the contact and only one equation per contact is solved self-consistently with the system of all equations:

$$\int_s \hat{n} \cdot [\vec{J}_p(\phi_F) + \vec{J}_n(\phi_F) + \vec{J}_D(\phi_F)]ds = \frac{(V_{\text{applied}} - \phi_F)}{R} \tag{114}$$

where s is a contact area used in a Sentaurus Device simulation to compute a total current through the contact.

When both a lump resistor R and a distributed resistance R_{d} are specified, ϕ_F is computed for each mesh vertex of the contact as a solution of the following equations, self-consistently with the system of all equations:

$$\hat{n} \cdot [\vec{J}_p(\phi_F) + \vec{J}_n(\phi_F) + \vec{J}_D(\phi_F)] = \frac{(V_{\text{internal}} - \phi_F)}{R_{\text{d}}} \tag{115}$$

$$\frac{V_{\text{applied}} - V_{\text{internal}}}{R} = \int_S \frac{V_{\text{internal}} - \phi_F}{R_{\text{d}}}ds \tag{116}$$

where V_{internal} depends on ϕ_F along the contact (on all contact vertices) and $\int_S \frac{V_{\text{internal}} - \phi_F}{R_{\text{d}}}ds$ is the total current on the contact.

NOTE   In 2D simulations, R must be specified in units of $\Omega\mu\text{m}$. In 3D simulations, R must be specified in units of Ω. R_{d} is given in Ωcm^2 (see Table 206 on page 1399).

To emulate the behavior of a Schottky contact [7], Schottky contact resistivity at zero bias was derived and a doping-dependent resistivity model of such contacts was obtained. This model is activated for Ohmic contacts by the keyword `DistResist=SchottkyResist` in the `Electrode` section. The model is expressed as:

$$R_{\rm d} = R_\infty \frac{300\,\rm K}{T_0} \exp\left(\frac{q\Phi_{\rm B}}{E_0}\right)$$

$$E_0 = E_{00} \coth\left(\frac{E_{00}}{kT_0}\right)$$

$$E_{00} = \frac{qh}{4\pi}\sqrt{\frac{|N_{\rm D,0} - N_{\rm A,0}|}{\varepsilon_{\rm s} m_{\rm t}}}$$

(117)

where:

- $\Phi_{\rm B}$ is the Schottky barrier (in this model, for electrons, this is the difference between the metal workfunction and the electron affinity of the semiconductor; for holes, this is the difference between the valence band energy of the semiconductor and the metal workfunction).

- R_∞ is the Schottky resistance for an infinite doping concentration at the contact (or zero Schottky barrier).

- $\varepsilon_{\rm s}$ is the semiconductor permittivity.

- $m_{\rm t}$ is the tunneling mass.

- T_0 is the device lattice temperature defined in the `Physics` section (see Table 233 on page 1427).

The parameters $\Phi_{\rm B}$, R_∞, and $m_{\rm t}$ can be mole dependent, and they can be specified in the region or material sections of the parameter file. If the parameters are mole independent, they also can be specified directly in the electrode section of the parameter file.

For example, if the contact `"top"` covers two semiconductor regions `"reg1"` and `"reg2"`, the mole dependency of parameter R_∞ can be defined as:

```
Region = "reg1" {
   SchottkyResistance {
      Xmax(0) = 0.0
      Xmax(1) = 0.6
      Electrode = "top" {
         Rinf = 2.4000e-09 , 5.2000e-09      # [Ohm*cm^2]
         Rinf(1) = 2.5000e-09 , 5.2000e-09   # [Ohm*cm^2]
      }
   }
}

Region = "reg2" {
   SchottkyResistance {
      Xmax(0) = 0.0
```

```
        Xmax(1) = 0.1
        Xmax(2) = 0.6
        Electrode = "top" {
           Rinf = 2.5000e-09 , 5.2000e-09      # [Ohm*cm^2]
           Rinf(1) = 2.6000e-09 , 5.2000e-09   # [Ohm*cm^2]
           Rinf(2) = 2.9000e-09 , 5.2000e-09   # [Ohm*cm^2]
        }
     }
  }
```

In the example, the parameter R_∞ of contact `"top"` is defined in `"reg1"` and `"reg2"` with different mole dependencies.

If the Schottky resistance parameters are not mole fraction dependent, the parameters can be specified regionwise or materialwise in the `SchottkyResistance` section:

```
Region = "reg1" {
   SchottkyResistance {
      Rinf = 2.4000e-09 , 5.2000e-09   # [Ohm*cm^2]
   }
}
```

For backward compatibility, the Schottky resistance parameters that are not mole fraction dependent also can be defined directly in the `Electrode` section of the Schottky resistive contact:

```
Electrode = "gate" {
   # no mole fraction dependency allowed
   SchottkyResistance {
      Rinf = 2.4000e-09 , 5.2000e-09   # [Ohm*cm^2]
      PhiB = 0.6        , 0.51         # [eV]
   }
}
```

When multiple definitions of the Schottky resistance parameters are found in the parameter file, a priority scheme is used:

1. If a `Region` section contains a `SchottkyResistance` subsection with an `Electrode` section, the parameters specified here are chosen.

2. If there is no `Region` section with a `SchottkyResistance` subsection having an `Electrode` specification, `Material` sections are searched next. If a `Material` section contains a `SchottkyResistance` subsection with an `Electrode` subsection, the parameters specified are chosen.

3. If there is no `Region` section or `Material` section with a `SchottkyResistance` subsection having an `Electrode` section, only constant parameters can be specified. First, the global `Electrode` sections are searched for constant parameters:

```
Electrode = "gate" {
   # no mole fraction dependency allowed
   SchottkyResistance {
      Rinf = 2.4000e-09 , 5.2000e-09   # [Ohm*cm^2]
   }
}
```

If this section is found, the parameters here are chosen. If not, a `Region` section with a `SchottkyResistance` subsection and constant parameters is searched for:

```
Region = "reg1" {
   SchottkyResistance {
      Rinf = 2.4000e-09 , 5.2000e-09   # [Ohm*cm^2]
   }
}
```

If a `Region` section is found, the parameters are chosen here. If not, a `Material` section with a `SchottkyResistance` subsection and constant parameters is the last possible specification:

```
Material = "Silicon" {
   SchottkyResistance {
      Rinf = 2.4000e-09 , 5.2000e-09   # [Ohm*cm^2]
   }
}
```

4. If nothing is specified at all, the default values are chosen, with their values:

a) $m_t = 0.19$, $R_\infty = 2.4 \times 10^{-9}$ Ωcm^2, $\Phi_B = 0.6$ eV for electrons

b) $m_t = 0.19$, $R_\infty = 5.2 \times 10^{-9}$ Ωcm^2, $\Phi_B = 0.51$ eV for holes [7]

These parameters can be specified independently in different sections as previously described. The priority scheme is applied independently of each of them.

When multiple regions are connected to a Schottky resist contact, the value of the Schottky resistance at the common vertices on the contact is taken as a maximum of the region Schottky resistances. In other words, the Schottky resistance at the common vertices is computed for each region with the region parameters, and the maximum value among regions is chosen.

In the case of alloys, parameters are interpolated from the composing materials. For example, in the case of $\text{Ge}_x\text{Si}_{1-x}$, the value of R_∞ is computed from the two side materials and the corresponding mole-fraction specification. The command file is:

```
Physics (Material = "SiliconGermanium") {   # Gex(x)Si(1-x)
   * Mole fraction material: SiGe(x=0) = Silicon
   * Mole fraction material: SiGe(x=1) = Germanium
```

```
      MoleFraction(
         xFraction = 0.35
      )
   }
```

The parameter file is:

```
   Material = "Silicon" {
      SchottkyResistance {
         Rinf = 2.3000e-09 , 5.1000e-09 # [Ohm*cm^2]
      }
   }

   Material = "Germanium" {
      SchottkyResistance {
         Rinf = 2.4000e-09 , 5.0000e-09 # [Ohm*cm^2]
      }
   }
```

The model is applied to each contact vertex and checks the sign of the doping concentration $N_{D,0} - N_{A,0}$. If the sign is positive, the electron parameters are used to compute R_d for the vertex. If the sign is negative, the hole parameters are used.

As an option, you can specify a constant metal workfunction parameter instead of a mole fraction–dependent Schottky barrier parameter Φ_B. In this case, Sentaurus Device computes the Schottky barrier Φ_B in Eq. 117 as the difference between the specified contact workfunction and the electron affinity of the semiconductor (in the case of n-type semiconductors), or as the difference between the valence band energy and the contact workfunction (in the case of p-type semiconductors). Although only a constant contact workfunction is allowed, the computed Schottky barrier Φ_B captures the mole-fraction dependency more physically through the electron affinity and the bandgap mole-fraction dependencies.

To use the metal contact workfunction option to compute the Schottky barrier Φ_B, specify the `Workfunction` keyword in the `SchottkyResistance` subsection, of the `Electrode` section, of the parameter file. For example, to compute the Schottky barrier Φ_B corresponding to a 4.1 eV workfunction at the contact `top2`, specify in the parameter file:

```
   Electrode = "top2" {
      SchottkyResistance {
         # PhiB = 0.6 , 0.51    # [eV]
         Workfunction = 4.1
      }
   }
```

In this case, the values of the Schottky barrier Φ_B in the parameter file (if specified by `PhiB`) are ignored because they are internally computed.

For convenience, the workfunction can also be specified in the contact section of the region or material:

```
Region = "reg2" {
   SchottkyResistance {
      Workfunction = 4.1
      Xmax(0) = 0.0
      Xmax(1) = 0.1
      Xmax(2) = 0.6
      Electrode = "top" {
         Rinf = 2.5000e-09 , 5.2000e-09     # [Ohm*cm^2]
         Rinf(1) = 2.6000e-09 , 5.2000e-09   # [Ohm*cm^2]
         Rinf(2) = 2.9000e-09 , 5.2000e-09   # [Ohm*cm^2]
      }
   }
}
```

In this case, note that the workfunction option is applied to `reg2` only. If the contact extends over multiple regions, the workfunction option can only be activated in certain regions by explicitly specifying `Workfunction` in the respective region.

When the workfunction option is specified in both the `Electrode` section and the `Region` or `Material` sections, the `Electrode` section takes precedence.

A more general model for Schottky resistance can be implemented using the Schottky resistance PMI (see Schottky Resistance Model on page 1288). In this case, Schottky-distributed resistance R_d can be an arbitrary function of lattice temperature, electron temperature, hole temperature, electron affinity, band gap, bandgap narrowing, conduction-band effective density-of-states, valence-band effective density-of-states, and effective intrinsic density, $R_d = R_d(T, T_n, T_p, \chi, E_g, E_{bgn}, N_C, N_V, n_{i,eff})$. The PMI model can access the built-in Schottky resistance model parameters (constant or mole fraction–dependent) using the vertex-based PMI support function `InitModelParameter()` (see Runtime Support for Vertex-Based PMI Models on page 1067).

Resistive Interfaces

A distributed resistance model is supported for metal–metal, semiconductor–semiconductor, and metal–semiconductor interfaces. The distributed resistance interface model is similar to the thermionic current model with the exponential dependency on the interface barrier height replaced by a linear dependency on the voltage drop across the interface. The interfaces are treated as discontinuous double-point interfaces.

The model is activated by specifying the keyword `eDistResistance` for electrons and the keyword `hDistResistance` for holes in the `Physics` section of the resistive interface. For

metal–metal interfaces, only `eDistResistance` is allowed because only electrons are involved in transport across the interface:

```
Physics (MaterialInterface="Germanium/Silicon") {
   eDistResistance=1e-3
   hDistResistance=1e-3
}
```

If the interface is between material 1 and material 2, in the following equations, it is assumed that the normal component of the carrier current density leaves material 1 and enters material 2. For semiconductor–semiconductor interfaces, the boundary conditions can be written as the following for electrons:

$$J_{n,2} = J_{n,1} \tag{118}$$

$$J_{n,1} = \frac{\Phi_{n,1} - \Phi_{n,2}}{R_{d,n}} \tag{119}$$

and for holes:

$$J_{p,2} = J_{p,1} \tag{120}$$

$$J_{p,1} = \frac{\Phi_{p,1} - \Phi_{p,2}}{R_{d,p}} \tag{121}$$

where $R_{d,n}$ and $R_{d,p}$ are the electron- and hole-distributed resistance at the interface.

For metal–metal resistive interfaces, the resistive boundary conditions take the form:

$$J_{n,2} = J_{n,1} \tag{122}$$

$$J_{n,1} = \frac{\Phi_{M,1} - \Phi_{M,2}}{R_{d,n}} \tag{123}$$

Finally, at metal–semiconductor interfaces, you have:

$$J_{n,1} = \frac{\Phi_{n,1} - \Phi_{M,2}}{R_{d,n}} \tag{124}$$

$$J_{p,1} = \frac{\Phi_{p,1} - \Phi_{M,2}}{R_{d,p}} \tag{125}$$

$$J_{M,2} = J_{n,1} + J_{p,1} \tag{126}$$

Like Schottky contacts, the behavior of a Schottky interface can be emulated using the doping-dependent resistivity model described by Eq. 117, p. 215. The model is activated for Ohmic metal–semiconductor interfaces by the keyword `DistResist=SchottkyResistance` in the `Physics` section of the interface:

```
Physics(MaterialInterface="AlGaAs/Aluminum") {
   DistResist=SchottkyResistance
}
```

The Schottky resistance parameters can be mole dependent or constant. When the parameter file contains multiple definitions of the Schottky resistance parameters, the same priority scheme used for contacts is applied.

As for the contacts, you can specify a constant metal workfunction parameter instead of a mole fraction–dependent Schottky barrier parameter Φ_B. The syntax is similar to contacts, but the `Workfunction` keyword must be specified in the `RegionInterface` section or the `MaterialInterface` section instead of the `Electrode` section.

A doping-dependent Schottky barrier model is supported for metal–semiconductor Schottky barriers. Image force lowering of the potential energy barrier is included in Schottky contacts. The model is based on the distributed resistance interface model. The Schottky barrier height is dependent on the doping on the semiconductor side.

> **NOTE**   This model works at the metal–semiconductor interface. It does not work for contacts.

The effects of image force rounding of the potential energy barrier are included. The magnitude of the bias-dependent image force lowering ($\Delta\varphi$), relative to the band bending (E_b), is defined as [8]:

$$\frac{\Delta\varphi}{E_b} = \left[16\pi\left(\frac{E_b}{E_{11}}\right)^{3/2}\frac{x_m}{\omega}\right]^{-1/2}\left(1 + 3\frac{x_m}{\omega}\right) \tag{127}$$

$$E_{11} = 9.05 \times 10^{-7}\left[\frac{N}{K_s K_d^2}\right]^{1/3} \tag{128}$$

$$\frac{x_m}{\omega} = \frac{2}{3} + \frac{1}{3}\cos\frac{\delta}{3} - \frac{1}{\sqrt{3}}\sin\frac{\delta}{3} \tag{129}$$

$$\cos\delta = 1 - \frac{27}{32\pi(E_b/E_{11})^{3/2}} \tag{130}$$

where K_s is the static dielectric constant, K_d is the high-frequency dielectric constant, E_{11} is a constant of the material with the unit of energy, and N is the electron density.

The syntax can be used in either the `RegionInterface` or `MaterialInterface` section. You can activate the model by specifying the keyword `DistResist=SchottkyResistance` (or `eDistResistance=eSchottkyResistance` for electrons and `hDistResistance=hSchottkyResistance` for holes) and `SRDoping`. The keyword `DistResist=SchottkyResistance` (or `eDistResistance=eSchottkyResistance` and `hDistResistance=hSchottkyResistance`) activates the Schottky interface resistance model, and `SRDoping` activates the image-force potential lowering model in Schottky contacts. For example:

```
Physics(MaterialInterface="AlGaAs/Aluminum") {
   DistResist=SchottkyResistance
   SRDoping
}

Physics(MaterialInterface="AlGaAs/Aluminum") {
   eDistResistance=eSchottkyResistance
   hDistResistance=hSchottkyResistance
   SRDoping
}
```

A more general model for interface Schottky resistance can be implemented using the Schottky resistance PMI (see Schottky Resistance Model on page 1288). In this case, Schottky-distributed resistance R_d can be an arbitrary function of lattice temperature, electron temperature, hole temperature, electron affinity, band gap, bandgap narrowing, conduction-band effective density-of-states, valence-band effective density-of-states, and effective intrinsic density, $R_d = R_d(T, T_n, T_p, \chi, E_g, E_{bgn}, N_C, N_V, n_{i, eff})$. The PMI model can access the built-in Schottky resistance model parameters using the vertex-based PMI support function `InitModelParameter()` (see Runtime Support for Vertex-Based PMI Models on page 1067).

Boundaries Without Contacts

Outer boundaries of the device that are not contacts are treated with ideal Neumann boundary conditions:

$$\varepsilon \nabla \phi + \vec{P} = 0 \tag{131}$$

$$\vec{J}_n \cdot \hat{n} = 0 \qquad \vec{J}_p \cdot \hat{n} = 0 \tag{132}$$

Eq. 132 also applies to semiconductor–insulator interfaces.

Floating Contacts

Floating Metal Contacts

The charge on a floating contact (for example, a floating gate in an EEPROM cell) is specified in the `Electrode` section:

```
Electrode { ...
    { name="FloatGate" charge=1e-15 }
}
```

In the case of a floating metal contact (a contact not in touch with any semiconductor region), the electrostatic potential is determined by solving the Poisson equation with the following charge boundary condition:

$$\int \varepsilon \hat{n} \cdot \nabla \phi \, dS = Q \tag{133}$$

where $\hat{n}$ is the normal vector on the floating contact surface S, and Q is the specified charge on the floating contact. The electrostatic potential on the floating-contact surface is assumed to be constant.

An additional capacitance between floating contact and control contact is necessary if, for example, EEPROM cells are simulated in a 2D approximation, to account for the additional influence on the capacitance from the real 3D layout. The additional capacitance can be specified in the `Electrode` section using the keyword `FGcap`.

For example, if you have `ContGate` and `FloatGate` contacts, additional `ContGate/FloatGate` capacitance is specified as:

```
Electrode {
    { name="ContGate" voltage=10 }
    { name="FloatGate" charge=0 FGcap=(value=3e-15 name="ContGate") }
}
```

where `value` is the capacitance value between `FloatGate` and `ContGate`. For the 1D case, the capacitance unit is $F/\mu m^2$; for the 2D case, $F/\mu m$; and for the 3D case, F.

If the floating-contact capacitance is specified, Eq. 133 changes to:

$$\int \varepsilon \hat{n} \cdot \nabla \phi \, dS + C_{FC}(\phi_{CC} - \phi_{FC} + \phi_B) = Q \tag{134}$$

where:

- C_{FC} is the specified floating-contact capacitance.
- ϕ_{FC} is the floating-contact potential.
- ϕ_{CC} is the potential on the control electrode (specified in the `FGcap` statement).
- ϕ_B is a barrier specified in the `Electrode` section for the floating contact, which can be used as a fitting parameter (default value is zero).

> **NOTE** If the control contact is a metal, the value of ϕ_{CC} is defined by the applied voltage and the metal barrier/workfunction (see Contacts on Insulators on page 203). However, if the control contact touches a semiconductor region, ϕ_{CC} is equal to the applied voltage with an averaged built-in potential on the contact.

Floating contacts can have several capacitance values for different control contacts, for example:

```
Electrode {
   { name="source" voltage=0 }
   { name="ContGate" voltage=10 }
   { name="FloatGate" charge=0 FGcap( (value=3e-15 name="ContGate")
      (value=2e-15 name="source") }
}
```

In transient simulations, Sentaurus Device takes the charge specified in the `Electrode` section as an initial condition. After each time step, the charge is updated due to tunneling and hot-carrier injection currents. For a description of tunneling and hot-carrier injection, see Chapter 24 on page 715 and Chapter 25 on page 737, respectively.

Floating Semiconductor Contacts

Sentaurus Device can simulate floating semiconductor contacts by connecting an electrode with charge boundary condition to an insulated semiconductor region. Within that floating-contact region, Sentaurus Device solves the Poisson equation with the following charge boundary condition:

$$\int_{FC} [q(p - n + N_D - N_A) + \rho_{trap}]dV = Q_{FC} \tag{135}$$

where Q_{FC} denotes the total charge on the floating gate and ρ_{trap} is the charge density contributed by traps and fixed charges (see Chapter 17 on page 449). The integral is calculated over all nodes of the floating-contact region [9].

The charge Q_{FC} is a boundary condition that must be specified in a Sentaurus Device `Electrode` statement in exactly the same way as for a floating metal contact:

```
Electrode {
    { name="floating_gate" Charge=1e-14 }
}
```

It is also possible to use the charge as a goal in a `Quasistationary` command:

```
Quasistationary (Goal {Name="floating_gate" Charge = 1e-13})
    { Coupled {Poisson Electron} }
```

Sentaurus Device automatically identifies a floating semiconductor contact based on information in the geometry (`.tdr`) file. It is not necessary for the charge contact to cover the entire boundary of the floating semiconductor region. A small contact is sufficient if the floating region has the same doping type throughout. However, if both n-type and p-type volumes exist in the floating region, both volumes must be associated with the floating contact defining the floating region. This can be achieved by having a contact in touch with both volumes.

It is assumed that no current flows within the floating region. Therefore, the quasi-Fermi potential for electrons and holes is identical and constant within the floating region:

$$\Phi_n = \Phi_p = \Phi \tag{136}$$

Therefore, the electron and hole densities n and p are functions of the electrostatic potential ϕ and the quasi-Fermi potential Φ as discussed in Quasi-Fermi Potential With Boltzmann Statistics on page 175 and Fermi Statistics on page 176. Sentaurus Device does not solve the electron and hole continuity equations within a floating region.

In transient simulations, Sentaurus Device takes the charge specified in the `Electrode` section as an initial condition. After each time step, the charge is updated due to hot-carrier injection or tunneling currents including tunneling to traps. For a description of tunneling models and how to enable them, see Chapter 24 on page 715. For hot-carrier injection models, see Chapter 25 on page 737.

The floating-contact capacitance can be specified in the `Electrode` statement in exactly the same way as for the floating metal contact (see Floating Metal Contacts on page 223). The only difference is that the potential on the semiconductor floating contact is not always a constant. Therefore, defining a constant capacitance may not be strictly correct, and it gives only approximate results. Sentaurus Device uses the semiconductor floating-contact Fermi level to compute the charge associated with the floating-contact capacitance and solves an equilibrium problem (zero voltages and zero charges) at the beginning to find a reference Fermi level.

For plotting purposes, floating semiconductor contacts are handled differently from other electrodes. Instead of the voltage, the value of the quasi-Fermi potential Φ is displayed.

Thermal Boundary Conditions

Boundary Conditions for Lattice Temperature

For the solution of Eq. 67, p. 190, Eq. 68, p. 192, Eq. 69, p. 193, and Eq. 75, p. 196, thermal boundary conditions must be applied. Wachutka [10] is followed, but the difference in thermo-powers between the semiconductor and metal at Ohmic contacts is neglected. For free, thermally insulating, surfaces:

$$\kappa \hat{n} \cdot \nabla T = 0 \tag{137}$$

where $\hat{n}$ denotes a unit vector in the direction of the outer normal.

At thermally conducting interfaces, thermally resistive (nonhomogeneous Neumann) boundary conditions are imposed:

$$\kappa \hat{n} \cdot \nabla T = \frac{T_{ext} - T}{R_{th}} \tag{138}$$

where R_{th} is the external thermal resistance, which characterizes the thermal contact between the semiconductor and adjacent material.

For the special case of an ideal heat sink $(R_{th} \rightarrow 0)$, Dirichlet boundary conditions are imposed:

$$T = T_{ext} \tag{139}$$

By default, $R_{th} = 0$. Other values can be specified with the keyword `SurfaceResistance` in the specification of the `Thermode` (see Table 209 on page 1402). Alternatively, `SurfaceConductance` can be used to specify $1/R_{th}$.

When the lattice temperature equation is solved, the lattice temperature (`Temperature`) and lattice heat flux (`lHeatFlux`) at thermodes are added automatically to the `.plt` file in the corresponding `Thermode` section. The unit for heat flux is W for 3D, $W/\mu m$ for 2D, and $W/\mu m^2$ for 1D.

At insulator–insulator, insulator–semiconductor, semiconductor–semiconductor, metal–semiconductor, metal–metal, and metal–insulator interfaces, a distributed thermal resistance is supported as well.

This feature is activated by specifying the distributed resistance using the keyword `DistrThermalResist` in the `Physics` section of the respective interface. For example:

```
Physics (RegionInterface="reg1/reg2") {
   DistrThermalResist=1e-3
}
```

activates a distributed thermal resistance at the interface between region `"reg1"` and region `"reg2"` with the value $0.001 \; \text{cm}^2\text{K/W}$. As for thermionic emission, double points are used at the interfaces where distributed thermal resistance has been activated. In this case, double points allow a discontinuity in the lattice temperature on the two sides of the interface. Assuming an interface between materials 1 and 2 such that $\Delta T = T_2 - T_1 > 0$, if $\vec{S}_{\text{L},1}$ is the heat flux density entering material 1 and $\vec{S}_{\text{L},2}$ is the heat flux density leaving material 2, the thermal boundary condition at the interface between materials 1 and 2 can be written as:

$$\vec{S}_{\text{L},2} = \vec{S}_{\text{L},1} \tag{140}$$

$$\vec{S}_{\text{L},1} = \frac{T_2 - T_1}{R_{\text{d},\text{th}}} \tag{141}$$

where $R_{\text{d},\text{th}}$ is the interface-distributed resistance defined with `DistrThermalResist` as described here.

Boundary Conditions for Carrier Temperatures

For the carrier temperatures T_n and T_p, at the thermal contacts, fast relaxation to the lattice temperature (boundary condition $T_n = T_p = T$) is assumed.

For other boundaries, adiabatic conditions for carrier temperatures are assumed:

$$\kappa_n \hat{n} \cdot \nabla T_n = \kappa_p \hat{n} \cdot \nabla T_p = 0 \tag{142}$$

When the hydrodynamic model is used, the lattice temperature (`Temperature`), the lattice heat flux (`lHeatFlux`), and the carrier heat fluxes (`eHeatFlux` and `hHeatFlux`) at thermodes are added automatically to the `.plt` file in the corresponding `Thermode` section. The unit for heat fluxes is W for 3D, $W/\mu m$ for 2D, and $W/\mu m^2$ for 1D.

Periodic Boundary Conditions

The use of periodic boundary conditions (PBCs) can be helpful for simulations of periodic device structures, for example, lines or arrays of cells. Instead of building a periodic simulation domain, you can supply PBCs at the lower and upper boundary planes (perpendicular to the

main axis of the coordinate system) of a single cell. Periodicity of the solution means that the two boundary planes are virtually identified, thereby forming a PBC interface: The solution is (weakly) continuous across this interface, and currents (or fluxes in the general case) can flow from one side to the other.

You can select between two different numeric PBC approaches, referred to as the Robin PBC (RPBC) approach and mortar PBC (MPBC) approach. Both approaches support:

- Several transport models, namely, drift-diffusion, thermodynamic, and hydrodynamic transport.

- Both conforming and nonconforming geometries and meshes.

- Two-dimensional and 3D device structures.

- The conservation of the fluxes (for example, current conservation for the continuity equations).

- Both one-fold and two-fold periodicity, that is, PBC can be applied in one axis direction and simultaneously in two directions for 3D structures.

Robin PBC Approach

The RPBC approach uses a current (or flux) model between both sides of the PBC interface of the form:

$$\alpha(u_1 - u_2) - j_{12} = 0 \tag{143}$$

where:

- u_1 and u_2 are the solution variables of an equation at both sides of the PBC interface.

- j_{12} is the flux density of the equation across the PBC interface.

- α represents a user-provided tuning parameter. The tuning parameter allows you to determine how strongly the local current density across the interface reduces the discontinuity of the solution variable. A large α reduces the jumps of the solution variable, while for $\alpha = 0$, no continuity is enforced at all and no current will flow across the interface.

Mortar PBC Approach

In the MPBC approach, both sides of the PBC interface are effectively glued together on one side (the mortar side), while on the other side (the nonmortar side), a weak continuity condition for the equation potential (mostly, the solution variable) is imposed. Therefore, the MPBC approach is not symmetric with respect to the selection of the mortar side if the mesh is nonconforming. The side where the accuracy requirements are larger (and, typically, the mesh

is finer) should be selected as the mortar side. The equation potential for the carrier continuity equations are the corresponding quasi-Fermi potentials, while for the other equations, the solution variable is chosen. The MPBC approach does not require a current model across the PBC interface.

Specifying Periodic Boundary Conditions

Periodic boundary conditions are activated by using `PeriodicBC` in the global or device `Math` section. Table 211 on page 1403 provides a complete list of possible options.

Specifying Robin Periodic Boundary Conditions

RPBCs can be activated individually for all supported equations (see Electrostatic Potential on page 173, Chapter 8 on page 181, and Chapter 9 on page 189). The solution variable u of the selected equation (for example, the electrostatic potential ϕ of the Poisson equation), and the corresponding flux density j are listed in Table 32.

Table 32   Solution variables and fluxes used in periodic boundary conditions

u	j	Description
ϕ	$\varepsilon\nabla\phi$	Electrostatic Potential on page 173
n	$\vec{J}_n$	Chapter 8 on page 181
p	$\vec{J}_p$	
T_n	$\vec{S}_n$	Chapter 9 on page 189
T_p	$\vec{S}_p$	
T	$\kappa\nabla T$	Chapter 9 on page 189

An RPBC is typically activated by `PeriodicBC(<options>)`, where `<options>` provides a selection of the equations and boundaries. Multiple specifications of `<options>` are possible to select several equations: `PeriodicBC( (<options1>) ... (<optionsN>) )`.

>   **NOTE**   If the material parameters or the doping concentration differ on both sides of the interface, RPBC may result in nonphysical solutions.

An example of specifying RPBCs for different equations and boundaries is:

```
Math {
   PeriodicBC(
      (Direction=0 Coordinates=(-1.0 2.0))
      (Poisson Direction=1 Coordinates=(-1e50 1e50))
      (Electron Direction=1 Coordinates=(-1e50 1e50) Factor=2.e8)
```

```
        )
    }
```

Here, the first option applies periodic boundary conditions to all equations in the direction of the x-axis and for the coordinates $-1.0\,\mu m$ and $2.0\,\mu m$. The next two options specify periodic boundary conditions for the electron and hole continuity equations in the y-direction and for the device side coordinates. `Factor` determines the tuning parameter α in the flux density model and defaults to 1.e8.

Specifying Mortar Periodic Boundary Conditions

Periodic boundary conditions using the MPBC approach are activated in the global or device `Math` section by:

```
    PeriodicBC ( ( Type=MPBC Direction=1 MortarSide=Ymax ) )
```

`Direction` selects the coordinate axis where the PBC interface is created (that is, here the y-axis). `MortarSide` specifies that the plane at maximum coordinate values is taken as the mortar side (the default is the minimum coordinate plane). The maximum and minimum coordinate planes are extracted automatically. Using `MortarSide` implies the MPBC approach (making `Type` and `Direction` redundant), which means the following specification enables a two-fold MPBC simulation:

```
    PeriodicBC( ( MortarSide=Xmin MortarSide=Ymax ) )
```

Application Notes

Note that:

- The RPBC approach supports, in contrast to the MPBC approach, some flexibility with respect to the involved equations.

- The MPBC approach treats the PBC interface essentially as a heterointerface. Conductor regions touching the PBC interface are not supported in MPBC. Heterointerfaces touching the PBC interface are allowed, but there are cases where the periodicity is further relaxed.

- If the device structure forms a heterointerface at the PBC interface, the MPBC approach must be used. The RPBC approach provides nonphysical results.

Specialized Linear Solver for MPBC

Using MPBC in combination with iterative linear solvers (such as ILS), you may observe some convergence problems. If feasible, using a direct solver (such as PARDISO) should resolve the problem. Otherwise, an improved preconditioner or the use of extended precision improves the convergence behavior in many cases.

There is a specialized linear solver available for MPBC simulations that utilizes the advantages of the iterative solver ILS and improves the robustness of the simulations. This solver can be enabled by a (temporary) user interface. Specifying `UseSchurSolver` in the global `Math` section replaces the `Blocked` method by the specialized MPBC solver for all `Coupled` statements. `Coupled` statements using other methods are not affected. Note that this solver is not yet available for AC analysis.

Discontinuous Interfaces

Discontinuous interfaces generalize the framework used for the simulation of heterointerfaces at semiconductor–semiconductor interfaces (see Abrupt and Graded Heterojunctions on page 10 and Heterostructure Device Simulation on page 763). They build the basis for models generating discontinuities of physical quantities across region interfaces.

Representation of Physical Quantities Across Interfaces

Several interface conditions result in discontinuous physical quantities across these interfaces. An interface is a *discontinuous interface* if all physical quantities use a discontinuous representation across this interface. The continuity of selected quantities is guaranteed by applying (often implicitly) corresponding interface conditions. By default, the interface conditions at discontinuous interfaces imply continuity for the solution variable.

You can enforce every interface to be a discontinuous interface by using `Discontinuity` in any `Physics` section, for example:

```
Physics ( MaterialInterface= "Silicon/Oxide" ) {
   Discontinuity   * applies to all interfaces of the two materials
}

Physics ( Material= "Silicon" ) {
   Discontinuity   * applies to all interfaces to other materials
}
```

Discontinuous interfaces are allowed between any two regions, independent of their material or material group (semiconductor, insulator, or conductor). They are implicitly or explicitly used for the following interface models:

- `Dipole` (see Dipole Layer on page 174)
- `Discontinuity`
- `DistrThermalResist` (see Boundary Conditions for Lattice Temperature on page 226)
- `HeteroInterface` (see Abrupt and Graded Heterojunctions on page 10)

- `Thermionic, eThermionic, hThermionic` (see Heterostructure Device Simulation on page 763)
- Concept of 'semiconductor floating gate' (see Destination of Injected Current on page 738)
- Optics standalone simulations (see Controlling Computation of Optical Problem in Solve Section on page 572)

Interface Conditions at Discontinuous Interfaces

At general discontinuous interfaces (that is, involving arbitrary material groups), not all interface conditions are yet supported. So far, the interface conditions related to drift-diffusion, thermodynamic, and hydrodynamic transport are allowed. Simulations using only heterointerfaces (that is, semiconductor–semiconductor interfaces including the `HeteroInterface` flag) as discontinuous interfaces support the full set of transport equations and interface conditions. Note that a discontinuous semiconductor–semiconductor interface must be a heterointerface.

Critical Points

Geometric locations, where several interfaces intersect or an interface intersects the boundary or contact, are so-called critical points. At such critical points, not all interface conditions can be fulfilled, in general, and conflicts are resolved by implicit rules.

Critical points are supported if the set of discontinuous interfaces either is empty, or is the entire set of involved interfaces, or consists of heterointerfaces.

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CHAPTER 11 Transport in Metals, Organic Materials, and Disordered Media

This chapter describes transport in materials other than low-defect, inorganic semiconductors.

Singlet Exciton Equation

In organic semiconductor devices, besides the simulation of the electrical part consisting of solving the Poisson and continuity equations, the *singlet exciton equation* is introduced to account for optical properties of these materials related to Frenkel excitons.

This equation takes into account only singlet excitons because triplet excitons do not contribute directly to light emission. The equation models the dynamics of the generation, diffusion, recombination, and radiative decay of singlet excitons in organic semiconductors.

The singlet exciton equation, governing the transport of excitons in organic semiconductors, is given by:

$$\frac{\partial n_{se}}{\partial t} = R_{bimolec} + \nabla \cdot D_{se} \nabla n_{se} - \frac{n_{se} - n_{se}^{eq}}{\tau} - \frac{n_{se} - n_{se}^{eq}}{\tau_{trap}} - R_{se} \tag{144}$$

where:

- n_{se} is the singlet exciton density.
- $R_{bimolec}$ is the carrier bimolecular recombination rate acting as a singlet exciton generation term.
- D_{se} is the singlet exciton diffusion constant.
- τ, τ_{trap} are the singlet exciton lifetimes.
- R_{se} is the net singlet exciton recombination rate.

The first term on the right-hand side of Eq. 144 accounts for the creation of excitons through bimolecular recombination (see Bimolecular Recombination on page 444). The second term describes exciton diffusion; while radiative decay associated with light emission is accounted for by the third and fourth terms.

Nonradiative exciton destruction and conversion of excitons to free electron and free hole populations are described by the net exciton recombination rate (fifth term):

$$R_{se} = R_{se-nf} + R_{se-pf}$$
$$R_{se-nf} = (v_{se} + v_n)\sigma_{se-n}n_{se}n \tag{145}$$
$$R_{se-pf} = (v_{se} + v_p)\sigma_{se-p}n_{se}p$$

where:

- R_{se-nf}, R_{se-pf} are the exciton recombination rate due to free electron and free hole populations, respectively.

- $v_{se} = v_{se,0}$ is the exciton velocity.

- $v_n = v_{n,0}\sqrt{T/300\,\mathrm{K}}$ and $v_p = v_{p,0}\sqrt{T/300\,\mathrm{K}}$ are the electron and hole velocities. $v_{se,0}$, $v_{n,0}$, and $v_{p,0}$ are set in the parameter file.

- σ_{se-n} and σ_{se-p} are the reaction cross sections between the singlet exciton, and the electron and hole, respectively.

In addition, the net exciton recombination rate R_{se} may contain exciton interface dissociation rates converted to volume terms if the exciton interface dissociation model is activated (see Exciton Dissociation Model on page 445).

Boundary and Continuity Conditions for Singlet Exciton Equation

At electrodes and thermodes, equilibrium is assumed for the singlet exciton population:

$$n_{se}(T) = n_{se}^{eq}(T) = \gamma g_{ex}(N_C(T) + N_V(T))\exp\left(-\frac{E_{g,\mathrm{eff}} - E_{ex}}{kT}\right) \tag{146}$$

where $\gamma = 1/4$, and g_{ex} and E_{ex} are the singlet exciton degeneracy factor and binding energy, respectively.

Conditions for the singlet exciton equation at interfaces depend on the interface type. The interface type is dictated by the two regions adjacent to the interface.

For interfaces where the singlet exciton equation is solved only in one of the regions of the interface, the boundary conditions imposed are either Eq. 146 (default) or $\nabla n_{se} \cdot \hat{n} = 0$ (zero flux), depending on the user selection.

For a heterointerface where the singlet exciton equation is solved in both regions, the continuity conditions imposed are thermionic-like. In this case, you can select the barrier ΔE to be the

difference between the band gaps, the conduction bands, or the valence bands of the two regions.

Assuming that at heterointerfaces between materials 1 and 2 (that is, regions 1 and 2), $\Delta E > 0$ ($E_{g,2} > E_{g,1}$ for example), and $j_{se,2}$ is the singlet exciton flux leaving material 2 and $j_{se,1}$ is the singlet exciton flux entering material 1, the interface boundary condition can be written as:

$$
\begin{aligned}
j_{se,1} &= j_{se,2} \\
j_{se,2} &= v_{si}\left(n_{se,2} - n_{se,1}\exp\left(-\frac{\Delta E}{kT}\right)\right)
\end{aligned}
\tag{147}
$$

where $n_{se,2}$ and $n_{se,1}$ are the singlet exciton densities of materials 2 and 1 at the heterointerface. v_{si} is the organic heterointerface emission velocity defined in the parameter file.

Using the Singlet Exciton Equation

To activate the singlet exciton equation, the keyword `SingletExciton` must be specified in the `Coupled` statement of the `Solve` section (see Coupled Command on page 136). Then, the regions where the equation will be solved are selected by specifying the keyword `SingletExciton` with different options in the `Physics` section of the respective regions (by default, none of the regions is selected for solving the singlet exciton equation, so you must select at least one region).

The singlet exciton generation and recombination terms in Eq. 144 are switched off by default. They can be activated regionwise by specifying the corresponding keyword as an option for `Recombination` in the `SingletExciton` section of the respective region `Physics` section (see Table 254 on page 1449).

The keyword `Bimolecular` activates the bimolecular generation (first term). The keywords `Radiative` and `TrappedRadiative` switch on radiative decay of singlet excitons either directly or trap-assisted (third and fourth terms). Nonradiative exciton destruction (fifth term) is activated by `eQuenching` and `hQuenching`. An example is:

```
Physics(Region="EML-ETL") {
    SingletExciton(Recombination(Bimolecular eQuenching hQuenching))
}
```

For interfaces where the singlet exciton equation is solved only in one of the regions of the interface, the default boundary conditions are defined by Eq. 146.

To switch to zero flux boundary condition $\nabla n_{\mathrm{se}} \cdot \hat{n} = 0$, the keyword `FluxBC` must be specified as an option for `SingletExciton` in the interface `Physics` section:

```
Physics(RegionInterface="Region_0/Region_2") {
    SingletExciton(FluxBC)
}
```

For heterointerfaces, the default barrier type for the singlet exciton flux injection across the interface (defined in Eq. 147) is the bandgap energy difference.

The barrier can be switched to conduction band or valence band type by specifying the keyword `BarrierType` with the option `CondBand` or `ValBand` in the `SingletExciton` section of the heterointerface `Physics` section:

```
Physics(RegionInterface="Region_0/Region_2") {
    SingletExciton(BarrierType(CondBand)
}
```

Parameters used with the singlet exciton equation must be specified in the `SingletExciton` section of the parameter file.

Table 33   Parameters and their default values for singlet exciton equation

Symbol	Parameter name	Default value	Location	Unit
γ	gamma	0.25	region	1
τ	tau	1×10^{-7}	region	s
τ_{trap}	tau_trap	1×10^{-8}	region	s
L_{diff}	l_diff	1×10^{-3}	region	cm
$D_{\mathrm{se}} = L_{\mathrm{diff}}^2/\tau$			region	cm^2/s
$\sigma_{\mathrm{se}-n}$	ex_cXsection	1×10^{-8}	region	cm^2
$\sigma_{\mathrm{se}-p}$	ex_cXsection	1×10^{-8}	region	cm^2
E_{ex}	Eex	0.015	region	eV
g_{ex}	gex	4	region	1
$v_{\mathrm{se},0}$	vth	1×10^{7}	region	cm/s
$v_{n,0}$	vth_car	1×10^{3}	region	cm/s
$v_{p,0}$	vth_car	1×10^{3}	region	cm/s
v_{si}	vel	1×10^{8}	interface	cm/s

Transport in Metals

The simulation of current transport in metals or semi-metals is important for interconnection problems in ICs. The current density in metals is given by:

$$\vec{J}_\mathrm{M} = -\sigma(\nabla\Phi_\mathrm{M} + P\nabla T) \tag{148}$$

where:

- σ is the metal conductivity.
- Φ_M is the Fermi potential in the metal.
- P is the metal thermoelectric power.
- T is the lattice temperature.

The second term in Eq. 148 accounts for the Seebeck effect, and it is nonzero only when computation of metal thermoelectric power is enabled (see Thermoelectric Power (TEP) on page 913). For the steady-state case, $\nabla \cdot \vec{J}_\mathrm{M} = 0$. Therefore, the equation for the Fermi potential inside of metals is:

$$\nabla \cdot (\sigma(\nabla\Phi_\mathrm{M} + P\nabla T)) = 0 \tag{149}$$

The following temperature dependence is applied for $\rho = 1/\sigma$:

$$\rho = \rho_0(1 + \alpha_T(T - 273 \text{ K})) \tag{150}$$

All these resistivity parameters can be specified in the parameter file as:

```
Resistivity {
   *  Resist(T) = Resist0 * ( 1 + TempCoef * ( T - 273 ) )
      Resist0 = <value>      # [Ohm*cm]
      TempCoef = <value>     # [1/K]
}
```

No specific keyword is required in the command file because Sentaurus Device recognizes all conductor regions and applies the appropriate equations to these regions and interfaces. The metal conductivity equation Eq. 149 is a part of the `Contact` equation, which is solved automatically by default. If the keyword `NoAutomaticCircuitContact` is specified in the `Math` section or only the Poisson equation is solved, the `Contact` equation must be added explicitly in the `Coupled` statement to account for conductivity in metals.

To switch off current transport in metals, specify the keyword `-MetalConductivity` in the `Math` section.

Electric Boundary Conditions for Metals

The following boundary conditions are used:

- At contacts connected to metal regions, the Dirichlet condition $\Phi_M = V_{\text{applied}}$ is applied for the Fermi potential.

- Interface conditions always include the displacement current $\vec{J}_D$ to ensure conservation of current.

- For interfaces between metal and insulator, the equations are:

$$\vec{J}_M \cdot \hat{n} = \vec{J}_D \cdot \hat{n}$$
$$\phi = \Phi_M - \Phi_{MS} \tag{151}$$

where Φ_{MS} is the workfunction difference between the metal and an intrinsic semiconductor selected (internally by Sentaurus Device) as a reference material, and $\hat{n}$ is the unit normal vector to the interface. The electrostatic potential inside metals is computed as $\phi = \Phi_M - \Phi_{MS}$.

- At metal–semiconductor interfaces, by default, there is an Ohmic boundary condition. Schottky boundary conditions can be selected as an option.

The Ohmic boundary condition at metal–semiconductor interfaces reads:

$$\vec{J}_M \cdot \hat{n} = (\vec{J}_n + \vec{J}_p + \vec{J}_D) \cdot \hat{n}$$
$$\phi = \Phi_M + \phi_0$$
$$n = n_0$$
$$p = p_0 \tag{152}$$

where:

- ϕ_0 is the equilibrium electrostatic potential (the built-in potential).

- n_0 and p_0 are the electron and hole equilibrium concentrations (see Ohmic Contacts on page 201).

There are several options for the Schottky interface (refer to the equations in Schottky Contacts on page 204). The potential barrier between metal and semiconductor is computed automatically and the barrier tunneling (see Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722) and barrier lowering (see Barrier Lowering at Schottky Contacts on page 208) models can be applied.

To select these models, use the following syntax in the command file:

```
Physics(MaterialInterface = "Metal/Silicon") { Schottky eRecVelocity=1e6
   hRecVelocity=1e6 }
Physics(MaterialInterface = "Metal/Silicon") { Schottky BarrierLowering }
Physics(MaterialInterface = "Metal/Silicon") { Schottky }
```

The default values of the electron and hole surface recombination velocities are `eRecVel = 2.573e6` and `hRecVel = 1.93e6`, respectively. Similarly to `Electrode` conditions, if `Schottky` is not specified but the `SurfaceSRH` keyword is specified, Sentaurus Device will apply Ohmic boundary conditions to the electrostatic potential and the surface recombination for both electron and hole carrier current densities on such interfaces.

> **NOTE** At nonmetal interfaces, the keyword `SurfaceSRH` activates a different model from the one described in this section (see Surface SRH Recombination on page 404).

Both Ohmic and Schottky interfaces support a distributed resistance model similar to the one described in Resistive Contacts on page 213. If a distributed resistance is specified at the interface, a distributed voltage drop $\Delta\phi(R_\mathrm{d}) = R_\mathrm{d}(\vec{J}_n + \vec{J}_p + \vec{J}_\mathrm{D}) \cdot \hat{n}$ is applied to the existing boundary condition for potential, where $\Delta\phi(R_\mathrm{d})$ is the voltage drop across the interface, and R_d is the distributed resistance at the interface. In addition, for Ohmic interfaces, emulation of a Schottky interface using a doping-dependent resistivity model is possible. These options are activated as following:

```
# Distributed resistance at Ohmic interface
Physics(MaterialInterface = "Metal/Silicon") {DistResist=1e-6}
# Distributed resistance at Schottky interface
Physics(MaterialInterface = "Metal/Silicon") {Schottky DistResist=1e-6}
# Distributed resistance at Ohmic interface emulating a Schottky interface
Physics(MaterialInterface = "Metal/Silicon")
   {DistResist = SchottkyResist}
```

For Schottky interfaces, the distributed resistance model works with all other options previously described.

For all other metal boundaries, the Neumann condition $\vec{J}_\mathrm{M} \cdot \hat{n} = 0$ is applied.

> **NOTE** By default, Sentaurus Device computes output currents through a contact using integration over the associated wells. For metal contacts, the integration can be switched off and the local current can be used instead by specifying the keyword `DirectCurrent` in the `Math` section. This option may produce a wrong current at the metal contact.

Metal Workfunction

To specify the metal workfunction, use the `Bandgap` parameter set, for example:

```
Material = "Gold" {
   Bandgap { WorkFunction = 5 # [eV] }
}
```

It is also possible to account for workfunction variations within the metal.

If such variations can be characterized by mole-fraction variations and if the metal is treated as a mole fraction–dependent material (see Mole-Fraction Materials on page 15), then `WorkFunction` in the `Bandgap` parameter set can be specified as a mole fraction–dependent quantity, for example:

```
Material = "Metal" {
   Bandgap {
      Xmax(0)=0.0
      Xmax(1)=0.2
      WorkFunction(0) = 4.53# [eV]
      WorkFunction(1) = 4.38# [eV]
   }
}
```

The positional dependency of the workfunction in metals also can be specified directly in the `Physics` section of the command file using one of three different methods:

```
Physics (Material = "<name>" | Region = "<name>") {
   MetalWorkfunction (
      [ Workfunction=<wf> ] |
      [ Workfunction=(<wf_1>, <x_1>, <y_1>, <z_1>)
        Workfunction=(<wf_2>, <x_2>, <y_2>, <z_2>)
        ...
        Workfunction=(<wf_N>, <x_N>, <y_N>, <z_N>) ] |
      [ SFactor= "<dataset_name-or-pmi_model_name>" [Factor=<scale>]
        [Offset=<offset>] ]
   )
}
```

The first method (`Workfunction=<wf>`) simply specifies a constant workfunction value for the material or region that overrides any specification from the parameter file.

The next method allows the specification of an arbitrary number of workfunction–position quadruplets. The workfunction at a vertex in the metal is assigned the value of the workfunction from the quadruplet whose position is closest to the vertex.

Alternatively, the `SFactor` parameter can be used to specify a dataset name (which includes the PMI user fields `PMIUserField0` through `PMIUserField299`) from which the vertex workfunction values will be taken, or a space factor PMI model can be specified that calculates the vertex workfunction values directly (see Space Factor on page 1190). If `Factor=<scale>` is specified, the `SFactor` values are normalized and then are multiplied by this factor. If `Offset=<offset>` is specified, this value is added to the raw or scaled `SFactor` values.

Metal Workfunction Randomization

The workfunction in metal regions can be randomized using specifications in the command file:

```
Physics (Material = "<name>" | Region = "<name>") {
   MetalWorkfunction (
      Randomize (
         AverageGrainSize=<size>                  # [micrometers]
         GrainProbability=(<P1>, <P2>, ...)
         GrainWorkfunction=(<wf1>, <wf2>, ...)    #[eV]
         RandomSeed=<seed>
         AtInsulatorInterface
         UniformDistribution
      )
   )
}
```

The approach taken assumes that the metal consists of randomized grains of varying size and shape that can be characterized with an average grain size. It also assumes that the grains in the metal occur with a finite number of orientations, and the number of grains for each orientation can be characterized with a probability of occurrence. All grains of the same orientation are assumed to have the same workfunction, but the workfunction can be different for each orientation.

`AverageGrainSize` is used to determine the average number of grains for a region, which then is used as the expectation value for a Poisson distribution, random number generator to determine the actual number of grains for the region. Each grain can have a different shape and size.

An arbitrary number of `GrainProbability` values can be specified, but their sum must be equal to one. In addition, there must be a one-to-one correspondence between `GrainProbability` values and `GrainWorkfunction` values.

By default, the seed for the random number generator used in the randomization process is different for every simulation. However, `RandomSeed` can be specified if required. This allows a particular randomization to be repeated if the same seed is used in a subsequent simulation of the same device on the same computer.

The `AtInsulatorInterface` option confines the randomization to the metal–insulator interface vertices. However, the resulting workfunction values at the interface will be exactly the same as those obtained when the entire metal region is randomized.

The `UniformDistribution` option *attempts* to use grains with a uniform size that are distributed uniformly. The success of this is highly dependent on the grid used in the metal region.

The workfunction in metal regions can be saved in a plot file for visualization by specifying `MetalWorkfunction` in the `Plot` section of the command file.

Temperature in Metals

In metals, only the lattice temperature is defined. If the lattice temperature is solved, in metals, it obeys the following equation:

$$c_{\mathrm{L}}\frac{\partial T}{\partial t} - \nabla \cdot \kappa \nabla T = -\nabla \psi_{\mathrm{M}} \cdot \vec{J}_{\mathrm{M}} \tag{153}$$

where κ is the thermal conductivity (see Thermal Conductivity on page 901). If current transport in metals is switched off, the right-hand side of Eq. 153 vanishes. However, a heat flow in metals can still be simulated.

Conductive Insulators

Leakage currents in dielectrics can be modeled by allowing dielectrics to have conductive properties. The conductive insulator (leaky insulator) model implements dielectrics that have nonzero (but typically low) conductivity (a metal-like property), besides the pure dielectric properties.

In a conductive insulator, the electrostatic potential is computed using the Poisson equation, similar to a pure dielectric. As in metals, conductivity is modeled by the Fermi potential (solving Eq. 149) and then the leakage current is computed using Eq. 148. Since the model does not allow net charge in the conductive insulator, the Poisson equation remains unchanged by adding conductive properties to the insulator.

The equation for the Fermi potential inside a conductive insulator is the same used for metals (see Eq. 149), where σ is now the conductivity of the conductive insulator and $\Phi_{\mathrm{M}} = \Phi_{\mathrm{CI}}$ is the Fermi potential in the conductive insulator.

The following boundary conditions are used for this equation:

- At contacts connected to conductive insulator regions, the Dirichlet condition $\Phi_{CI} = V_{applied}$ is applied for the Fermi potential.

- Interface conditions always include the displacement current $\vec{J}_D$ in insulators, conductive insulators, and semiconductors to ensure conservation of current.

- For conductive insulator–semiconductor interfaces, Ohmic-like boundary conditions, thermionic-like boundary conditions, and boundary conditions for floating regions are available.

Leakage from or to a semiconductor to or from a conductive insulator is mainly determined by two factors: the conductive properties of the interface and the bulk resistivity of the conductive insulator. The bulk resistivity-limited conduction corresponds to the case when the current flow is limited by the high resistivity of the conductive insulator region, and the interface has zero resistivity. This case is modeled by the Ohmic-like boundary conditions:

$$
\begin{aligned}
\vec{J}_{CI} \cdot \hat{n} &= (\alpha \vec{J}_n + (1-\alpha)\vec{J}_p) \cdot \hat{n} \\
\Phi_{CI} &= \phi - \phi_0
\end{aligned}
\tag{154}
$$

where:

- Φ_{CI} and $\vec{J}_{CI}$ are the Fermi potential and current density on the interface.

- ϕ is the electrostatic potential (the solution of the Poisson equation in insulator and semiconductor regions).

- ϕ_0 is the built-in potential.

- $\hat{n}$ is the unit normal vector to the interface.

- $\vec{J}_n$ and $\vec{J}_p$ are the electron and hole currents on the semiconductor side of the interface.

- α is the fraction ($0 \leq \alpha \leq 1$) of the current density of the conductive insulator going to the electron current density.

Thermionic-like emission at the interface models the case where conduction is limited by both interface properties and the bulk resistivity of the conductive insulator. Thermionic boundary conditions read:

$$
\begin{aligned}
\vec{J}_{CI} \cdot \hat{n} &= (\vec{J}_{n,\,th} + \vec{J}_{p,\,th}) \cdot \hat{n} \\
\vec{J}_{n,\,th} &= aq\left[v_n(T_n)n - v_n(T)\left(\frac{T}{T_n}\right)^{1.5} N_C \exp\left(\frac{E_F^{CI} - E_C}{kT}\right) \right] \\
\vec{J}_{p,\,th} &= aq\left[v_p(T_p)p - v_p(T)\left(\frac{T}{T_p}\right)^{1.5} N_V \exp\left(\frac{E_V - E_F^{CI}}{kT}\right) \right]
\end{aligned}
\tag{155}
$$

where:

- $\vec{J}_{n,\,\text{th}}$ and $\vec{J}_{p,\,\text{th}}$ are the electron and hole thermionic-emission current densities on the interface from the semiconductor side.

- $v_n(T) = (kT/2\pi m_n)^{0.5}$ and $v_p(T) = (kT/2\pi m_p)^{0.5}$ are 'emission velocities' at the interface.

- T, T_n, and T_p are the lattice, electron and hole temperatures, respectively.

- E_F^CI, E_C, and E_V are the conductive insulator Fermi-level energy, conduction band energy, and valence band energy, respectively.

- a is a constant set through the parameter file, which has the default value of 2.

By using a conductive insulator layer between a semiconductor floating region and a semiconductor region, leakage from a semiconductor floating-gate can be emulated. The boundary condition used in this case is:

$$\vec{J}_\text{CI} \cdot \hat{n} = -\sigma \nabla \Phi \qquad (156)$$

where Φ is the Fermi potential close to the interface. In this case, during transient simulations, the charge update on the floating gate is computed as $J_\text{CI}\Delta t$, where J_CI is the total current at the conductive insulator–floating gate interface, and Δt is the current time step. The activation of this type of boundary condition is automatic if the boundary condition at the conductive insulator–semiconductor floating-gate interface is Ohmic and the simulation is transient (to allow for charging and discharging of the floating gate).

The model is activated by using the keyword `CondInsulator` in the `Physics` section to make the dielectric conductive and by adding the `CondInsulator` equation in the `Solve` section to actually solve the Fermi potential:

```
Physics(Region="insulator"){
   ...
   CondInsulator
   ...
}

Solve {
   ...
   Coupled {Poisson Electron Hole Contact CondInsulator}
   ...
}
```

The parameters for the resistivity of conductive insulators (see Eq. 150) are specified in the `Resistivity` parameter set:

```
Material = "Si3N4" {
   Resistivity {
      * Resist(T) = Resist0 * (1 + TempCoef * (T-273))
```

```
        Resist0 = 3.0e9       # [Ohm*cm]
        TempCoef = 43.0e-4    # [1/K]
    }
}
```

Boundary conditions according to Eq. 154 are used by default. The parameter α in Eq. 154 is given by the value of curw in the CondInsCurr parameter set:

```
MaterialInterface = "Si3N4/AlGaN" {
    CondInsCurr {
        curw = 1.0   # [1]
    }
}
```

Thermionic emission at the semiconductor–conductive insulator interface is enabled by adding eThermionic or hThermionic in the Physics section:

```
Physics(MaterialInterface="Si3N4/AlGaN") {
    *----- Insulator/AlGaN -----
    ...
    eThermionic
    hThermionic
    ...
}
```

where the parameter a (see Eq. 155) is specified in the parameter file:

```
MaterialInterface = "Si3N4/AlGaN" {
    ThermionicEmission {
        A = 2, 2
    }
}
```

For nonthermionic interfaces, an equilibrium solution is needed internally to solve the CondInsulator equation. The equilibrium solution is computed automatically by a nonlinear iteration. Sentaurus Device allows you to specify numeric parameters of the nonlinear iteration as options to the keyword EquilibriumSolution in the Math section (see Equilibrium Solution on page 175 and Table 220 on page 1421). The following example forces the Newton solver to solve up to 100 iterations:

```
Math {
    ...
    EquilibriumSolution(Iterations=100)
    ...
}
```

CHAPTER 12 Semiconductor Band Structure

This chapter discusses the relevance of band structure to the simulation of semiconductor devices.

For device simulation, the most fundamental property of a semiconductor is its band structure. Realistic band structures are complex and can be fully accounted for only in Monte Carlo simulations (refer to the *Sentaurus™ Device Monte Carlo User Guide*). In Sentaurus Device, the band structure is simplified to four quantities: the energies of the conduction and valence band edges (or, in a different parameterization, band gap and electron affinity), and the density-of-states masses for electrons and holes (or, parameterized differently, the band edge density-of-states). The models for these quantities are discussed in Band Gap and Electron Affinity and Effective Masses and Effective Density-of-States on page 261.

Intrinsic Density

The band gap and band edge density-of-states are summarized in the intrinsic density $n_i(T)$ (for undoped semiconductors):

$$n_i(T) = \sqrt{N_C(T)N_V(T)} \exp\left(-\frac{E_g(T)}{2kT}\right) \tag{157}$$

and the effective intrinsic density (including doping-dependent bandgap narrowing):

$$n_{i,\,eff} = n_i \exp\left(\frac{E_{bgn}}{2kT}\right) \tag{158}$$

In devices that contain different materials, the electron affinity χ (see Band Gap and Electron Affinity) is also important. Along with the band gap, it determines the alignment of conduction and valence bands at material interfaces.

Band Gap and Electron Affinity

The band gap is the difference between the lowest energy in the conduction band and the highest energy in the valence band. The electron affinity is the difference between the lowest energy in the conduction band and the vacuum level.

Selecting the Bandgap Model

Sentaurus Device supports different bandgap models: `BennettWilson`, `delAlamo`, `OldSlotboom`, and `Slotboom` (the same model with different default parameters), `JainRoulston`, and `TableBGN`. The bandgap model can be selected in the `EffectiveIntrinsicDensity` statement in the `Physics` section, for example:

```
Physics {
   EffectiveIntrinsicDensity(BandGapNarrowing (Slotboom))
}
```

activates the `Slotboom` model. The default model is `BennettWilson`.

By default, bandgap narrowing is active. Bandgap narrowing can be switched off with the keyword `NoBandGapNarrowing`:

```
Physics {
   EffectiveIntrinsicDensity(NoBandGapNarrowing)
}
```

> **NOTE** To plot the band gap including the bandgap narrowing, specify `EffectiveBandGap` in the `Plot` section of the command file. The quantity that Sentaurus Device plots when `BandGap` is specified does not include bandgap narrowing.

Table 36 on page 260 and Table 37 on page 261 list the model parameters available for calibration (see Bandgap and Electron-Affinity Models).

Bandgap and Electron-Affinity Models

Sentaurus Device models the lattice temperature–dependence of the band gap as [1]:

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T + \beta} \tag{159}$$

where $E_g(0)$ is the bandgap energy at $0\,\text{K}$, and α and β are material parameters (see Table 36 on page 260).

To allow $E_g(0)$ to differ for different bandgap models, it is written as:

$$E_g(0) = E_{g,0} + \delta E_{g,0} \tag{160}$$

$E_{g,0}$ is an adjustable parameter common to all models. For the `TableBGN` and `JainRoulston` models, $\delta E_{g,0} = 0$. Each of the other models offers its own adjustable parameter for $\delta E_{g,0}$ (see Table 36 on page 260).

The effective band gap results from the band gap reduced by bandgap narrowing:

$$E_{g,eff}(T) = E_g(T) - E_{bgn} \tag{161}$$

The electron affinity χ is the energy separation between the conduction band and the vacuum. For `BennettWilson`, `delAlamo`, `OldSlotboom`, `Slotboom`, and `TableBGN`, the affinity is temperature dependent and is affected by bandgap narrowing:

$$\chi(T) = \chi_0 + \frac{(\alpha + \alpha_2)T^2}{2(T + \beta + \beta_2)} + \texttt{Bgn2Chi} \cdot E_{bgn} \tag{162}$$

where χ_0 and `Bgn2Chi` are adjustable parameters (see Table 36 on page 260). `Bgn2Chi` defaults to 0.5 and, therefore, bandgap narrowing splits equally between conduction and valence bands.

In the case of the `JainRoulston` model, the electron affinity depends also on the doping concentration (especially at high dopings) because bandgap narrowing is doping dependent:

$$\chi(T, N_{A,0}, N_{D,0}) = \chi_0 + \frac{(\alpha + \alpha_2)T^2}{2(T + \beta + \beta_2)} + E_{bgn}^{cond} \tag{163}$$

where E_{bgn}^{cond} is the shift in the conduction band due to the `JainRoulston` bandgap narrowing and χ_0 is an adjustable parameter as previously defined.

The main difference of the bandgap models is how they handle bandgap narrowing. Bandgap narrowing in Sentaurus Device has the form:

$$E_{bgn} = \Delta E_g^0 + \Delta E_g^{Fermi} \tag{164}$$

where ΔE_g^0 is determined by the particular bandgap narrowing model used, and ΔE_g^{Fermi} is an optional correction to account for carrier statistics (see Eq. 178, p. 259).

Bandgap Narrowing for Bennett–Wilson Model

Bandgap narrowing for the Bennett–Wilson [2] model (keyword `BennettWilson`) in Sentaurus Device reads:

$$\Delta E_g^0 = \begin{cases} E_{ref}\left[\ln\left(\frac{N_{tot}}{N_{ref}}\right)\right]^2 & N_{tot} \geq N_{ref} \\ 0 & \text{otherwise} \end{cases} \tag{165}$$

The model was developed from absorption and luminescence data of heavily doped n-type materials. The material parameters E_{ref} and N_{ref} are accessible in the `Bennett` parameter set in the parameter file of Sentaurus Device (see Table 37 on page 261).

Bandgap Narrowing for Slotboom Model

Bandgap narrowing for the Slotboom model (keyword `Slotboom` or `OldSlotboom`) (the only difference is in the parameters) in Sentaurus Device reads:

$$\Delta E_g^0 = E_{\text{ref}}\left[\ln\left(\frac{N_{\text{tot}}}{N_{\text{ref}}}\right) + \sqrt{\left(\ln\left(\frac{N_{\text{tot}}}{N_{\text{ref}}}\right)\right)^2 + 0.5}\right] \tag{166}$$

The models are based on measurements of $\mu_n n_i^2$ in n-p-n transistors (or $\mu_p n_i^2$ in p-n-p transistors) with different base doping concentrations and a 1D model for the collector current [3]–[6]. The material parameters E_{ref} and N_{ref} are accessible in the `Slotboom` and `OldSlotboom` parameter sets in the parameter file (see Table 37 on page 261).

Bandgap Narrowing for del Alamo Model

Bandgap narrowing for the del Alamo model (keyword `delAlamo`) in Sentaurus Device reads:

$$\Delta E_g^0 = \begin{cases} E_{\text{ref}}\ln\left(\dfrac{N_{\text{tot}}}{N_{\text{ref}}}\right) & N_{\text{tot}} \geq N_{\text{ref}} \\ 0 & \text{otherwise} \end{cases} \tag{167}$$

This model was proposed [7]–[11] for n-type materials. The material parameters E_{ref} and N_{ref} are accessible in the `delAlamo` parameter set in the parameter file (see Table 37 on page 261).

Bandgap Narrowing for Jain–Roulston Model

Bandgap narrowing for the Jain–Roulston model (keyword `JainRoulston`) in Sentaurus Device is implemented based on the literature [12] and is given by:

$$\Delta E_g^0 = A \cdot N_{\text{tot}}^{1/3} + B \cdot N_{\text{tot}}^{1/4} + C \cdot N_{\text{tot}}^{1/2} + D \cdot N_{\text{tot}}^{1/2} \tag{168}$$

where A, B, C, and D are material-dependent coefficients that can be specified in the parameter file.

The coefficients A, B, C, and D are derived from the quantities defined and described in the literature [12]:

$$A = 1.83 \frac{\Lambda}{N_b^{1/3}} \frac{aR}{\left(\frac{3}{4\pi}\right)^{1/3}} \quad [\text{eV} \cdot \text{cm}] \tag{169}$$

$$B = \frac{0.95 R a^{3/4}}{\left(\frac{3}{4\pi}\right)^{1/4}} \quad [\text{eV} \cdot \text{cm}^{3/4}] \tag{170}$$

$$C = \frac{1.57 R a^{3/2}}{N_b \left(\frac{3}{4\pi}\right)^{1/2}} \quad [\text{eV} \cdot \text{cm}^{3/2}] \tag{171}$$

$$D = \frac{1.57 R_{(\text{mino})} a^{3/2}}{N_b \left(\frac{3}{4\pi}\right)^{1/2}} \quad [\text{eV} \cdot \text{cm}^{3/2}] \tag{172}$$

where a is the effective Bohr radius, R is the Rydberg energy, N_b is the number of valleys in the conduction or valence band, $R_{(\text{mino})}$ is the Rydberg energy for the minority carrier band, and Λ is a correction factor.

In general, papers on bandgap narrowing define the Jain–Roulston bandgap narrowing as $\Delta E_g^0 = C_1 \cdot N_{\text{tot}}^{1/3} + C_2 \cdot N_{\text{tot}}^{1/4} + C_3 \cdot N_{\text{tot}}^{1/2}$. Comparing this definition to Eq. 168, the coefficients C_1, C_2, and C_3 can be mapped to the ones of Sentaurus Device: $C_1 = A$, $C_2 = B$, and $C_3 = C + D$.

If, on the other hand, C_1, C_2, and C_3 are given, then computing the corresponding Sentaurus Device coefficients A, B, C, and D requires splitting C_3 into C and D using Eq. 171 and Eq. 172.

Sentaurus Device needs four coefficients instead of three to compute $E_{\text{bgn}}^{\text{cond}}$ and the doping-dependent affinity (Eq. 163) internally. The expression of $E_{\text{bgn}}^{\text{cond}}$ is given by:

$$E_{\text{bgn}}^{\text{cond}} = \begin{cases} A \cdot N_{\text{tot}}^{1/3} + C \cdot N_{\text{tot}}^{1/2} & N_{D,0} > N_{A,0} \\ B \cdot N_{\text{tot}}^{1/4} + D \cdot N_{\text{tot}}^{1/2} & \text{otherwise} \end{cases} \tag{173}$$

The coefficients A, B, C, and D are specified in the `JainRoulston` section of the parameter file:

```
Material = "Silicon" {
   JainRoulston {
      * n-type
      A_n = 1.02e-8      # [eV cm]
      B_n = 4.15e-7      # [eV cm^(3/4)]
      C_n = 1.45e-12     # [eV cm^(3/2)]
      D_n = 1.48e-12     # [eV cm^(3/2)]
      * p-type
      A_p = 1.11e-8      # [eV cm]
      B_p = 4.79e-7      # [eV cm^(3/4)]
      C_p = 3.23e-12     # [eV cm^(3/2)]
      D_p = 1.81e-12     # [eV cm^(3/2)]
   }
}
```

Table 34   Coefficients and their default values for Jain–Roulston bandgap narrowing model

Symbol	Parameter name	Default value for material				Unit
		Si	Ge	GaAs	All others	
A	A_n	1.02e-8	7.30e-9	1.65e-8	0.0	eVcm
	A_p	1.11e-8	8.21e-9	9.77e-9	0.0	eVcm
B	B_n	4.15e-7	2.57e-7	2.38e-7	0.0	eVcm$^{3/4}$
	B_p	4.79e-7	2.91e-7	3.87e-7	0.0	eVcm$^{3/4}$
C	C_n	1.45e-12	2.29e-12	1.83e-11	0.0	eVcm$^{3/2}$
	C_p	3.23e-12	3.58e-12	3.41e-12	0.0	eVcm$^{3/2}$
D	D_n	1.48e-12	2.03e-12	7.25e-11	0.0	eVcm$^{3/2}$
	D_p	1.81e-12	2.19e-12	4.84e-13	0.0	eVcm$^{3/2}$

Table Specification of Bandgap Narrowing

It is possible to specify bandgap narrowing by using a table, which can be defined in the `TableBGN` parameter set. This table gives the value of bandgap narrowing as a function of donor or acceptor concentration, or total concentration (the sum of acceptor and donor concentrations).

When specifying acceptor and donor concentrations, the total bandgap narrowing is the sum of the contributions of the two dopant types. If only acceptor or only donor entries are present in the table, the bandgap narrowing contribution for the missing dopant type vanishes. Total concentration and donor or acceptor concentration must not be specified in the same table.

Each table entry is a line that specifies a concentration type (`Donor`, `Acceptor`, or `Total`) with a concentration in cm^{-3}, and the bandgap narrowing for this concentration in eV. The actual bandgap narrowing contribution for each concentration type is interpolated from the table, using a scheme that is piecewise linear in the logarithm of the concentration.

For concentrations below (or above) the range covered by table entries, the bandgap narrowing of the entry for the smallest (or greatest) concentration is assumed, for example:

```
TableBGN {
   Total 1e16, 0
   Total 1e20, 0.02
}
```

means that for total doping concentrations below $10^{16} cm^{-3}$, the bandgap narrowing vanishes, then increases up to $20\,meV$ at $10^{20} cm^{-3}$ concentration and maintains this value for even greater concentrations. The interpolation is such that, in this example, the bandgap narrowing at $10^{18} cm^{-3}$ is $10\,meV$.

Tabulated default parameters for bandgap narrowing are available only for GaAs. For all other materials, you can specify the tabulated data in the parameter file.

> **NOTE** It is not possible to specify mole fraction–dependent bandgap narrowing tables. In particular, Sentaurus Device does not relate the parameters for ternary compound semiconductor materials to those of the related binary materials.

Schenk Bandgap Narrowing Model

`BennettWilson`, `delAlamo`, `OldSlotboom`, `Slotboom`, `JainRoulston`, and `TableBGN` are all doping-induced bandgap narrowing models. They do not depend on carrier concentrations. High carrier concentrations produced in optical excitation or high electric field injection can also cause bandgap narrowing. This effect is referred to as plasma-induced bandgap narrowing.

The Schenk bandgap narrowing model described in [13] also takes into account the plasma-induced narrowing effect in silicon. In this model, the bandgap narrowing is the sum of two parts:

- An exchange-correlation part, which is a function of plasma density and temperature.
- An ionic part, which is a function of activated doping concentration, plasma density, and temperature.

Sentaurus Device supports two versions of the Schenk model: a simplified version where bandgap narrowing is computed at $T = 0\,K$ and does not depend on temperature, and the full model where temperature dependence is accounted for. You can switch from the simplified

model (the default) to the full model by setting `IsSimplified=-1` in the Schenk bandgap narrowing section of the parameter file.

The full-model exchange correlation and ionic terms are described by:

$$\Delta_a^{xc}(n, p, T) = -\frac{(4\pi)^3 n_\Sigma^2 \left[\left(\frac{48n_a}{\pi g_a}\right)^{1/3} + c_a \ln(1 + d_a n_p^{p_a})\right] + \left(\frac{8\pi\alpha_a}{g_a}\right)n_a \Upsilon^2 + \sqrt{8\pi n_\Sigma}\Upsilon^{5/2}}{(4\pi)^3 n_\Sigma^2 + \Upsilon^3 + b_a\sqrt{n_\Sigma}\Upsilon^2 + 40n_\Sigma^{3/2}\Upsilon} \tag{174}$$

$$\Delta_a^{i}(N_{tot}, n, p, T) = -\frac{N_{tot}[1 + U^i(n_\Sigma, \Upsilon)]}{\sqrt{\Upsilon n_\Sigma/(2\pi)}[1 + h_a\ln(1 + \sqrt{n_\Sigma}/\Upsilon) + j_a U^i(n_\Sigma, \Upsilon)n_p^{3/4}(1 + k_a n_p^{q_a})]} \tag{175}$$

and, for the simplified model by:

$$\Delta_a^{xc}(n, p, T= 0) = -\left[\left(\frac{48n_a}{\pi g_a}\right)^{1/3} + c_a\ln(1 + d_a n_p^{p_a})\right] \tag{176}$$

$$\Delta_a^{i}(N_{tot}, n, p, T= 0) = -N_{tot}\frac{0.799\alpha_a}{n_p^{3/4}} \tag{177}$$

where $a = e, h$ is the index for the carrier type, $\Upsilon = kT/Ry_{ex}$, $n_\Sigma = n + p$, $n_p = \alpha_e n + \alpha_h p$, and $U^i(n_\Sigma, \Upsilon) = n_\Sigma^2/\Upsilon^3$. The default values (silicon) and units for the parameters that can be changed in Sentaurus Device in this model are listed in Table 35 on page 258.

Sentaurus Device implements the Schenk bandgap narrowing model using the framework of the density gradient model (see Density Gradient Model on page 294). If you want to suppress the quantization corrections contained in this model, set the density gradient model parameter $\gamma = 0$ (see Eq. 231, p. 295).

The Schenk model is switched on separately for electrons (conduction band correction) and holes (valence band correction). The complete bandgap narrowing correction is the sum of conduction and valence band corrections, and it can be obtained by switching on the Schenk model for both electrons and holes.

First, in the `Physics` section of silicon regions, `SchenkBGN_elec` must be specified as the `LocalModel` (that is, the model for Λ_{PMI} in Eq. 231, p. 295) for `eQuantumPotential` (conduction bandgap correction), and `SchenkBGN_hole` must be specified as the `LocalModel` for `hQuantumPotential` (valence band correction).

In addition, because the Schenk model is a bandgap narrowing model itself, all other models must be switched off by specifying the keyword `NoBandGapNarrowing` as the argument for `EffectiveIntrinsicDensity`:

```
Physics(Region = "Region1_Si") {
   ...
   EffectiveIntrinsicDensity (NoBandGapNarrowing)
   eQuantumPotential(LocalModel=SchenkBGN_elec)
   hQuantumPotential(LocalModel=SchenkBGN_hole)
   ...
}
```

Apart from switching on quantum corrections in the `Physics` section, the equations for quantum corrections must be solved to compute the corrections. This is performed by specifying `eQuantumPotential` (for electrons) or `hQuantumPotential` (for holes) or both in the `Solve` section:

```
Solve {
   Coupled (LineSearchDamping=0.01){Poisson eQuantumPotential}
   Coupled {Poisson eQuantumPotential hQuantumPotential}
   quasistationary ( Goal {name="base" voltage=0.4}
                     Goal {name="collector" voltage=2.0}
                     Initialstep=0.1 Maxstep=0.1 Minstep=1e-6
                    )
      {coupled {poisson electron hole eQuantumPotential hQuantumPotential}}
}
```

Finally, to ignore the quantization corrections by the density gradient model, in the parameter file, γ is set to zero. Then, the Schenk model parameter `IsSimplified` is set to `1` if the simplified model ($T = 0\,\mathrm{K}$) is used or `-1` for the full model (temperature dependent):

```
Material = "Silicon" {
   ...
   *turn off everything in density gradient model except
   *apparent band-edge shift
   QuantumPotentialParameters {gamma = 0 , 0}
   ...
   SchenkBGN_elec {
      ...
      * Selects simplified model (1) or complete Schenk model (-1)
      IsSimplified = 1
   }
   SchenkBGN_hole {
      ...
      * Selects simplified model (1) or complete Schenk model (-1)
      IsSimplified = 1
   }
}
```

The Schenk bandgap narrowing model is specifically for silicon. Sentaurus Device permits the model parameters to be changed in the parameter file (the `SchenkBGN_elec` and `SchenkBGN_hole` sections) as an option for also using this bandgap narrowing model for other materials. A full description of the parameters is given in the literature [13] and their default values are summarized in Table 35.

The Schenk bandgap narrowing can be visualized by specifying the data entry `eSchenkBGN` or `hSchenkBGN` or both in the `Plot` section of the command file.

Table 35   Default parameters for Schenk bandgap narrowing model

Symbol	Parameter name	Default value (silicon)	Unit
SchenkBGN_elec			
α_e	alpha_e	0.5187	1
g_e	g_e	12	1
Ry_{ex}	Ry_ex	16.55	meV
a_{ex}	a_ex	3.719e-7	cm
b_e	b_e	8	1
c_e	c_e	1.3346	1
d_e	d_e	0.893	1
p_e	p_e	0.2333	1
h_e	h_e	3.91	1
j_e	j_e	2.8585	1
k_e	k_e	0.012	1
q_e	q_e	0.75	1
SchenkBGN_hole			
α_h	alpha_h	0.4813	1
g_h	g_h	4	1
Ry_{ex}	Ry_ex	16.55	meV
a_{ex}	a_ex	3.719e-7	cm
b_h	b_h	1	1
c_h	c_h	1.2365	1
d_h	d_h	1.1530	1
p_h	p_h	0.2333	1

Table 35   Default parameters for Schenk bandgap narrowing model (Continued)

Symbol	Parameter name	Default value (silicon)	Unit
h_h	h_h	4.20	1
j_h	j_h	2.9307	1
k_h	k_h	0.19	1
q_h	q_h	0.25	1

Bandgap Narrowing With Fermi Statistics

Parameters for bandgap narrowing are often extracted from experimental data assuming Maxwell–Boltzmann statistics. However, in the high-doping regime for which bandgap narrowing is important, Maxwell–Boltzmann statistics differs significantly from the more realistic Fermi statistics.

The bandgap narrowing parameters are, therefore, systematically affected by using the wrong statistics to interpret the experiment. For use in simulations that do not use Fermi statistics, this 'error' in the parameters is desirable, as it partially compensates the error by using the 'wrong' statistics in the simulation. However, for simulations using Fermi statistics, this compensation does not occur.

Therefore, Sentaurus Device can apply a correction to the bandgap narrowing to reduce the errors introduced by using Maxwell–Boltzmann statistics for the interpretation of experiments on bandgap narrowing (see Eq. 164, p. 251):

$$\Delta E_g^{\text{Fermi}} \ = \ k300\text{K}\left[\ln\left(\frac{N_V N_C}{N_{A,0} N_{D,0}}\right) + F_{1/2}^{-1}\left(\frac{N_{A,0}}{N_V}\right) + F_{1/2}^{-1}\left(\frac{N_{D,0}}{N_C}\right)\right] \tag{178}$$

where the right-hand side is evaluated at $300\,\text{K}$.

By default, correction Eq. 178 is switched on for simulations using Fermi statistics and switched off (that is, $\Delta E_g^{\text{Fermi}} = 0$) for simulations using Maxwell–Boltzmann statistics. To switch off the correction in simulations using Fermi statistics, specify `EffectiveIntrinsicDensity(NoFermi)` in the `Physics` section of the command file. This is recommended if you use parameters for bandgap narrowing that have been extracted assuming Fermi statistics. Sometimes for III–IV materials, the correction Eq. 178 is too large, and it is recommended to switch it off in these cases. For Maxwell–Boltzmann statistics, `EffectiveIntrinsicDensity(NoFermi)` or `EffectiveIntrinsicDensity()` means that the correction of Eq. 178 is set to zero.

Bandgap Parameters

The band gap $E_{g,0}$ and values of $\delta E_{g,0}$ for each model are accessible in the `BandGap` section of the parameter file, in addition to the electron affinity χ_0 and the temperature coefficients α and β. As an extension to what Eq. 159 and Eq. 162 suggest, the parameters $E_{g,0}$ and χ_0 can be specified at any reference temperature T_{par}. By default, $T_{par} = 0\,\text{K}$.

To prevent abnormally low (or negative) band gap, the calculated value of the band gap E_g (which may include bandgap narrowing and stress effects) is limited if $E_g < E_{g,min} + \delta E_{g,min}$:

$$E_{g,\text{limited}} = E_{g,min} + \delta E_{g,min} \exp[(E_g - E_{g,min} - \delta E_{g,min})/\delta E_{g,min}] \tag{179}$$

Table 36   Bandgap models: Parameters and their default values for silicon

Symbol	Parameter name	Default	Unit	Band gap at 0 K $E_{g,0} + \delta E_{g,0} + \dfrac{\alpha T_{par}^2}{\beta + T_{par}}$	Reference
$E_{g,0}$	Eg0	1.1696	eV	–	Eq. 160, p. 250
$\delta E_{g,0}$	dEg0(Bennett)	0.0	eV	1.1696	Eq. 160
	dEg0(Slotboom)	-4.795×10^{-3}	eV	1.1648	
	dEg0(OldSlotboom)	-1.595×10^{-2}	eV	1.1537	
	dEg0(delAlamo)	-1.407×10^{-2}	eV	1.1556	
α	alpha	4.73×10^{-4}	eV/K	–	Eq. 159, p. 250, Eq. 162, p. 251
α_2	alpha2	0	eV/K	–	Eq. 162
β	beta	636	K	–	Eq. 159, Eq. 162
β_2	beta2	0	K	–	Eq. 162
χ_0	Chi0	4.05	eV	–	Eq. 162
Bgn2Chi	Bgn2Chi	0.5	1	–	Eq. 162
T_{par}	Tpar	0	K	–	
$E_{g,min}$	EgMin	0	eV	–	Eq. 179
$\delta E_{g,min}$	dEgMin	0.01	eV	–	Eq. 179

Table 37 summarizes the silicon default parameters for the analytic bandgap narrowing models available in Sentaurus Device.

Table 37   Bandgap narrowing models: Parameters and their default values for silicon

Symbol	Parameter	Bennett	Slotboom	Old Slotboom	del Alamo	Unit
E_{ref}	Ebgn	6.84×10^{-3}	6.92×10^{-3}	9.0×10^{-3}	18.7×10^{-3}	eV
N_{ref}	Nref	3.162×10^{18}	1.3×10^{17}	1.0×10^{17}	7.0×10^{17}	cm^{-3}

Effective Masses and Effective Density-of-States

Sentaurus Device provides two options for computing carrier effective masses and densities of states. The first method, selected by specifying `Formula=1` in the parameter file, computes an effective density-of-states (DOS) as a function of carrier effective mass. The effective mass may be either independent of temperature or a function of the temperature-dependent band gap. The latter is the most appropriate model for carriers in silicon and is the default for simulations of silicon devices.

In the second method, selected by specifying `Formula=2` in the parameter file the effective carrier mass is computed as a function of a temperature-dependent density-of-states. The default for simulations of GaAs devices is `Formula=2`.

Electron Effective Mass and DOS

Formula 1

The lattice temperature–dependence of the DOS effective mass of electrons is modeled by:

$$m_n = 6^{2/3}(m_t^2 m_l)^{1/3} + m_m \tag{180}$$

where the temperature-dependent effective mass component $m_t(T)$ is best described in silicon by the temperature dependence of the energy gap [14]:

$$\frac{m_t(T)}{m_0} = a \frac{E_g(0)}{E_g(T)} \tag{181}$$

The coefficient a and the mass m_l are defined in the parameter file with the default values provided in Table 38 on page 262. The parameter m_m, which defaults to zero, allows m_n to be defined as a temperature-independent quantity if required.

The effective densities of states (DOS) in the conduction band N_C follows from:

$$N_C(m_n, T_n) = 2.5094 \times 10^{19} \left(\frac{m_n}{m_0}\right)^{\frac{3}{2}} \left(\frac{T_n}{300\,\mathrm{K}}\right)^{\frac{3}{2}} \mathrm{cm}^{-3} \tag{182}$$

Formula 2

If `Formula=2` is specified in the parameter file, the value for the DOS is computed from $N_C(300\,\mathrm{K})$, which is read from the parameter file:

$$N_C(T_n) = N_C(300\,\mathrm{K}) \left(\frac{T_n}{300\,\mathrm{K}}\right)^{\frac{3}{2}} \tag{183}$$

and the electron effective mass is simply a function of $N_C(300\,\mathrm{K})$:

$$\frac{m_n}{m_0} = \left(\frac{N_C(300\,\mathrm{K})}{2.5094 \times 10^{19}\,\mathrm{cm}^{-3}}\right)^{\frac{2}{3}} \tag{184}$$

Electron Effective Mass and Conduction Band DOS Parameters

Table 38 lists the default coefficients for the electron effective mass and conduction band DOS models. The values can be modified in the `eDOSMass` parameter set.

NOTE The default setting for the `Formula` parameter depends on the materials, for example, it is equal to 1 for silicon and 2 for GaAs.

Table 38   Default coefficients for effective electron mass and DOS models

Option	Symbol	Parameter name	Electrons	Unit
Formula=1	a	a	0.1905	1
	m_1	ml	0.9163	1
	m_m	mm	0	1
Formula=2	$N_C(300\,\mathrm{K})$	Nc300	2.890×10^{19}	cm^{-3}

Hole Effective Mass and DOS

Formula 1

For the DOS effective mass of holes, the best fit in silicon is provided by the expression [15]:

$$\frac{m_p(T)}{m_0} = \left(\frac{a + bT + cT^2 + dT^3 + eT^4}{1 + fT + gT^2 + hT^3 + iT^4}\right)^{\frac{2}{3}} + m_{\mathrm{m}} \tag{185}$$

where the coefficients are listed in Table 39 on page 264. The parameter m_{m}, which defaults to zero, allows m_p to be defined as a temperature-independent quantity. The effective DOS for holes N_{V} follows from:

$$N_{\mathrm{V}}(m_p, T_p) = 2.5094 \times 10^{19} \left(\frac{m_p}{m_0}\right)^{\frac{3}{2}} \left(\frac{T_p}{300\,\mathrm{K}}\right)^{\frac{3}{2}} \mathrm{cm}^{-3} \tag{186}$$

Formula 2

If `Formula=2` in the parameter file, the temperature-dependent DOS is computed from $N_{\mathrm{V}}(300\,\mathrm{K})$ as given in the parameter file:

$$N_{\mathrm{V}}(T_p) = N_{\mathrm{V}}(300\,\mathrm{K})\left(\frac{T_p}{300\,\mathrm{K}}\right)^{\frac{3}{2}} \tag{187}$$

and the effective hole mass is given by:

$$\frac{m_p}{m_0} = \left(\frac{N_{\mathrm{V}}(300\,\mathrm{K})}{2.5094 \times 10^{19}\,\mathrm{cm}^{-3}}\right)^{\frac{2}{3}} \tag{188}$$

Hole Effective Mass and Valence Band DOS Parameters

The model coefficients for the hole effective mass and valence band DOS can be modified in the parameter set `hDOSMass`. Table 39 on page 264 lists the default parameter values.

> **NOTE** The default setting for the `Formula` parameter depends on the materials, for example, it is equal to 1 for silicon and it is equal to 2 for GaAs.

Table 39   Default coefficients for hole effective mass and DOS models

Option	Symbol	Parameter name	Holes	Unit
Formula=1	a	a	0.4435870	1
	b	b	0.3609528×10^{-2}	K^{-1}
	c	c	0.1173515×10^{-3}	K^{-2}
	d	d	0.1263218×10^{-5}	K^{-3}
	e	e	0.3025581×10^{-8}	K^{-4}
	f	f	0.4683382×10^{-2}	K^{-1}
	g	g	0.2286895×10^{-3}	K^{-2}
	h	h	0.7469271×10^{-6}	K^{-3}
	i	i	0.1727481×10^{-8}	K^{-4}
	m_{m}	mm	0	1
Formula=2	$N_{\mathrm{V}}(300\,\mathrm{K})$	Nv300	3.140×10^{19}	cm^{-3}

Gaussian Density-of-States for Organic Semiconductors

Gaussian density-of-states (DOS) has been introduced to better represent electron and hole effective DOS in disordered organic semiconductors. Within the Gaussian disorder model, electron and hole DOS are represented by:

$$\Gamma(E) = \frac{N_{\mathrm{t}}}{\sqrt{2\pi}\sigma_{\mathrm{DOS}}} \exp\left(-\frac{(E - E_0)^2}{2\sigma_{\mathrm{DOS}}^2}\right) \tag{189}$$

where N_{t} is the total number of hopping sites with $N_{\mathrm{t}} = N_{\mathrm{LUMO}}$ for electrons (LUMO is the lowest unoccupied molecular orbital) and $N_{\mathrm{t}} = N_{\mathrm{HOMO}}$ for holes (HOMO is the highest occupied molecular orbital), E_0 and σ_{DOS} are the energy center and the width of the DOS distribution, respectively.

Electron and hole densities in the most general case (Fermi–Dirac statistics) then are computed using Gaussian distribution from Eq. 189 as:

$$\frac{n}{N_{\mathrm{LUMO}}} = \frac{1}{\sqrt{2\pi}\sigma_n} \int_{-\infty}^{\infty} \exp\left(-\frac{(E - E_{0n})^2}{2\sigma_n^2}\right) \frac{1}{1 + e^{(E - E_{\mathrm{F},n})/(kT)}} dE = G_n(\zeta_n;\hat{s}_n) \tag{190}$$

$$\frac{p}{N_{\text{HOMO}}} = \frac{1}{\sqrt{2\pi}\sigma_p} \int\limits_{-\infty}^{\infty} \exp\left(-\frac{(E - E_{0p})^2}{2\sigma_p^2}\right) \frac{1}{1 + e^{(E_{F,p} - E)/(kT)}} dE = G_p(\zeta_p;\hat{s}_p) \qquad (191)$$

where $\zeta_n = \dfrac{E_{F,n} - E_{0n}}{kT}$, $\zeta_p = \dfrac{E_{0p} - E_{F,p}}{kT}$, $\hat{s}_n = \dfrac{\sigma_n}{kT}$, $\hat{s}_p = \dfrac{\sigma_p}{kT}$.

Sentaurus Device computes Gauss–Fermi integrals $G_n(\zeta_n;\hat{s}_n)$ and $G_p(\zeta_p;\hat{s}_p)$ using an analytic approximation [16]. The approximation covers both the nondegenerate and degenerate cases:

$$G_c(\zeta_c;\hat{s}_c) = \begin{cases} \dfrac{\exp\left(\dfrac{\hat{s}_c^2}{2} + \zeta_c\right)}{1 + \exp(K(\hat{s}_c)(\zeta_c + \hat{s}_c^2))} & \zeta_c \le -\hat{s}_c^2 \quad \text{(nondegenerate region)} \\[4mm] \dfrac{1}{2}erfc\left(-\dfrac{\zeta_c}{\hat{s}_c\sqrt{2}}H(\hat{s}_c)\right) & \zeta_c > -\hat{s}_c^2 \qquad \text{(degenerate region)} \end{cases} \qquad (192)$$

where the index c is n or p, and the analytic functions H and K are given by:

$$H(s) = \frac{\sqrt{2}}{s}\text{erfc}^{-1}\left(\exp\left(-\frac{s^2}{2}\right)\right) \qquad (193)$$

$$K(s) = 2\left(1 - \frac{H(s)}{s}\sqrt{\frac{2}{\pi}}\exp\left[\frac{1}{2}s^2(1 - H^2(s))\right]\right) \qquad (194)$$

The model is activated regionwise, materialwise, or globally by specifying the keyword `GaussianDOS_Full` in the respective `Physics` section together with the `Fermi` keyword in the global `Physics` section:

```
Physics(Region="Organic_sem1") {
    GaussianDOS_full
}

Physics {
    Fermi
}
```

The model parameters used in Eq. 190 and Eq. 191 are listed in Table 40 on page 266. They can be specified in the `GaussianDOS_full` section of the parameter file.

Table 40   Gaussian DOS model parameters

Parameter symbol	Parameter name	Default value	Unit
N_{t} N_{LUMO} (electron) N_{HOMO} (hole)	Nt	1×10^{21} 1×10^{21}	cm^{-3}
σ_{DOS} σ_n σ_p	sigmaDOS	0.052 0.052	eV
$E_{0n} = E_0 - E_C$ (electron) $E_{0p} = E_V - E_0$ (hole)	E0	0.1 0.1	eV

In the case of nondegenerate semiconductors (Maxwell–Boltzmann approximation can be used for carrier densities), a simplified version based on a correction of standard densities-of-states N_C and N_V is available as well. The densities-of-states are corrected so that equivalent carrier densities are obtained when Gaussian densities-of-states described by are used instead of standard densities-of-states. Introducing the notations:

$$
\begin{aligned}
A_{\mathrm{e}} &= \frac{\sigma_n^2}{2k^2} \\[4pt]
B_{\mathrm{e}} &= \frac{E_{0n} - E_C}{k} \\[4pt]
C_{\mathrm{e}} &= \frac{E_{0n} - E_C}{\sqrt{2}\sigma_n} \\[4pt]
A_{\mathrm{h}} &= \frac{\sigma_p^2}{2k^2} \\[4pt]
B_{\mathrm{h}} &= \frac{E_V - E_{0p}}{k} \\[4pt]
C_{\mathrm{h}} &= \frac{E_V - E_{0p}}{\sqrt{2}\sigma_p}
\end{aligned}
\tag{195}
$$

the electron and hole effective DOS are computed in the Maxwell–Boltzmann approximation as:

$$
N_{\mathrm{C}}(T) = \frac{N_{\mathrm{LUMO}}}{2}\exp\!\left(\frac{A_{\mathrm{e}}}{T^2} - \frac{B_{\mathrm{e}}}{T}\right)\mathrm{erfc}\!\left(\frac{\sqrt{A_{\mathrm{e}}}}{T} - C_{\mathrm{e}}\right)
\tag{196}
$$

and:

$$
N_{\mathrm{V}}(T) = \frac{N_{\mathrm{HOMO}}}{2}\exp\!\left(\frac{A_{\mathrm{h}}}{T^2} - \frac{B_{\mathrm{h}}}{T}\right)\mathrm{erfc}\!\left(\frac{\sqrt{A_{\mathrm{h}}}}{T} - C_{\mathrm{h}}\right)
\tag{197}
$$

The simplified model can be activated regionwise or globally by specifying the keyword `GaussianDOS` for `EffectiveMass` in the `Physics` section of the command file:

```
Physics(Region="Organic_sem1") {
   EffectiveMass(GaussianDOS)
}
```

The model parameters used in Eq. 189, p. 264 and Eq. 195 and their default values are summarized in Table 41.

Table 41   Simplified Gaussian DOS model parameters

Parameter symbol		Parameter name	Default value	Unit
N_{t}	N_{LUMO} (electron)	N_LUMO	$1{\times}10^{21}$	cm^{-3}
	N_{HOMO} (hole)	N_HOMO	$1{\times}10^{21}$	
σ_{DOS}	σ_n	sigmaDOS_e	0.052	eV
	σ_p	sigmaDOS_h	0.052	
$E_{0cn} = E_0 - E_{\text{C}}$		E0_c	0.1	eV
$E_{0v} = E_{\text{V}} - E_0$		E0_v	0.1	

Multivalley Band Structure

Eq. 43 and Eq. 44, p. 177 give a dependency of electron and hole concentrations on the quasi–Fermi level for a single-valley representation of the semiconductor band structure. Stress-induced change of the silicon band structure and the nature of low bandgap materials require you to consider several valleys in the conduction and valence bands to compute the correct dependency of the carrier concentration on the quasi–Fermi level.

With the parabolic band assumption and Fermi–Dirac distribution function applied to each valley, the multivalley electron and hole concentrations are represented as follows:

$$n = N_{\text{C}} F_{\text{MV},n}\left(\frac{E_{\text{F},n} - E_{\text{C}}}{kT}\right) = N_{\text{C}} \sum_{i=1}^{N_n} g_n^i F_{1/2}\left(\frac{E_{\text{F},n} - E_{\text{C}} - \Delta E_n^i}{kT}\right) \tag{198}$$

$$p = N_{\text{V}} F_{\text{MV},p}\left(\frac{E_{\text{V}} - E_{\text{F},p}}{kT}\right) = N_{\text{V}} \sum_{i=1}^{N_p} g_p^i F_{1/2}\left(\frac{\Delta E_p^i + E_{\text{V}} - E_{\text{F},p}}{kT}\right) \tag{199}$$

where N_n and N_p are the electron and hole numbers of valleys, g_n^i and g_p^i are the electron and hole DOS valley factors, and ΔE_n^i and ΔE_p^i are the electron and hole valley energy shifts

relative to the band edges E_C and E_V, respectively. All other variables in these equations are the same as in Eq. 43 and Eq. 44, p. 177. Without Fermi statistics, the Fermi–Dirac integrals $F_{1/2}$ in these equations are replaced by exponents that correspond to the Boltzmann statistics for each valley.

Similarly to the Fermi statistics, the inverse functions of $F_{MV,n}$ and $F_{MV,p}$ are used to define the variables γ_n and γ_p that bring an additional drift term with $\nabla(\ln \gamma)$ as it is expressed in Eq. 47 and Eq. 48, p. 177:

$$\gamma_n = \frac{n}{N_C} \exp\left(-F_{MV,n}^{-1}\left(\frac{n}{N_C}\right)\right) \tag{200}$$

$$\gamma_p = \frac{p}{N_V} \exp\left(-F_{MV,p}^{-1}\left(\frac{p}{N_V}\right)\right) \tag{201}$$

To compute the inverse functions $F_{MV,n}^{-1}\left(\frac{n}{N_C}\right)$ and $F_{MV,p}^{-1}\left(\frac{p}{N_V}\right)$, an internal Newton solver is used.

Together with the fast Joyce–Dixon approximation of the Fermi–Dirac integral $F_{1/2}$, the multivalley model of Sentaurus Device provides an option for a numeric integration over the energy to compute the carrier density using Gauss–Laguerre quadratures. This extends applicability of the model to account for band nonparabolicity (see Nonparabolic Band Structure) and the MOSFET channel quantization effect using the multivalley MLDA model (see Modified Local-Density Approximation on page 300). To control the accuracy and CPU time of such a numeric integration, it is possible to set a user-defined number of integration points in the Gauss–Laguerre quadratures.

Nonparabolic Band Structure

The Fermi–Dirac integral $F_{1/2}$ assumes a typical parabolic band approximation where an energy dependency of the DOS is approximated with $\sqrt{\varepsilon}$. Usually, such a simple approximation is valid only in the vicinity of the band minima. Generally, the isotropic nonparabolicity parameter α is introduced into the dispersion relation as follows: $\varepsilon(1 + \alpha\varepsilon) = (\hbar k)^2/(2m)$, where k is the wavevector, and m is the effective mass.

With such a dispersion, the multivalley carrier density is computed similarly to Eq. 198 and Eq. 199, but $F_{1/2}$ is replaced by the following integral:

$$F_{1/2}^\alpha(\eta, T) = \int_0^\infty \frac{(1 + 2kT\alpha\varepsilon)\sqrt{\varepsilon(1 + kT\alpha\varepsilon)}}{1 + e^{\varepsilon - \eta}} d\varepsilon \tag{202}$$

where η is the carrier quasi Fermi energy defined by Eq. 49 and Eq. 50, p. 177. Compared to $F_{1/2}$, the above integral explicitly depends on the carrier temperature T, which is accounted for in hydrodynamic and thermodynamic problems.

The more general case of nonparabolic bands can be accounted for with the six-band k · p band-structure model for holes (see Strained Hole Effective Mass and DOS on page 833). The model considers three hole bands (the heavy-hole, light-hole, and split-off bands) and the DOS of band n is given generally by:

$$D_n(\varepsilon) = \frac{2}{(2\pi)^3} \oint_{\varepsilon_n(\kappa) = \varepsilon} \frac{dS}{|\nabla_\kappa \varepsilon_n(\kappa)|} \tag{203}$$

Therefore, accounting for Fermi–Dirac carrier distribution over the energy, the total hole concentration in the valence band can be expressed as:

$$p(E_{F,p}, T) = \sum_i \int_0^\infty \frac{D_i(\varepsilon)}{1 + \exp\left(\dfrac{\varepsilon - \Delta E_p^i - E_V + E_{F,p}}{kT}\right)} d\varepsilon \tag{204}$$

where variable notations correspond to ones in Eq. 199 and integrals over the energy in Eq. 204 are computed numerically using Gauss–Laguerre quadrature. Similar to the parabolic case, without Fermi statistics, the Fermi–Dirac distribution function in Eq. 202 and Eq. 204 is replaced by the Boltzmann one.

Bandgap Widening

The bandgap widening effect is related to the carrier geometric confinement, which is important to account for in ultrathin layer semiconductor structures. Typically, the electrons in the Γ-valley of III–V materials have a very small effective mass, which leads to increased geometric confinement in such materials. This effect in the model is accounted for by the simple assumption that the carrier DOS in Eq. 202 and Eq. 203, and in the Fermi–Dirac integrals of Eq. 198 and Eq. 199, is zero up to the first subband energy ε_1 computed analytically for the infinite barrier rectangular quantum well with the layer thickness size L_z. Mostly, this option is designed to work together with the MLDA quantization model (see MLDA Model on page 300).

Moreover, the multivalley band structure with this bandgap widening model could be used with other quantization models, such as the Density Gradient Model on page 294.

The first subband energy for nonparabolic bands is computed for each valley i as follows:

$$\varepsilon_1^i = \frac{-1 + \sqrt{1 + \frac{2\alpha^i}{m_q^i}\left(\frac{\hbar\pi}{L_z}\right)^2}}{2\alpha^i} \tag{205}$$

where α^i is the band nonparabolicity, L_z is the layer thickness, and m_q^i is the quantization mass computed automatically along the confinement direction or specified in the valley definition. To account for ε_1^i in the density integrals Eq. 202 and Eq. 203, the DOS energy is replaced by $\varepsilon + \varepsilon_1^i$. Various options to compute the layer thickness automatically or to define it explicitly are described in Geometric Parameters on page 361 and Using MLDA on page 304.

Monte Carlo Density-of-States

To have consistency between the continuity transport models (see Carrier Transport in Semiconductors on page 181) and the Monte Carlo method (refer to the *Sentaurus™ Device Monte Carlo User Guide*), there is an option to use Monte Carlo DOS in the multivalley model. The Monte Carlo DOS is computed for the full semiconductor band structure used in Monte Carlo simulations. If the DOS $D_i(\varepsilon)$ is computed for various bands in the conduction band, the electron density can be expressed as:

$$n(E_{F,n}, T) = \sum_i \int_0^\infty \frac{D_i(\varepsilon)}{1 + \exp\left(\frac{\varepsilon + \Delta E_n^i + E_C - E_{F,n}}{kT}\right)} d\varepsilon \tag{206}$$

where $E_{F,n}$ is the electron quasi-Fermi energy, and ΔE_n^i is the difference between the energy of band i and the conduction band edge. A similar expression works for the hole density (see Eq. 204).

Using Multivalley Band Structure

Multivalley statistics is activated with the keyword `MultiValley` in the `Physics` section. If the model must be activated only for electrons or holes, the keywords `eMultiValley` and `hMultiValley` can be used, respectively. The model can be defined regionwise as well.

For testing and comparison purposes, the numeric Gauss–Laguerre integration (mentioned in Nonparabolic Band Structure on page 268) can be activated for the Fermi–Dirac integral $F_{1/2}$.

To set such an integration, the keyword `DensityIntegral` must be used as in the following statement:

```
Physics { (e|h)Multivalley(DensityIntegral) }
```

Similarly, to activate the carrier density computation that accounts for nonparabolicity as in Eq. 202, the following statement must be used:

```
Physics { (e|h)Multivalley(Nonparabolicity) }
```

To activate the six-band $k \cdot p$ band-structure model for holes described in Strained Hole Effective Mass and DOS on page 833 and Nonparabolic Band Structure on page 268, the following should be specified:

```
Physics { hMultivalley(kpDOS) }
```

This statement will create three hole bands (light, heavy, and spin-orbit) in the multivalley model. The parameters affecting the six-band $k \cdot p$ band-structure model (see Eq. 965, p. 833 for the DOS mass and Eq. 203, p. 269) include the deformation potentials of the model for hole bands (`adp`, `bdp`, `ddp`, and `dso`) and the Luttinger parameters (`gamma_1`, `gamma_2`, and `gamma_3`). All parameters can be specified in the `LatticeParameters` section of the parameter file and can be mole fraction dependent. These parameters define relaxed hole bands and the stress-induced change (see Deformation of Band Structure on page 826).

To activate the two-band $k \cdot p$ band-structure model for electrons described in Strained Electron Effective Mass and DOS on page 831 (where three Δ_2 valleys will be created), specify:

```
Physics { eMultivalley(kpDOS) }
```

The parameters affecting the two-band $k \cdot p$ band-structure model for Δ_2 valleys (see Eq. 952–Eq. 955) include the deformation potentials of the $k \cdot p$ model for electron bands (`xis`, `dbs`, `xiu`, and `xid`), the Sverdlov $k \cdot p$ parameter (`Mkp`), and the relaxed nonparabolicity α_0 (this is accounted for only with the `Nonparabolicity` keyword in the `eMultivalley` statement). These parameters can be specified in the `LatticeParameters` section of the parameter file. In addition, the Δ_2 valley effective masses (`me_l0` and `me_t0`) can be defined in the `StressMobility` section. All parameters can be mole fraction dependent. These parameters define three relaxed Δ_2 valleys and the stress-induced change (see Deformation of Band Structure on page 826).

To control the number of Gauss–Laguerre integration points (the default is 30, which gives a good compromise between accuracy of the numeric integration and CPU time), the global `Math` statement must be used:

```
Math { DensityIntegral(30) }
```

For non $k \cdot p$ bands, all multivalley model parameters are defined in the `MultiValley` section of the parameter file. You can define an arbitrary number of valleys; however, by default, for example for silicon, Sentaurus Device defines three Δ_2 electron valleys and two hole valleys as follows:

```
MultiValley{
   eValley"Delta1"(1,0,0)(ml=0.914, mt=0.196, energy=0, degeneracy=2,
                          alpha=0.5, xiu=9.16, xid=0.77)
   eValley"Delta2"(0,1,0)(ml=0.914, mt=0.196, energy=0, degeneracy=2,
                          alpha=0.5, xiu=9.16, xid=0.77)
   eValley"Delta3"(0,0,1)(ml=0.914, mt=0.196, energy=0, degeneracy=2,
                          alpha=0.5, xiu=9.16, xid=0.77)
   hValley"LH"(m=0.16, energy=0, degeneracy=1)
   hValley"HH"(m=0.49, energy=0, degeneracy=1)
}
```

The above definition of `"Delta"` valleys represents a most general way to define valleys in the multivalley band structure. For example, the valley `"Delta1"` defines an ellipsoidal valley with the effective masses $m_l = 0.914$ and $m_t = 0.196$, its main axis oriented in the <100> direction, the nonparabolicity $\alpha = 0.5\,\mathrm{eV}^{-1}$, the degeneracy equal to 2, zero energy shift ΔE_n from the conduction band edge, and the deformation potentials Ξ_u, Ξ_d, which are used to have a stress effect in the valley energy using the linear deformation potential model (see Eq. 945 in Deformation of Band Structure on page 826).

The general valley definition allows also another parameter m_q that could redefine the quantization mass computed automatically by the multivalley MLDA model (see Modified Local-Density Approximation on page 300). The hole valleys above are assumed to be simple spherical ones with no stress dependency. This is a huge simplification compared to the six-band $k \cdot p$ model.

> **NOTE** With both the `Multivalley(parfile)` and `Multivalley` options, only valleys defined in the `Multivalley` section of the parameter file (or default material-specific ones) will be used. With the `Multivalley` section in the parameter file, all default valleys will be ignored and only valleys defined in the parameter file will be used.

> **NOTE** With the `Multivalley(kpDOS)` option in the `Physics` section, all multivalley model parameters (N_n, N_p, g_n^i, g_p^i, ΔE_n^i, and ΔE_p^i) are defined and described by stress models in Multivalley Band Structure on page 835. This case ignores all valleys defined in the parameter file. To use the $k \cdot p$ bands together with valleys in the parameter file, specify:
>
> `Multivalley(kpDOS parfile)`

> **NOTE** The option `eMultivalley(kpDOS parfile)` can be used, for example, for SiGe applications where the two-band $k \cdot p$ model brings three Δ_2 valleys, but four L-valleys are taken from the parameter file. Generally, it is a useful option to combine $k \cdot p$ and analytic valleys, but you must be careful not to double-count the Δ_2 valleys because, by default, the parameter file for SiGe has analytic Δ_2 valleys as well. So, these valleys must be removed from the `Multivalley` section of the parameter file. However, if no `Multivalley` section is defined in the parameter file, the default valleys are still used and there may be double-counting (see previous notes).

To account for the bandgap widening effect as in Eq. 205, the `ThinLayer` keyword must be in the `MultiValley` statement, and the `LayerThickness` statement must be set. All `LayerThickness` options are described in LayerThickness Command on page 310 where generally the layer thickness can be extracted automatically for defined regions. In addition, some specific options can be found in Using MLDA on page 304 for non-1D confinement, but practically, if the geometric confinement is mostly 1D, such a setting could be as simple as:

```
LayerThickness( Thickness = L_z )
Multivalley( ThinLayer )
```

To activate the use of the Monte Carlo DOS in the multivalley model, specify one of the following options:

```
Physics { (e|h)Multivalley(mcDOS("mcdos_file_name")) }
```

or:

```
Physics { (e|h)Multivalley(mcDOS) }
File { mcDOS="mcdos_file_name" }
```

To save the Monte Carlo DOS file, use `CreateDOSFile=1` or `CreateDOSFile=2` in the `MonteCarlo` statement of the command file (refer to the *Sentaurus™ Device Monte Carlo User Guide*). The DOS saved in the file can be solely the DOS of the full conduction and valence bands (`CreateDOSFile=1`) or the DOS of separate bands (`CreateDOSFile=2`). For the DOS of separate bands, the multivalley model will search for bands with the same energy minima and will combine such bands into one in the multivalley model (to speed up related numeric density integrations). The saved Monte Carlo DOS file will be named `<MonteCarloOut>.dostot.dat`, where `MonteCarloOut` is an output field of the Monte Carlo simulations in the `File` section of the input file.

> **NOTE** Currently, the `mcDOS` option in the `Multivalley` statement cannot be used with any other option. Therefore, the Monte Carlo DOS (bands) cannot be combined with analytic and $k \cdot p$ bands, and with the multivalley `MLDA` and `ThinLayer` quantization models.

There are two options for the model parameters g_n^i and g_p^i. By default, these parameters are defined by the effective masses from the `(e|h)Valley` statement, and such a definition removes the dependency on N_C and N_V (defined by Effective Masses and Effective Density-of-States on page 261) in Eq. 198 and Eq. 199:

$$g_{n,p}^i = \frac{2.5094 \times 10^{19}}{N_{C,V}} d^i \sqrt{\frac{m_l^i m_t^i m_t^i}{m_0 m_0 m_0}} \left(\frac{T_{n,p}}{300\,\text{K}}\right)^{\frac{3}{2}} \tag{207}$$

Another option is to use `Multivalley(RelativeToDOSMass)`. In this case, the parameters g_n^i and g_p^i define the carrier density relative to the effective DOS N_C and N_V:

$$g_{n,p}^i = \frac{d^i \sqrt{m_l^i m_t^i m_t^i}}{\sum\limits_{k=1}^{N} d^k \sqrt{m_l^k m_t^k m_t^k} \exp\left(\mp\frac{\Delta E_{n,p}^k}{kT}\right)} \tag{208}$$

where ΔE_n^k and ΔE_p^k are the valley energy shifts in reference to the band edge (positive for the conduction band and negative for the valence band).

If all valley energy shifts equal zero, Eq. 208 provides the single-valley condition where, as usual, only the effective DOS and band edge define the semiconductor band structure and carrier concentration.

The valley definition allows you to have mole fraction–dependent valley parameters. The following example shows the definition for two valleys (Δ_2 and L) and with two mole fraction intervals in SiGe material:

```
MultiValley{
    Xmax(0)  = 0.0
    Xmax(1)  = 0.85
    Xmax(2)  = 1.0

    eValley"Delta1"(1,0,0)(ml=0.914 mt=0.196 energy=0 alpha=0.5 degeneracy=2
                         xiu=9.16 xid=0.77)
    eValley"L1"(1,1,1)(ml=1.69 mt=0.13 energy=1.1 alpha=0.5 degeneracy=1
                    xiu=11.5 xid=-6.58)
    eValley"Delta1"(1)(ml=0.914 mt=0.196 energy=0 alpha=0.5 degeneracy=2
                    xiu=9.16 xid=0.77)
    eValley"L1"(1)(ml=1.768 mt=0.0967 energy=0 alpha=0.5 degeneracy=1
                xiu=11.5 xid=-6.58)
    eValley"Delta1"(2)(ml=0.915 mt=0.201 energy=0.19 alpha=0.5 degeneracy=2
                    xiu=9.42 xid=-0.54)
    eValley"L1"(2)(ml=1.768 mt=0.0967 energy=0 alpha=0.5 degeneracy=1
                xiu=11.5 xid=-6.58)
}
```

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CHAPTER 13   Incomplete Ionization

This chapter discusses how incomplete ionization is accounted for in Sentaurus Device.

Overview

In silicon, with the exception of indium, dopants can be considered to be fully ionized at room temperature because the impurity levels are sufficiently shallow. However, when impurity levels are relatively deep compared to the thermal energy kT, incomplete ionization must be considered. This is the case for indium acceptors in silicon and nitrogen donors and aluminum acceptors in silicon carbide. In addition, for simulations at reduced temperatures, incomplete ionization must be considered for all dopants. For these situations, Sentaurus Device has an ionization probability model based on activation energy. The ionization (activation) is computed separately for each species present.

All doping species for Sentaurus Device are defined in the file datexcodes.txt. To add new doping species or to modify an existing specification, see Doping Specification on page 11.

Using Incomplete Ionization

The incomplete ionization model is activated with the keyword IncompleteIonization in the Physics section:

```
Physics{ IncompleteIonization }
```

The incomplete ionization model for selected species is activated with the additional keyword Dopants:

```
Physics{ IncompleteIonization(Dopants = "Species_name1 Species_name2 ...") }
```

For example, the following command line activates the model only for boron:

```
Physics{ IncompleteIonization(Dopants = "BoronActiveConcentration") }
```

The incomplete ionization model can be specified in region or material physics (see Region-Specific and Material-Specific Models on page 18). In this case, the model is activated only in these regions or materials.

Using `DonorPlusConcentration` and `AccepMinusConcentration` in the `Plot` section of the device, you can visualize the ionized donor and acceptor concentrations, respectively.

> **NOTE**   Incomplete ionization is implemented in terms of traps and, therefore, is affected by setting the trap occupation explicitly (see Explicit Trap Occupation on page 468). Use named traps to avoid affecting dopant ionization by settings intended for 'real' traps only.

Multiple Lattice Sites

In certain semiconductors, dopants may occupy different lattice sites, resulting in different activation energies for incomplete ionization. An example is 6H-SiC where nitrogen can occupy either a hexagonal site h, or a cubic site k_1 or k_2.

For the most accurate results, the doping concentration at each lattice site must be modeled by a different doping species. This approach works as follows:

- Introduce new doping species in the `datexcodes.txt` file to describe the doping concentrations in each lattice site (see Doping Specification on page 11). To model the nitrogen doping in 6H-SiC, you may introduce the following species:

  - `Nitrogen_h_Concentration`

  - `Nitrogen_k1_Concentration`

  - `Nitrogen_k2_Concentration`

- Provide a TDR doping file with the concentrations for the new doping species.

- Provide incomplete ionization model parameters for the new doping species (see Physical Model Parameters on page 281).

In many cases, it is sufficient to specify the average occupation probability of the various lattice sites. For example, you may assume that nitrogen doping in 6H-SiC occupies the hexagonal site h and the cubic sites k_1 or k_2 with equal probability.

Sentaurus Device supports this simplification using a `Split` specification in the command file:

```
Physics {
   IncompleteIonization (
      Split (
         Doping = "NitrogenConcentration"
         Weights = (0.3333 0.3333 0.3334)
      )
   )
}
```

NOTE The sum of the weights must be one.

With a `Split` specification, it is no longer necessary to introduce new doping species in the `datexcodes.txt` file. Instead, Sentaurus Device generates the necessary doping species as required and initializes them based on the occupation probabilities. In the example, Sentaurus Device introduces the following doping species automatically:

- `NitrogenConcentration_split1`
- `NitrogenActiveConcentration_split1`
- `NitrogenPlusConcentration_split1`
- `NitrogenConcentration_split2`
- `NitrogenActiveConcentration_split2`
- `NitrogenPlusConcentration_split2`
- `NitrogenConcentration_split3`
- `NitrogenActiveConcentration_split3`
- `NitrogenPlusConcentration_split3`

NOTE The generated doping species also can be used in a device plot (see Device Plots on page 122).

The corresponding parameters can then be specified in the parameter file as described in Physical Model Parameters on page 281:

```
Ionization {
    Species ("NitrogenConcentration_split1") {
        E_0 = 0.1
        alpha = 2.5e-8
        g = 2
        Xsec = 1e-12
    }
    ...
}
```

Incomplete Ionization Model

The concentration of ionized impurity atoms is given by Fermi–Dirac distribution:

$$N_{\mathrm{D}} = \frac{N_{\mathrm{D},0}}{1 + g_{\mathrm{D}}\exp\left(\dfrac{E_{\mathrm{F},n} - E_{\mathrm{D}}}{kT}\right)} \quad \text{for } N_{\mathrm{D},0} < N_{\mathrm{D,crit}} \tag{209}$$

$$N_{\mathrm{A}} = \frac{N_{\mathrm{A},0}}{1 + g_{\mathrm{A}}\exp\!\left(\dfrac{E_{\mathrm{A}} - E_{\mathrm{F},p}}{kT}\right)} \quad \text{for } N_{\mathrm{A},0} < N_{\mathrm{A,crit}} \tag{210}$$

where $N_{\mathrm{D},0}$ and $N_{\mathrm{A},0}$ are the substitutional (active) donor and acceptor concentrations, g_{D} and g_{A} are the degeneracy factors for the impurity levels, and E_{D} and E_{A} are the donor and acceptor ionization (activation) energies.

In the literature [1], incomplete ionization in SiC material has been considered and another general distribution function has been proposed, which can be expressed as:

$$N_{\mathrm{D}} = \frac{N_{\mathrm{D},0}}{1 + G_{\mathrm{D}}(T)\exp\!\left(\dfrac{E_{\mathrm{F},n} - E_{\mathrm{C}}}{kT}\right)} \tag{211}$$

$$N_{\mathrm{A}} = \frac{N_{\mathrm{A},0}}{1 + G_{\mathrm{A}}(T)\exp\!\left(-\dfrac{E_{\mathrm{F},p} - E_{\mathrm{V}}}{kT}\right)} \tag{212}$$

where $G_{\mathrm{D}}(T)$ and $G_{\mathrm{A}}(T)$ are the ionization factors discussed in [2][3]. These factors can be defined by a PMI (see [1] and Example: Matsuura Incomplete Ionization Model on page 1225).

By comparing Eq. 209 and Eq. 210 to Eq. 211 and Eq. 212, it can be seen that, in the case of the Fermi distribution function, the ionization factors can be written as:

$$G_{\mathrm{D}}(T) = g_{\mathrm{D}} \cdot \exp\!\left(\frac{\Delta E_{\mathrm{D}}}{kT}\right) , \ \Delta E_{\mathrm{D}} = E_{\mathrm{C}} - E_{\mathrm{D}} \ \text{ and } \ G_{\mathrm{A}}(T) = g_{\mathrm{A}} \cdot \exp\!\left(\frac{\Delta E_{\mathrm{A}}}{kT}\right) , \ \Delta E_{\mathrm{A}} = E_{\mathrm{A}} - E_{\mathrm{V}} \tag{213}$$

In Sentaurus Device, the basic variables are potential, electron concentration, and hole concentration. Therefore, it is more convenient to rewrite Eq. 209 and Eq. 210 in terms of the carrier concentration instead of the quasi-Fermi levels:

$$N_{\mathrm{D}} = \frac{N_{\mathrm{D},0}}{1 + g_{\mathrm{D}}\dfrac{n}{n_1}} , \ \text{with } n_1 = N_{\mathrm{C}}\exp\!\left(-\frac{\Delta E_{\mathrm{D}}}{kT}\right) \ \text{for } N_{\mathrm{D},0} < N_{\mathrm{D,crit}} \tag{214}$$

$$N_{\mathrm{A}} = \frac{N_{\mathrm{A},0}}{1 + g_{\mathrm{A}}\dfrac{p}{p_1}} , \ \text{with } p_1 = N_{\mathrm{V}}\exp\!\left(-\frac{\Delta E_{\mathrm{A}}}{kT}\right) \ \text{for } N_{\mathrm{A}} < N_{\mathrm{A,crit}} \tag{215}$$

The expressions for n_1 and p_1 in these two equations are valid for Boltzmann statistics and without quantization. If Fermi–Dirac statistics or a quantization model (see Chapter 14 on page 283) is used, n_1 and p_1 are multiplied by the coefficients γ_n and γ_p defined in Eq. 47 and Eq. 48, p. 177 (see Fermi Statistics on page 176). For $N_{\mathrm{D/A}} > N_{\mathrm{D/A, crit}}$, the dopants are assumed to be completely ionized, in which case, every donor and acceptor species is

considered in the Poisson equation. The values of $N_{D,crit}$ and $N_{A,crit}$ can be adjusted in the parameter file of Sentaurus Device.

The donor and acceptor activation energies are effectively reduced by the total doping in the semiconductor. This effect is accounted for in the expressions:

$$\Delta E_D = \Delta E_{D,0} - \alpha_D \cdot N_{tot}^{1/3} \tag{216}$$

$$\Delta E_A = \Delta E_{A,0} - \alpha_A \cdot N_{tot}^{1/3} \tag{217}$$

where $N_{tot} = N_{A,0} + N_{D,0}$ is the total doping concentration. In transient simulations, the terms:

$$\frac{\partial N_D}{\partial t} = \sigma_D v_{th}^n \left[\frac{n_1}{g_D} N_{D,0} - \left(n + \frac{n_1}{g_D} \right) N_D \right] \tag{218}$$

$$\frac{\partial N_A}{\partial t} = \sigma_A v_{th}^p \left[\frac{p_1}{g_A} N_{A,0} - \left(p + \frac{p_1}{g_A} \right) N_A \right] \tag{219}$$

are included in the continuity equations ($v_{th}^{n,p}$ denote the carrier thermal velocities).

Physical Model Parameters

The values of the dopant level $E_{A/D,0}$, the doping-dependent shift parameter $\alpha_{A/D}$, the impurity degeneracy factor $g_{A/D}$, and the cross section $\sigma_{A/D}$ are accessible in the parameter set Ionization.

For each ionized doping species, the Ionization parameter set must contain a separate subsection where the parameters $E_{A/D,0}$, $\alpha_{A/D}$, $g_{A/D}$, and $\sigma_{A/D}$ are defined. For example, for the dopant BoronConcentration, described in Doping Specification on page 11, for the material SiC, the parameter set is:

```
Material = "SiC" {
   ...
   Ionization {
      ...
      Species ("BoronConcentration") {
         type  = acceptor
         E_0   = 0.2
         alpha = 3.1e-8
         g     = 4
         Xsec  = 1.0e-12
      }
```

```
    }
  }
```

The field `type` can be omitted because the dopant type is specified in the `datexcodes.txt` file. It is used here for informative purposes only.

Table 42   Default coefficients for incomplete ionization model for dopants in silicon

Symbol	Parameter name	Default value for species *									Unit
		As	P	Sb	B	Al	In	N	NDopant	PDopant	
$E_{A/D,0}$	E_*_0	0.054	0.045	0.039	0.045	0.045	0.16	0.045	0.045	0.045	eV
$\alpha_{A/D}$	alpha_*	3.1×10^{-8}									eVcm
$g_{A/D}$	g_*	2	2	2	4	4	4	2	2	4	1
$\sigma_{A/D}$	Xsec_*	1.0×10^{-12}									cm^2
$N_{D,crit}$	NdCrit	1.0×10^{22}									cm^{-3}
$N_{A,crit}$	NaCrit	1.0×10^{22}									cm^{-3}

References

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CHAPTER 14 Quantization Models

This chapter describes the features that Sentaurus Device offers to model quantization effects.

Some features of current MOSFETs (oxide thickness, channel width) have reached quantum-mechanical length scales. Therefore, the wave nature of electrons and holes can no longer be neglected. The most basic quantization effects in MOSFETs are the shift of the threshold voltage and the reduction of the gate capacity. Tunneling, another important quantum effect, is described in Chapter 24 on page 715.

Overview

To include quantization effects in a classical device simulation, Sentaurus Device introduces a potential-like quantity Λ_n in the classical density formula:

$$n \;=\; N_C F_{1/2}\!\left(\frac{E_{F,\,n}-E_C-\Lambda_n}{kT_n}\right) \tag{220}$$

An analogous quantity Λ_p is introduced for holes.

The most important effects related to the density modification (due to quantization) can be captured by proper models for Λ_n and Λ_p. Other effects (for example, single electron effects) exceed the scope of this approach.

Sentaurus Device implements five quantization models, that is, five different models for Λ_n and Λ_p. They differ in physical sophistication, numeric expense, and robustness:

- The van Dort model is a numerically robust, fast, and proven model (see van Dort Quantization Model on page 284). It is only suited to bulk MOSFET simulations. While important terminal characteristics are well described by this model, it does not give the correct density distribution in the channel.

- The 1D Schrödinger equation is a physically sophisticated quantization model (see 1D Schrödinger Solver on page 285). It can be used for MOSFET simulation, and quantum well and ultrathin SOI simulation. Simulations with this model tend to be slow and often lead to convergence problems, which restrict its use to situations with small current flow. Therefore, the Schrödinger equation is used mainly for the validation and calibration of other quantization models.

■ For 3D structures, an external 2D Schrödinger solver can be used to provide a quantization model (see External 2D Schrödinger Solver on page 292). This is the physically most sophisticated approach, but requires a high computation time and a complicated setup, and provides reduced numeric robustness.

■ The density gradient model (see Density Gradient Quantization Model on page 294) is numerically robust, but significantly slower than the van Dort model. It can be applied to MOSFETs, quantum wells and SOI structures, and gives a reasonable description of terminal characteristics and charge distribution inside a device. Compared to the other quantization models, it can describe 2D and 3D quantization effects.

■ The modified local-density approximation (MLDA) model (see Modified Local-Density Approximation on page 300) is a numerically robust and fast model. It can be used for bulk MOSFET simulations and thin SOI simulations. Although it sometimes fails to calculate the accurate carrier distribution in the saturation regions because of its one-dimensional characteristic, it is suitable for three-dimensional device simulations because of its numeric efficiency.

■ The quantum-well quantization model (see Quantum-Well Quantization Model on page 309) can be applied to semiconductor quantum wells with a width that does not vary very much over the device. It approximates the solution by the solution for a trapezoidal potential.

van Dort Quantization Model

van Dort Model

The van Dort model [1] computes Λ_n of Eq. 220 as a function of $\left| \hat{n} \cdot \vec{F} \right|$, the electric field normal to the semiconductor–insulator interface:

$$\Lambda_n = \frac{13}{9} \cdot k_{\text{fit}} \cdot G(\vec{r}) \cdot \left(\frac{\varepsilon \varepsilon_0}{4kT} \right)^{1/3} \cdot \left| \left| \hat{n} \cdot \vec{F} \right| - E_{\text{crit}} \right|^{2/3} \tag{221}$$

and likewise for Λ_p. k_{fit} and E_{crit} are fitting parameters.

The function $G(\vec{r})$ is defined by:

$$G(\vec{r}) = \frac{2 \cdot \exp\left(-a^2(\vec{r})\right)}{1 + \exp\left(-2a^2(\vec{r})\right)} \tag{222}$$

where $a(\vec{r}) = l(\vec{r})/\lambda_{\text{ref}}$ and $l(\vec{r})$ is a distance from the point $\vec{r}$ to the interface. The parameter λ_{ref} determines the distance to the interface up to which the quantum correction is relevant. The quantum correction is applied to those carriers (electrons or holes) that are drawn towards the interface by the electric field; for the carriers driven away from the interface, the correction is 0.

Using the van Dort Model

To activate the model for electrons or holes, specify the `eQCvanDort` or `hQCvanDort` flag in the `Physics` section:

```
Physics { ... eQCvanDort}
```

Table 43 lists the parameters in the `vanDortQMModel` parameter set. The default value of λ_{ref} is from the literature [1]. Other parameters were obtained by fitting the model to experimental data for electrons [1] and holes [2].

Table 43   Default parameters for van Dort quantum correction model

Symbol	Electrons		Holes		Unit
k_{fit}	`eFit`	2.4×10^{-8}	`hFit`	1.8×10^{-8}	eV cm
E_{crit}	`eEcritQC`	10^5	`eEcritQC`	10^5	V/cm
λ_{ref}	`dRef`	2.5×10^{-6}	`dRef`	2.5×10^{-6}	cm

By default, in Eq. 221, $\hat{n}$ is the normal to the closest semiconductor–insulator interface. The interface can be specified explicitly by `EnormalInterface` in the `Math` section (see Normal to Interface on page 355).

1D Schrödinger Solver

To use the 1D Schrödinger solver:

1. Construct a special purpose 'nonlocal' mesh (see Nonlocal Mesh for 1D Schrödinger on page 286).

2. Activate the Schrödinger solver on the nonlocal line mesh with appropriate parameters (see Using 1D Schrödinger on page 287).

Sometimes, especially for heteromaterials, the physical model parameters need to be adapted (see 1D Schrödinger Parameters on page 287).

> **NOTE** The 1D Schrödinger solver is time consuming and often causes converge problems. Furthermore, small-signal analysis (see Small-Signal AC Analysis on page 96) and noise and fluctuation analysis (see Chapter 23 on page 675) are not possible when using this solver.

Nonlocal Mesh for 1D Schrödinger

The specification of the nonlocal mesh determines where in the device the 1D Schrödinger equation can be solved. This section summarizes the features that are typically needed to obtain a correct nonlocal mesh for the 1D Schrödinger equation. For more information about constructing nonlocal meshes, see Nonlocal Meshes on page 146.

To generate a nonlocal mesh, specify `NonLocal` in the global `Math` section. Options to `NonLocal` control the construction of the nonlocal mesh. For example:

```
Math {
   NonLocal "NLM" (
      RegionInterface="gateoxide/channel"
      Length=10e-7
      Permeation=1e-7
      Direction=(0 1 0) MaxAngle=5
      -Transparent(Region="gateoxide")
   )
}
```

generates a nonlocal mesh named `"NLM"` at the interface between region `gateoxide` and `channel`. The nonlocal lines extend 10 nm (according to `Length`) to one side of the interface and 1 nm (according to `Permeation`) to the other side. The segments of the nonlocal lines on the two sides are handled differently; see below. In the example, `Direction` and `MaxAngle` restrict the nonlocal mesh to lines that run along the y-axis, with a tolerance of $5°$. `Direction` defines a vector that is typically perpendicular to the interface; therefore, the specification above is appropriate for an interface in the xz plane.

For nonlocal meshes constructed for the Schrödinger equation, the `-Transparent` switch is important. In the above example, it suppresses the construction of nonlocal lines for which the section with length `Length` passes through `gateoxide`. Therefore, Sentaurus Device only constructs nonlocal lines that extend 10 nm into `channel` and 1 nm into `gateoxide`, and suppresses the nonlocal lines that extend 1 nm into `channel` and 10 nm into `gateoxide`. Without the `-Transparent` switch, Sentaurus Device would construct both line types and, therefore, would solve the Schrödinger equation not only in the channel, but also in the poly gate (provided that a poly gate exists and `gateoxide` is thinner than 10 nm).

Using 1D Schrödinger

To activate the 1D Schrödinger equation for electrons or holes, specify the `Electron` or `Hole` switch as an option to `Schroedinger` in the global `Physics` section. For example:

```
Physics {
   Schroedinger "NLM" (Electron)
}
```

activates the Schrödinger equation for electrons on the nonlocal mesh named `"NLM"`.

Additional options to `Schroedinger` determine numeric accuracy, details of the density computation, and which eigenstates will be computed. Table 320 on page 1485 lists the optional keywords.

`MaxSolutions`, `Error`, and `EnergyInterval` support the option `electron` or `hole`. For example, the specification `MaxSolutions=30` sets the value for both electrons and holes. The specifications `MaxSolutions(electron)=2` and `MaxSolutions(hole)=3` set different values for electrons and holes.

By default, Sentaurus Device only computes bound states, that is, states with an energy that is below the largest value of the potential both left and right of the point with minimal potential. If, according to this definition, no bound states exist, the quantum corrections will be disabled. With the `EnergyInterval` parameter, this behavior can be changed to compute all states with an energy up to the specified value above the lowest potential point.

For backward compatibility, you can define `Schroedinger` in an interface-specific or a contact-specific `Physics` section; in this case, omit the nonlocal mesh name. The specification applies to an unnamed nonlocal mesh that has been constructed for the same location (see Unnamed Meshes on page 152).

1D Schrödinger Parameters

Typically, the Schrödinger equation must be solved repeatedly, with different masses and potential profiles, resulting in a number of distinct 'ladders' of eigenenergies. For example, the six-fold degenerate, anisotropic conduction band valleys in silicon require the Schrödinger equation to be solved up to three times with different parameters. Sentaurus Device allows you to specify the number of ladders and the associated parameters explicitly, or it can extract the number of ladders and the parameters from other parameters and the nonlocal line direction automatically.

Parameters for the Schrödinger equation are region specific. The Schrödinger equation must not be solved across regions with fundamentally different band structures. Sentaurus Device displays an error message if band structure compatibility is violated.

Explicit Ladder Specification

Any number of `eLadder(` $m_{z,\nu}$, $m_{xy,\nu}$, d_ν , ΔE_ν `)` (for electrons) or `hLadder(` $m_{z,\nu}$, $m_{xy,\nu}$, d_ν , ΔE_ν `)` (for holes) specifications is possible in the `SchroedingerParameters` parameter set. The ν-th specification for a particular carrier type defines the quantization mass $m_{z,\nu}$, the mass perpendicular to the quantization direction $m_{xy,\nu}$, the ladder degeneracy d_ν , and a nonnegative band edge shift ΔE_ν .

The parameter pair `ShiftTemperature` in the `SchroedingerParameters` parameter set is given in kelvin and determines the temperatures T_{ref} for electrons and holes that enter scaling factors applied to $m_{xy,\nu}$. The scaling factors ensure that the masses for the Schrödinger equation are consistent with the density-of-states masses. For electrons, the scaling factor is:

$$\frac{m_n^{3/2}}{\sum_\nu d_\nu m_{xy,\nu} m_{z,\nu}^{1/2} \exp(-\Delta E_\nu / k T_{ref})} \tag{223}$$

and likewise for holes. T_{ref} defaults to a large value. When $T_{ref} = 0$, scaling is disabled.

Automatic Extraction of Ladder Parameters

When no explicit ladder specification is present, Sentaurus Device attempts to extract the required parameters automatically. The `formula` parameter pair in the `SchroedingerParameters` parameter set specifies which expressions for the masses to use. If an explicit ladder specification is present, `formula` for the respective carrier type is ignored, and only the explicit ladder specification is accounted for.

For each carrier, if the formula is 0, Sentaurus Device uses the isotropic density-of-states mass as both the quantization mass and the mass perpendicular to it.

For electrons, if the formula is 1, Sentaurus Device uses the anisotropic (silicon-like) masses specified in the `eDOSMass` parameter set. The quantization mass for the conduction band valley ν reads:

$$\frac{1}{m_{z,\nu}} = \sum_{i=1}^{3} \frac{z_i^2}{m_{i,\nu}} \tag{224}$$

where $m_{i,\nu}$ are the effective mass components for valley ν , and z_i are the coefficients of the unit normal vector pointing in the quantization direction, expressed in the crystal coordinate

system. The `LatticeParameters` parameter set determines the relation to the mesh coordinate system (see Crystal and Simulation Coordinate Systems on page 781).

For holes, 'warped' band structure (formula 1), or heavy-hole and light-hole masses (formula 2) are available (see Table 44). For the former, the quantization mass is given by:

$$m_{z,\nu} = \frac{m_0}{A \pm \sqrt{B + C \cdot \left(z_1^2 z_2^2 + z_2^2 z_3^2 + z_3^2 z_1^2 \right)}} \tag{225}$$

For the latter, `ml` and `mh` (given as multiples of m_0) determine directly the masses for the light-hole and heavy-hole bands.

The masses $m_{xy,\nu}$ are chosen to achieve the same density-of-states mass as used in classical simulations. For electrons:

$$m_{xy,\nu} = \frac{m_n^{3/2}}{m_{z,\nu}^{1/2} n_\nu} \tag{226}$$

where n_ν is the number of band valleys (or bands). The expression for holes is analogous.

`SchroedingerParameters` offers a parameter pair `offset` to model the lifting of the degeneracy of band minima in strained materials. Unless exactly two ladders exist, `offset` must be zero. Positive offsets apply to the electron ladder with lower degeneracy or the heavy-hole band; negative values apply to the electron ladder of higher degeneracy or the light-hole band. The modulus of the value is added to the band edge for the respective ladder, moving it away from mid-gap, while the other ladder remains unaffected. For holes, the shift is taken into account in the scaling of $m_{xy,\nu}$ as it is in Eq. 223.

Table 44   Parameters for hole effective masses in Schrödinger solver

Formula	Symbol	Parameter name	Default value	Unit
1	A	A	4.22	1
	B	B	0.6084	1
	C	C	23.058	1
2	m_1	ml	0	1
	m_h	mh	0	1

Visualizing Schrödinger Solutions

To visualize the results obtained by the Schrödinger equation, Sentaurus Device offers special keywords for the `NonLocalPlot` section (see Visualizing Data Defined on Nonlocal Meshes on page 148).

To plot the wavefunctions, specify `WaveFunction` in the `NonLocalPlot` section. Sentaurus Device plots wavefunctions in units of $\mu m^{-1/2}$. To plot the eigenenergies, specify `EigenEnergy`; Sentaurus Device plots them in units of eV. The names of the curves in the output have two numeric indices. The first index denotes the ladder index and the second index denotes the number of zeros of the wavefunction (see ν and j in Eq. 227).

Without further specification, Sentaurus Device will plot all eigenenergies and wavefunctions it has computed. The `Electron` and `Hole` options to `WaveFunction` and `EigenEnergy` restrict the output to the wavefunctions and eigenenergies for electrons and holes, respectively.

The `Electron` and `Hole` options have a sub-option `Number=<int>` to restrict the output to a certain number of states of lowest energy. For example:

```
NonLocalPlot(
   (0 0)
){
   WaveFunction(Electron(Number=3) Hole)
}
```

will plot all hole wavefunctions and the three lowest-energy electron wavefunctions for the nonlocal mesh line close to the coordinate (0, 0, 0).

To plot the overlap integrals between all pairs of the computed wavefunctions on a nonlocal line, specify `OverlapIntegral` in the `NonLocalPlot` section.

1D Schrödinger Model

Omitting x- and y-coordinates for simplicity, the 1D Schrödinger equation for electrons is:

$$\left(-\frac{\partial}{\partial z}\frac{\hbar^2}{2m_{z,\nu}(z)}\frac{\partial}{\partial z} + E_C(z) + \Delta E_\nu\right)\Psi_{j,\nu}(z) = E_{j,\nu}\Psi_{j,\nu}(z) \tag{227}$$

where z is the quantization direction (typically, the direction perpendicular to the silicon–oxide interface in a MOSFET), ν labels the ladder, ΔE_ν is the (region-dependent) energy offset for the ladder ν, $m_{z,\nu}$ is the effective mass component in the quantization direction, $\Psi_{j,\nu}$ is the j-th normalized eigenfunction, and $E_{j,\nu}$ is the j-th eigenenergy.

From the solution of this equation, the density is computed as:

$$n(z) = \frac{kT(z)}{\pi\hbar^2}\sum_{j,\nu}|\Psi_{j,\nu}(z)|^2 d_\nu m_{xy,\nu}(z)\left[F_0\left(\frac{E_{F,n}(z)-E_{j,\nu}}{kT(z)}\right) - F_0\left(\frac{E_{F,n}(z)-E_{\max,\nu}}{kT(z)}\right)\right] + \sum_\nu n_{cl,\nu} \qquad (228)$$

where $m_{xy,\nu}$ is the mass component perpendicular to the quantization direction and d_ν is the degeneracy for ladder ν. For the parameters $m_{z,\nu}$, $m_{xy,\nu}$, d_ν, and ΔE_ν, see 1D Schrödinger Parameters on page 287.

If `DensityTail=MaxEnergy`, $E_{\max,\nu}$ in Eq. 228 is the energy of the highest computed subband for ladder ν; otherwise, it is an estimate of the energy of the lowest not computed subband. $n_{cl,\nu}$ is the contribution to the classical density for ladder ν by energies above $E_{\max,\nu}$.

At the ends of the nonlocal line, Sentaurus Device optionally smoothly blends from the classical density to the density according to Eq. 228. Equating the resulting density to Eq. 220 determines Λ_n.

The Schrödinger equation is solved over a finite domain $[z_-,z_+]$. At the endpoints of this domain, the boundary condition:

$$\frac{\Psi'_{j,\nu}}{\Psi_{j,\nu}} = \mp\frac{\sqrt{2m_{z,\nu}|E_{j,\nu}-E_C|}}{\hbar} \qquad (229)$$

is applied, where for the upper sign, all position-dependent functions are taken at z_+ and, for the lower sign, at z_-.

1D Schrödinger Application Notes

Note that:

- Convergence problems: Near the flatband condition, minor changes in the band structure can change the number of bound states between zero and one. By default, Sentaurus Device computes only bound states and, therefore, this change switches from a purely classical solution to a solution with quantization. To avoid the large change in density that this transition can cause, set `EnergyInterval` to a nonzero value (for example, 1). Then, a few unbound states are computed and a hard transition is avoided.

- The Schrödinger solver uses an iterative method. If this iterative method fails to converge, the solution of the coupled system of all equations will not be accepted, even if the RHS and the error as reported in the log file are small.

- Always include a part of the 'barrier' in the nonlocal line on which the Schrödinger equation is solved. In a MOSFET, besides the channel region, solve the Schrödinger equation in a part of the oxide adjacent to the channel (for example, 1 nm deep). Use the

`Permeation` option to `NonLocal` to achieve this (see Nonlocal Mesh for 1D Schrödinger on page 286). Failure to solve in a part of the oxide adjacent to the channel blinds the Schrödinger solver to the barrier. It does not know the electrons are confined and the quantization effects are not obtained.

External 2D Schrödinger Solver

For 3D structures, Sentaurus Device can connect to external 2D Schrödinger solvers to compute the quantum-mechanical density correction. Sentaurus Device interpolates solution-dependent data, such as band edges, quasi-Fermi potentials, and temperature, to 2D cross sections of the device, and passes it to the 2D Schrödinger solvers. From this information and their own configuration, the 2D Schrödinger solvers compute quantum-mechanical densities and pass them back to Sentaurus Device. Using these densities and Eq. 220, p. 283, Sentaurus Device computes the quantum potentials Λ_n and Λ_p. Then, the quantum potentials are interpolated to the 3D device mesh and are used in subsequent calculations.

The connection to the external 2D Schrödinger solver is defined in the global `Physics` section:

```
ExternalSchroedinger <string> (
   NumberOfSlices=<int>       * required parameter, at least two
   Carriers = <carrierlist>   * required parameter
   Volume=<string>            * optional
   SBandCommandFile=<string>  * optional
   DampingLength=<float>      * in um, default 0.005
   MaxMismatch=<float>        * in um, default 1e-4
)
```

The string after `ExternalSchroedinger` is a name used to establish the connection to the 2D Schrödinger solver processes. Two Sentaurus Device processes running concurrently on the same computer, in the same working directory, must not use the same value for this name.

`NumberOfSlices` is the number of 2D slices (cross sections) of the 3D mesh on which to solve the 2D Schrödinger equation. The slices themselves are provided to Sentaurus Device by the 2D Schrödinger solver processes. They must correspond to cuts of the 3D mesh Sentaurus Device is using, that is, at the same point, the 3D mesh and the 2D slices must have the same region. Sentaurus Device checks this condition, with a tolerance that can be changed with the `MaxMismatch` parameter.

To allow users to perform 3D simulations of a symmetric structure with a reduced mesh, the interface to the external 2D Schrödinger solver takes the `ThinLayer(Mirror)` specification into account (see Geometric Parameters of LayerThickness Command on page 312). Note, however, that the 2D Schrödinger solver still needs the full 2D slices.

Slices are numbered from zero to `NumberOfSlices-1`. This number is used to refer to slices individually, for example, in error messages. The number also is used by the 2D Schrödinger solvers to identify a particular slice.

The carrier types to which you apply a quantum correction are specified by `Carriers`. Possible values are `(Electron)`, `(Hole)`, and `(Electron Hole)` to apply the correction to electrons only, holes only, or both, respectively.

The quantum correction is only applied to semiconductors. If specified, the application is further restricted to the named volume given by `Volume` (for named volumes, see Random Band Edge Fluctuations on page 688). Within that domain, the quantum correction from the 2D slices is interpolated to the volume enclosed by the slices. With increasing distance from the enclosed volume, the quantum correction is damped. For vertices farther outside the enclosed volume than the distance specified with `DampingLength`, the 2D Schrödinger quantum corrections Λ_n and Λ_p are zero.

> **NOTE** For typical MOSFET applications, the 2D Schrödinger solver is used mostly to account for the quantization in the active channel area. However, the source and drain regions can use other simpler quantum-correction models such as density gradient (see Density Gradient Quantization Model on page 294) or MLDA (see Modified Local-Density Approximation on page 300). For such a combination, the parameter `DampingLength` is also used in the density gradient or MLDA quantum corrections (Λ_{nO} and Λ_{pO}) to have a smooth transition between these corrections. The parameter defines a position-dependent damping α_{SE} (which is equal to 1 inside the 2D Schrödinger domain and goes to 0 at `DampingLength` distance from that domain), and the combined quantum corrections are computed as $\alpha_{SE}\Lambda_n + (1 - \alpha_{SE})\Lambda_{nO}$ and $\alpha_{SE}\Lambda_p + (1 - \alpha_{SE})\Lambda_{pO}$.

If `SBandCommandFile` is used to provide the name of a command file for Sentaurus Band Structure, Sentaurus Device automatically starts Sentaurus Band Structure processes with this command file. Sentaurus Device passes to each process the number of the slice it handles on the command line.

Otherwise, users are responsible for starting the 2D Schrödinger solver processes, which must be started in the same working directory on the same computer as the Sentaurus Device process that connects to them.

See Sentaurus™ Device Monte Carlo User Guide, Using Sentaurus Band Structure as an External Schrödinger Solver for Sentaurus Device on page 213 for details about the 2D Schrödinger solver.

Application Notes

One crucial step in using the interface to external 2D Schrödinger solvers is to decide the number and the placement of the slices. Usually, the quantum corrections are applied to the channel of a device. The slices at least must resolve the shape of the cross section of the channel.

Using the quantum potentials Λ_n and Λ_p as the quantities that are interpolated between slices, interpolation becomes insensitive to potential and quasi-Fermi potential drops along the channel. Therefore, for devices with a uniform channel cross section, one slice close to either end of the channel should be sufficient to obtain sufficient accuracy.

> **NOTE** The placement of the slices is not specified in Sentaurus Device. The only information specified in the Sentaurus Device command file about the slices it their number. The placement of the slices is the responsibility of the external 2D Schrödinger solvers. Therefore, their configuration must be consistent with the 3D mesh used by Sentaurus Device.

Similarly, the exact model for quantization, as well as band structure information beyond the band edges, is not specified by Sentaurus Device, but by the configuration of the 2D Schrödinger solvers.

Density Gradient Quantization Model

Density Gradient Model

For the density gradient model [3][4], Λ_n in Eq. 220 is given by a partial differential equation:

$$\Lambda_n = -\frac{\gamma \hbar^2}{12 m_n}\left\{ \nabla^2 \ln n + \frac{1}{2}(\nabla \ln n)^2 \right\} = -\frac{\gamma \hbar^2}{6 m_n}\frac{\nabla^2 \sqrt{n}}{\sqrt{n}} \tag{230}$$

where $\gamma = \gamma_0 \cdot \gamma_{\mathrm{pmi}}$ is a fit factor. The γ_0 is solution independent. It is dependent on the mole fraction and the distance to the nearest insulating surface (option `AutoOrientation`). The additional factor γ_{pmi} (solution dependent) can be defined by a PMI (see Gamma Factor for Density Gradient Model on page 1283).

Introducing the reciprocal thermal energy $\beta = 1/kT_n$, the mass-driving term $\Phi_m = -kT_n \ln(N_C/N_{\text{ref}})$ (with an arbitrary normalization constant N_{ref}) and the potential-like quantity $\overline{\Phi} = E_C + \Phi_m + \Lambda_n$, Eq. 230 can be rewritten and generalized as:

$$\Lambda_n = -\frac{\hbar^2 \gamma}{12 m_n} \{ \nabla \cdot \alpha(\xi \nabla \beta E_{F,n} - \nabla \beta \overline{\Phi} + (\eta - 1)q\nabla \beta \phi)$$

$$+ \vartheta(\xi \nabla \beta E_{F,n} - \nabla \beta \overline{\Phi} + (\eta - 1)q\nabla \beta \phi) \cdot \alpha(\xi \nabla \beta E_{F,n} - \nabla \beta \overline{\Phi} + (\eta - 1)q\nabla \beta \phi) \} + \Lambda_{\text{PMI}} \tag{231}$$

with the default parameters $\xi = \eta = 1$, $\vartheta = 1/2$, and α is a symmetric matrix that defaults to one. In insulators, Sentaurus Device does not compute the Fermi energy; therefore, in insulators, $\xi = \eta = 0$. By default, Sentaurus Device uses Eq. 231, which for Fermi statistics deviates from Eq. 230, even when $\xi = \eta = 1$ and $\vartheta = 1/2$. The density-based expression Eq. 230 is available as an option (see Using the Density Gradient Model on page 296).

In Eq. 231, Λ_{PMI} is a locally dependent quantity computed from a user-specified PMI model (see Apparent Band-Edge Shift on page 1144), from the Schenk bandgap narrowing model (see Schenk Bandgap Narrowing Model on page 255), or from apparent band-edge shifts caused by multistate configurations (see Apparent Band-Edge Shift on page 483). By default, $\Lambda_{\text{PMI}} = 0$.

At Ohmic contacts, interfaces to metals with Ohmic boundary conditions, resistive contacts, and current contacts, the boundary condition $\Lambda_n = \Lambda_{\text{PMI}}$ is imposed. At Schottky contacts, gate contacts, interfaces to metals with Schottky boundary conditions, and external boundaries, homogeneous Neumann boundary conditions are used:
$\hat{n} \cdot \alpha(\xi \nabla \beta E_{F,n} - \nabla \beta \overline{\Phi} + (\eta - 1)q\nabla \beta \phi) = 0$.

At internal interfaces between regions where the density gradient equation is solved, $\overline{\Phi}$ and $\hat{n} \cdot \alpha(\xi \nabla \beta E_{F,n} - \nabla \beta \overline{\Phi} + (\eta - 1)q\nabla \beta \phi)$ must be continuous.

At internal interfaces between a region where the equation is solved (indicated below by 0^-) and a non-metal region where it is not solved (0^+), an inhomogeneous Neumann boundary condition obtained from the analytic solution of the 1D step problem is applied:

$$\hat{n} \cdot \nabla \Lambda_n = \sqrt{\frac{24 m_n(0^+)\overline{\alpha}k^3 T_n^3}{\hbar^2 \gamma(0^+)}[E_C(0^+) - E_C(0^-) - \Lambda_n]} f\left(\frac{2\vartheta(0^+)}{kT_n}[\Lambda_n - E_C(0^+) + E_C(0^-)] \right) \tag{232}$$

where $f(x) = \sqrt{[(\exp x - 1)/x - 1]/x}$ and $\overline{\alpha} = \det[\alpha(0^+)]^{1/3}$.

Optionally, Sentaurus Device offers a modified mobility to improve the modeling of tunneling through semiconductor barriers:

$$\mu = \frac{\mu_{\text{cl}} + r\mu_{\text{tunnel}}}{1 + r} \tag{233}$$

where μ_{cl} is the usual (classical) mobility as described in Chapter 15 on page 317, μ_{tunnel} is a fit parameter, and $r = \max(0, n/n_{cl} - 1)$. Here, n_{cl} is the 'classical' density (see Eq. 404). In this modification, for $n > n_{cl}$, the additional carriers (density $n - n_{cl}$) are considered as tunneling carriers that are subject to a different mobility μ_{tunnel} than the classical carriers (density n_{cl}).

Using the Density Gradient Model

The density gradient equation for electrons and holes is activated by the `eQuantumPotential` and `hQuantumPotential` switches in the `Physics` section. Use `-eQuantumPotential` and `-hQuantumPotential` to switch off the equations. These switches can also be used in regionwise or materialwise `Physics` sections. In metal regions, the equations are never solved. For a summary of available options, see Table 294 on page 1470.

The `Ignore` switch to `eQuantumPotential` and `hQuantumPotential` instructs Sentaurus Device to compute the quantum potential, but not to use it. `Ignore` is intended for backward compatibility to earlier versions of Sentaurus Device.

The `Resolve` switch enables a numeric approach that handles discontinuous band structures, at moderately refined interfaces that are not heterointerfaces, more accurately than the default approach.

The switch `Density` to `eQuantumPotential` and `hQuantumPotential` activates the density-based formula Eq. 230 instead of the potential-based formula Eq. 231. If this option is used, the parameters ξ and η must both be 1.

The `LocalModel` option of `eQuantumPotential` and `hQuantumPotential` specifies the name of a PMI model (see Physical Model Interface on page 1043) or the Schenk bandgap narrowing model (see Schenk Bandgap Narrowing Model on page 255) for Λ_{PMI} in Eq. 231. An additional apparent band-edge shift contribution can be added if the corresponding model of a multistate configuration is switched on (see Apparent Band-Edge Shift on page 483).

The `BoundaryCondition` option of the `eQuantumPotential` and `hQuantumPotential` specifications in metal interface-specific or electrode-specific `Physics` sections allows you to explicitly specify the boundary condition for the quantum potential, overriding the default boundary condition. Possible values are `Dirichlet` and `Neumann`, to enforce homogeneous Dirichlet and Neumann boundary conditions, respectively.

Apart from activating the equations in the `Physics` section, the equations for the quantum corrections must be solved by using `eQuantumPotential` or `hQuantumPotential`, or both in the `Solve` section. For example:

```
Physics {
   eQuantumPotential
}
Plot {
   eQuantumPotential
}
Solve {
   Coupled { Poisson eQuantumPotential }
   Quasistationary (
      DoZero InitialStep=0.01 MaxStep=0.1 MinStep=1e-5
      Goal { Name="gate" Voltage=2 }
   ){
      Coupled { Poisson Electron eQuantumPotential }
   }
}
```

The quantum corrections can be plotted. To this end, use `eQuantumPotential`, or `hQuantumPotential`, or both in the `Plot` section.

To activate the mobility modification according to Eq. 233, specify the `Tunneling` switch to `Mobility` in the `Physics` section of the command file. Specify μ_{tunnel} for electrons and holes by the `mutunnel` parameter pair in the `ConstantMobility` parameter set.

The parameters γ, ϑ, ξ, and η are available in the `QuantumPotentialParameters` parameter set. The parameters can be specified regionwise and materialwise. They cannot be functions of the mole fraction in heterodevices. In insulators, ξ is always assumed as zero, regardless of user specifications.

The diagonal of α in the crystal coordinate system (see Crystal and Simulation Coordinate Systems on page 781) is determined by the parameter pairs `alpha[1]`, `alpha[2]`, and `alpha[3]` (for the x-direction, y-direction, and z-direction, respectively) in the `QuantumPotentialParameters` parameter set. Unless α is a multiple of the unit matrix, Sentaurus Device solves an anisotropic problem. For example:

```
QuantumPotentialParameters {
   alpha[1] = 1    1
   alpha[2] = 0.5  0.5
}
```

decreases the quantization effect along the y-direction to half, for both electrons and holes.

The anisotropic density-gradient equation supports the `AverageAniso` approximation (see Chapter 28 on page 779) and the tensor grid approximation (see Tensor Grid Option on

). For the latter, `TensorGridAniso` must be selected as the numeric method in the `Math` section, and either `eQuantumPotential` or `hQuantumPotential` must be specified as an option of `Aniso` in the `Physics` section, for example:

```
Physics { Aniso (eQuantumPotential) }
Math { TensorGridAniso(Aniso) }
```

Named Parameter Sets for Density Gradient

The `QuantumPotentialParameters` parameter set can be named. For example, in the parameter file, you can write:

```
QuantumPotentialParameters "myset" { ... }
```

to declare a parameter set with the name `myset`. To use a named parameter set, specify its name with `ParameterSetName` as an option to either `eQuantumPotential` or `hQuantumPotential` in the command file, for example:

```
Physics {
   eQuantumPotential (ParameterSetName = "myset")
}
```

By default, the unnamed parameter set is used.

Auto-Orientation for Density Gradient

The `eQuantumPotential` and `hQuantumPotential` models support the auto-orientation framework (see Auto-Orientation Framework on page 37) that switches between different named parameter sets based on the orientation of the nearest interface. This can be activated by specifying `AutoOrientation` as an argument to either `eQuantumPotential` or `hQuantumPotential` in the command file:

```
Physics {
   eQuantumPotential (AutoOrientation)
}
```

Density Gradient Application Notes

Note that:

- Fitting parameters: The parameter γ has been calibrated only for silicon. The quantum correction affects the densities and field distribution in a device. Therefore, parameters for mobility and recombination models that have been calibrated to classical simulations (or simulations with the van Dort model) may require recalibration.

- Evaluation box: You can improve convergence by solving the density gradient equations only within regions that are adequately meshed for that task. For example, in FinFETs, it is understood that, for a fin situated on a large substrate, given the oppressive cost of meshing the surface of the substrate to density gradient standards, it is beneficial to solve the equations only in the fin.

  This works well if the fin can be specified as a unique region that coincides with the domain over which the quantum potential is useful. However, in structures formed by Sentaurus Process, such precise registration of regions may not be possible.

  An alternate approach is to reduce the quantum potential in parts of a region that are not of interest. In this approach, the parameter γ effectively attenuates the quantum potential outside the 'Box' where the solution of quantum potential may cause convergence issues. The corresponding command file can be written as:

  ```
  Math {
   eQPBox({MinX=0.042 MaxX=0.045 MinY=0.008 MaxY=0.015 Attenuation_Length=1e-3}
          {MinX=0.022 MaxX=0.027 MinY=0.002 MaxY=0.004 Attenuation_Length=2e-3}
   )
   hQPBox({MinX=0.042 MaxX=0.045 MinY=0.008 MaxY=0.015 Attenuation_Length=2e-3}
          {MinX=0.022 MaxX=0.027 MinY=0.002 MaxY=0.004 Attenuation_Length=4e-3}
   )
  }
  ```

  The parameter γ is effectively attenuated using an error function for each of the six specified domain boundaries. `Attenuation_Length` determines the decay of the transition, where 0 is abrupt, and the default value is 1e-3 μm.

- Tunneling: The density gradient model increases the current through the semiconducting potential barriers. However, this effect is not a trustworthy description of tunneling through the barrier. To model tunneling, use one of the dedicated models that Sentaurus Device provides (see Chapter 24 on page 715). To suppress unwanted tunneling or to fit tunneling currents despite these concerns, consider using the modified mobility model according to Eq. 233.

- Convergence: In general and particularly for the density gradient corrections, solving additional equations worsens convergence. Typically, it is advisable to solve the equations for the quantum potentials whenever the Poisson equation is solved (using a `Coupled` statement). Usually, the best strategy to obtain an initial solution at the beginning of the simulation is to do a coupled solve of the Poisson equation and the quantum potentials, without the current and temperature equations.

  To obtain this initial solution, it is sometimes necessary that you set the `LineSearchDamping` optional parameter (see Damped Newton Iterations on page 139) to a value less than 1; a good value is 0.01.

  Often, using initial bias conditions that induce a current flow work well for a classical simulation, but do not work when the density gradient model is active. In such cases, start

from equilibrium bias conditions and put an additional voltage ramping at the beginning of the simulation.

If an initial solution is still not possible, consider using Fermi statistics (see Fermi Statistics on page 176). Check grid refinement and pay special attention to interfaces between insulators and highly doped semiconductor regions. For classical simulations, the refinement perpendicular to such interfaces is often not critical, whereas for quantum mechanical simulations, quantization introduces variations at small length scales, which must be resolved.

- Avalanche: The combination of using the density gradient model with an avalanche model can sometimes degrade convergence. An option is available in the `Math` section that can often result in better convergence in this situation:

  `Math {RefDens_QuantumPotential=<`n_0`>}`

  where n_0 is the carrier concentration below which the effects of quantum corrections are reduced.

- Speed: Activate the equations only for regions where the quantum corrections are physically needed. For example, usually, the density gradient equations do not need to be computed in insulators. Using the model selectively, typically, also benefits convergence.

- By default, the DOS mass used in the expressions of the density gradient method ignores the effects of strain (see Strained Effective Masses and Density-of-States on page 830). This is accomplished by using the expression $m_n = m_{n0} + \nu \cdot \Delta m_n$ with a default value of $\nu = 0$, where m_{n0} is the unstrained mass and Δm_n is the change in mass due to strain. The parameter ν can be specified in the `QuantumPotentialParameters` parameter set.

Modified Local-Density Approximation

MLDA Model

The modified local-density approximation (MLDA) model is a quantum-mechanical model that calculates the confined carrier distributions that occur near semiconductor–insulator interfaces [5]. It can be applied to both inversion and accumulation, and simultaneously to electrons and holes. It is based on a rigorous extension of the local-density approximation and provides a good compromise between accuracy and runtime.

Following Paasch and Übensee [5], the confined electron density at a distance z from a Si–SiO$_2$ interface is given, under Fermi statistics, by:

$$n_{\mathrm{MLDA}}(\eta_n) = N_{\mathrm{C}}\left(\frac{2}{\sqrt{\pi}}\right)\int_0^\infty d\varepsilon \frac{\sqrt{\varepsilon}}{1 + \exp[(\varepsilon - \eta_n)]}[1 - j_0(2z\sqrt{\varepsilon}/\lambda_n)] \tag{234}$$

where η_n is given by Eq. 49, p. 177, j_0 is the 0th-order spherical Bessel function, and $\lambda_n = \sqrt{\hbar^2 / 2 m_{qn} k T_n}$ is the electron thermal wavelength which depends on the quantization mass m_{qn}. The integrand of Eq. 234 is very similar to the classical Fermi integrand, with an additional factor describing confinement for small z. A similar equation is applied to holes.

Sentaurus Device provides two MLDA model options:

- One option is the simple original model that uses only one user-defined parameter λ per carrier type.

- The second option (considered in detail in the next section) accounts for the multivalley/band property of the electron and hole band structures.

For the simple model, in Boltzmann statistics, Eq. 234 simplifies to the following expression for the electron density (the hole density is similar):

$$n_{\text{MLDA}}(\eta_n) = N_C \exp(\eta_n)[1 - \exp(-(z/\lambda_n)^2)] \tag{235}$$

Interface Orientation and Stress Dependencies

The MLDA model allows you to consider a dependency of the quantization effect on interface orientation and stress. Mainly, such dependencies come from mass anisotropy and stress related valley/band energy change.

Mass anisotropy has been considered in the literature [6] where ellipsoidal type of bands, which correspond to three electron Δ_2-valleys in silicon, were used. The main result of the article is that Eq. 234 is still valid for each of three electron Δ_2-valleys with the effective DOS equal to $N_C/3$. Another result is that the quantization mass of each valley m_{qn}^i should be computed as a rotation of the inverse mass tensor from the crystal system (where the tensor is diagonal) to another one where one axis is perpendicular to the interface and the mass component, which corresponds to the axis, should be taken as m_{qn}^i. Considering three electron Δ_2-valleys, Eq. 234 could be rewritten as follows:

$$n_{\text{MLDA}}(\eta_n, z) = \sum_{i=1}^{3} \int_0^\infty \frac{D_n^i(\varepsilon, z)}{1 + \exp(\varepsilon - \eta_n - \Delta\eta^i)} d\varepsilon$$

$$D_n^i(\varepsilon, z) = N_C g_n^i \left(\frac{2}{\sqrt{\pi}}\right) \sqrt{\varepsilon} \left[1 - j_0\left(2z\sqrt{\frac{2m_{qn}^i k T_n \varepsilon}{\hbar^2}}\right)\right] \tag{236}$$

where:

- $D_n^i(\varepsilon, z)$ is the electron DOS of valley i with a dependency on the normalized energy ε and on the distance to the interface z.

- g_n^i is defined by Eq. 207, p. 274 or Eq. 208, p. 274; however, in the case of stress, $N_C g_n^i$ is defined by Eq. 956, p. 832.

■ $\Delta\eta^i$ represents the stress-induced valley energy change (see Deformation of Band Structure on page 826).

Similar to Eq. 236, the same multivalley MLDA quantization model could be applied to holes with hole bands defined in the `MultiValley` section of the parameter file described in Multivalley Band Structure on page 267, but such spherical or ellipsoidal hole bands do not produce a correct dependency of the hole quantization on the interface orientation. Therefore, for holes, the six-band $k \cdot p$ band structure is used. The bulk six-band $k \cdot p$ model is described in [14][15] of Chapter 31 on page 821. An extension of the MLDA model is formulated for arbitrary bands and applied to the six-band $k \cdot p$ band structure [7].

The DOS of one hole band is written generally as follows:

$$D^i(\varepsilon, z) \;=\; \frac{2}{(2\pi)^3}\oint \frac{dS}{\left|\nabla_k \varepsilon^i(\vec{k})\right|}\left[1 - \exp\left(i2z\gamma_{\mathrm{kp}}\sum_j k_j \frac{w_{j3}(\vec{k})}{w_{33}(\vec{k})}\right)\right] \tag{237}$$

where:

■ $\varepsilon^i(\vec{k})$ is a hole band dispersion of the bulk six-band $k \cdot p$ model (the model considers three bands: heavy holes, light holes, and the spin-orbit split-off band holes).

■ The surface integral is in k-space over isoenergy surface S defined by $\varepsilon^i(\vec{k}) \;=\; \varepsilon$.

■ w_{ij} are components of the reciprocal mass tensor computed locally on the isoenergy surface.

■ γ_{kp} is a fitting parameter that accounts for the nonparabolicity of hole bands in the MLDA model.

The hole density near the interface is computed similarly to the electron one in Eq. 236, but with the DOS from Eq. 237. The interface orientation and stress dependencies of the hole quantization are defined naturally by the physical property of the six-band $k \cdot p$ model.

Heterojunctions

Originally, the MLDA quantization model was developed to describe the carrier density at semiconductor–insulator interfaces where a zero density (wavefunction) assumption on the interface is a reasonable approximation due to a typically high-band offset between the semiconductor and insulator. Such an assumption is mostly incorrect if the model is applied to heterojunctions where the band offset between two semiconductors is small. To apply the MLDA model to heterojunctions [8], you can use a wave penetration length in the model:

$$z_0 \;=\; \frac{\hbar}{\sqrt{2m\Delta\varepsilon}} \tag{238}$$

where m is the carrier (electron or hole) effective mass of the low-bandgap semiconductor, and $\Delta\varepsilon$ is the band offset between two semiconductors (in the conduction or valence band). According to [8], the penetration length z_0 is simply added to the interface distance z in Eq. 234–Eq. 237.

Nonparabolic Bands and Geometric Quantization

Other effects that can play an important role, for example, in III–V semiconductors are the band nonparabolicity and geometric quantization in thin-layer structures. For the bulk case, the carrier density computation with the nonparabolic bands is described in Nonparabolic Band Structure on page 268.

To account for this effect and 1D geometric quantization (between two parallel interfaces that confine the carriers) in the MLDA model, the DOS in Eq. 236 must be replaced with the following [9]:

$$D_n^i(\varepsilon, z) \ = \ N_C g_n^i\left(\frac{2}{\sqrt{\pi}}\right)(1 + 2kT_n\alpha^i\varepsilon')\sqrt{\varepsilon'(1 + kT_n\alpha^i\varepsilon')}\,[\,1 - j_0(zK) - j_0((L_z - z)K) + j_0(L_zK)\,]$$

$$K \ = \ 2\sqrt{\frac{2m_{qn}^i kT_n\varepsilon'(1 + kT_n\alpha^i\varepsilon')}{\hbar^2}} \qquad \varepsilon' \ = \ \varepsilon + \frac{\varepsilon_1}{kT_n} \qquad \varepsilon_1 \ = \ \frac{-1 + \sqrt{1 + \frac{2\alpha^i}{m_{qn}^i}\left(\frac{\hbar\pi}{L_z}\right)^2}}{2\alpha^i} \tag{239}$$

where:

- α^i is the band nonparabolicity.
- L_z is a distance between the parallel interfaces.
- ε_1 is the first subband energy of the infinite-barrier quantum well with size L_z.

Eq. 239 assumes that the DOS is equal to zero up to the first subband energy ε_1 and this gives an effect of bandgap widening in thin-layer structures.

For the hole six-band $k \cdot p$ bands in Eq. 237, geometric quantization is accounted for similarly by using the first subband energy ε_1. In this case, the quantization mass in ε_1 is taken to be energy dependent along the quantization direction, which comes from the reciprocal mass tensor w_{ij} used in Eq. 237.

This MLDA quantization option is implemented using the multivalley carrier density model described in Multivalley Band Structure on page 267. It uses all of the valley and mass parameter definitions of the multivalley model in the `MultiValley` section of the parameter file. In addition, it applies a numeric integration of Eq. 234, Eq. 236 based on Gauss–Laguerre quadratures as described in Nonparabolic Band Structure on page 268. The numeric integration is applied to both Fermi–Dirac statistics and Boltzmann statistics. By default, the model automatically finds the closest interface and accounts for its orientation by recomputing the

quantization mass for each valley and channel mesh point. The interface orientation is found using a vector normal to the interface and an orientation of the simulation coordinate system in reference to the crystal system defined in the `LatticeParameters` section of the parameter file (see Crystal and Simulation Coordinate Systems on page 781). For fitting purposes, you have an option to define a specific quantization mass for each valley using the parameter file (see Using MLDA).

Using MLDA

To activate the multivalley orientation–dependent model, the keyword `MLDA` must be used in the `MultiValley` statement of the `Physics` section:

```
Physics { MultiValley(MLDA) }
```

To activate the model only for electrons or holes, use `eMultiValley(MLDA)` or `hMultiValley(MLDA)`, respectively.

You can modify parameters of the model in the `MultiValley` section of the parameter file (see Using Multivalley Band Structure on page 270). By default, longitudinal and transverse effective masses are specified in the `(e|h)Valley` sections. These masses form the inverse mass tensor in the valley ellipsoidal coordinate system, which is rotated to the interface system, and is used to compute the quantization mass m_q. For users who want to define a constant quantization mass per valley, ignoring automatic interface orientation dependency, there is an option to define it in the `Valley` statement:

```
MultiValley { (e|h)Valley(mq = m_q) }
```

To activate the multivalley MLDA model based on the six-band $k \cdot p$ band structure for holes (see Eq. 237) or the two-band $k \cdot p$ model for Δ_2 electron valleys, an additional keyword must be used:

```
Physics { MultiValley(MLDA kpDOS) }
```

In this case, all $k \cdot p$ model parameters are defined in the `LatticeParameters` section of the parameter file (see Using Strained Effective Masses and DOS on page 834). The fitting parameter γ_{kp} in Eq. 237 should be specified as a value of the parameter `hkpDOSfactor` in the `MLDAQMModel` section of the parameter file as follows:

```
MLDAQMModel{
    hkpDOSfactor = 0.4
    ekpDOSfactor = 1.0
}
```

The parameter `ekpDOSfactor` can be used as a fitting parameter for the electron multivalley MLDA model (as a factor to z in Eq. 236) if `eMultiValley(MLDA kpDOS)` is specified in

the `Physics` section of the command file. To use the multivalley MLDA model for both $k \cdot p$ bands and valleys defined in the parameter file, `MultiValley(MLDA kpDOS parfile)` must be used.

To apply the MLDA model to heterojunctions, the penetration length z_0 (see Eq. 238) must be specified (default is zero) in the parameter file for electrons and holes separately. This length is considered to be a fitting parameter specific for heterojunctions, and Eq. 238 should be used only as a reference. For example, with a 5 Å penetration, the penetration length can be specified as:

```
MLDAQMModel{
    ePenetration = 5e-8   # [cm]
    hPenetration = 5e-8   # [cm]
}
```

To activate the multivalley MLDA model with nonparabolic bands (Eq. 239), the keywords `Multivalley(MLDA Nonparabolicity)` must be specified. If the nonparabolicity should be ignored only in the MLDA part of the model (in the Bessel functions j_0 of Eq. 239), you must use `MLDA(-Nonparabolicity)`.

To have the geometric quantization accounted for as in Eq. 239 (the part dependent on the quantization length L_z), the `ThinLayer` keyword must be in the `MultiValley` statement and the `LayerThickness` statement must be set. All `LayerThickness` options are described in LayerThickness Command on page 310 where generally the layer thickness (the quantization length L_z) can be extracted automatically for defined regions. Practically, if the geometric quantization is mostly 1D, such a setting can be as simple as:

```
LayerThickness( Thickness = L_z )
Multivalley(MLDA ThinLayer)
```

For more complicated cases, such as for rectangular nanowires, the geometric quantization at corners is important and the following statements with automatic extraction of the quantization length L_z can be used:

```
LayerThickness( MaxFitWeight = 0.35 DimensionWeight = 1.0 )
Multivalley(MLDA ThinLayer)
```

The parameter `DimensionWeight` is specific to the model where the first subband energy ε_1 is used, as in Eq. 239. This parameter works as a factor to ε_1 and is designed as a fitting factor to effectively account for multidimensional quantization. Its default value is 1, but it should be increased with a reduction of the nanowire size.

To plot the electron and hole effective quantum corrections of the quantization models activated in the `Multivalley` statement (`MLDA` and `ThinLayer`), the `eMVQMBandgapShift` and `hMVQMBandgapShift` keywords must be present in the `Plot` section.

By default, the MLDA model looks for all semiconductor–insulator interfaces and calculates the normal distance z in Eq. 234–Eq. 237 to the nearest interface. The MLDA model also uses the `EnormalInterface` option and the `GeometricDistances` option (see Normal to Interface on page 355). To improve numerics if there is a coarse mesh in highly doped regions, there is an option to compute an averaged distance from a vertex to the interface based on element volumes and interface distances of elements, which contain the vertex (surrounding elements). The option is implemented only for the multivalley MLDA and has an adjusting parameter that can be specified as follows:

```
Math{
    MVMLDAcontrols(AveDistanceFactor = 0.05)
}
```

The default value of the parameter is 0.05 but, if it is equal to zero, the normal distance z is not modified by such averaging. If the parameter is unit, the distance z will be computed as an averaged distance using the normal distances of all vertices of the surrounded semiconductor elements with element–vertex volume weights.

To control a distance from the interface where the multivalley MLDA models will be applied, use the following statement:

```
Math {
    MVMLDAcontrols(MaxIntDistance = 1e-6)
}
```

The default value of `MaxIntDistance` is 10^{-6} cm.

To control the multivalley MLDA models by the doping concentration (for example, to exclude partially source/drain regions), the following command can be used:

```
Math {
    MVMLDAcontrols(MaxDoping4Majority = 1e19)
}
```

where `MaxDoping4Majority` defines the maximum doping concentration where the multivalley MLDA models are applied for majority carriers. For example, if `MaxDoping4Majority` is equal to zero, it excludes source/drain regions completely and the models are applied only for minority carriers. The default value of `MaxDoping4Majority` is 10^{22} cm^{-3}, that is, there are no limitations related to the doping concentration.

If the statement `hMultivalley(MLDA kpDOS)` is activated, the model performs an initial computation of energy-dependent data based on the bulk six-band k · p dispersion model. This computation may be time consuming, especially for 3D simulations and with the `hSubband` model active (see Mobility Modeling on page 838).

To separate this initial computation from bias ramping, there is an option to save and load the energy-dependent data file, for example:

```
Math { MVMLDAcontrols(Save = "file_name") }
Math { MVMLDAcontrols(Load = "file_name") }
```

If `LoadWithInterpolation = "file_name"` is used, then the saved data file could have a mesh different to the simulation one, and this option will interpolate the data to the simulation mesh.

In addition, to exclude source/drain or other regions, the keyword `MLDAbox` can be used to define the range of the interface from which the MLDA distance function is calculated:

```
Math{
    EnormalInterface(
        regionInterface=["SemiRegion/InsulRegion"]
        materialInterface=["OxideAsSemiconductor/Silicon"]
    )
    * single MLDAbox
    MLDAbox( MinX=-0.1, MaxX=0.1, MinY=-0.01, MaxY=0.01 )
    * multiple MLDAbox
    MLDAbox( { MinX=-0.1, MaxX=0.1, MinY=-0.01, MaxY=0.01 }
        { MinX=-0.1, MaxX=0.1, MinY= 0.05, MaxY=0.06 } )
}
```

The unit of the parameters `MinX`, `MaxX`, `MinY`, and `MaxY` in the `MLDAbox` is micrometer.

To activate the simple MLDA model (with one parameter λ per carrier type), use the keyword `MLDA` in the `Physics` section. To activate the model for electrons or holes only, use `eMLDA` or `hMLDA`. The model also can be specified in the regionwise or materialwise `Physics` section, and can be switched off by using `-MLDA`, `-eMLDA`, or `-hMLDA`.

By default, the thermal wavelength is computed from the thermal wavelengths at $300\,\text{K}$ as $\lambda = \lambda_{300}\sqrt{300\,\text{K}/T_n}$; alternatively, $\lambda = \lambda_{300}$ can be used.

To activate or deactivate the temperature dependence of the thermal wavelength, the `LambdaTemp` switch can be specified as an option to `MLDA`:

```
Physics {
    MLDA (                  * eMLDA | hMLDA for one carrier
        -LambdaTemp    * switch off temperature dependency
    )
}
```

Table 45 lists the coefficients for this model. The default values of λ_{300} were determined by comparison with the Schrödinger equation solver at 23.5 Å and 25.0 Å for electrons and holes, respectively. These parameters are accessible in the `MLDA` parameter set.

Table 45   Default coefficients for MLDA model

Symbol	Electrons		Holes		Unit
λ_{300}	`eLambda`	23.5×10^{-8}	`hLambda`	25×10^{-8}	cm

To plot the electron and hole effective quantum corrections of the simple MLDA model (see Eq. 234), the `eMLDAQuantumPotential` and `hMLDAQuantumPotential` keywords must be present in the `Plot` section.

MLDA Application Notes

Note that:

- For each carrier type, only one of the two MLDA options (either multivalley `(e|h)MultiValley(MLDA)` or only `(e|h)MLDA`) can be used in the `Physics` section.

- The multivalley MLDA model can be used to compute stress-related mobility change (see Mobility Modeling on page 838) and, therefore, it is required to be switched on for these mobility models. However, for some cases, other quantum models may be needed in the carrier density computation. For such cases, the multivalley MLDA model can be activated for all models except the density as follows:

      (e|h)MultiValley(MLDA -Density)

  Such activation (exclusion of the multivalley option from the density computation) is global for the whole device even if it appears in one region of the device only.

- Theoretically, the MLDA model should give zero carrier density at the semiconductor–insulator interface. However, since the zero carrier density results in various numeric problems, the actual values of carrier density at the interface calculated by the program are very small but greater than zero. This is achieved by assuming a very thin transition layer (one-hundredth of an ångström) between the insulator and the semiconductor.

- MLDA quantization is switched off at contacts and at a small distance to the contacts (to avoid numeric and physical inconsistencies). By default, the distance to the contacts (where the model is switched off) is 75 Å.

  To change the distance, use `MLDAMinDistanceToContact=<number>` (in units of μm) in the `Math` section.

Quantum-Well Quantization Model

The quantum-well quantization model is activated in the `Physics` section for semiconductor regions using the `eDensityCorrection` and `hDensityCorrection` options of `QWLocal`:

```
Physics(Region = "well") {
   QWLocal(
      eDensityCorrection
      hDensityCorrection
   )
}
```

For additional options of `QWLocal`, see Localized Quantum-Well Model on page 978 and Table 250 on page 1446.

The 'quantum well' is composed of all regions in which this model is active. Sentaurus Device computes the local thickness t of the quantum well and, together with the local electric field F, computes the electron density as:

$$n = \frac{kT}{t\hbar^2\pi}\sum_{\nu}d_{\nu}m_{xy,\,\nu}\sum_{j}F_0\left(\frac{E_{F,\,n}-\tilde{E}_C-E_{j,\,\nu}(F,t)}{kT}\right) \tag{240}$$

A similar expression is used for holes. In Eq. 240, j runs over all subbands of band ν. The eigenenergy $E_{j,\nu}(F,t)$ is measured relative to the band edge $\tilde{E}_C$ at the center of the well. $E_{j,\,\nu}(F,t)$ and $\tilde{E}_C$ are computed from the local field F and the local band edge E_C, assuming that the field in the well is constant and equal to F, and that the barriers limiting the well are symmetric and are given by the average barrier height of the entire quantum well.

During Newton iterations, large fields can occur, which can cause the `QWLocal` implementation to take a lot of time and memory. With the `MaxElectricField` parameter of `QWLocal`, you can set a cutoff value for the field. The default is 10^6 V/cm. To ensure that the cutoff does not affect the result, you can check that, for the converged solution, the electric field in the well does not exceed the cutoff.

Contrary to the 1D Schrödinger solver (see 1D Schrödinger Parameters on page 287), which can extract the number of ladders and its parameters automatically, an explicit ladder specification (see Explicit Ladder Specification on page 288) is required in the parameter file. The number of bands in the ladders must be the same over the entire quantum well and in the regions adjacent to it. To specify the number of subbands to be computed for electrons, heavy holes, and light holes, use the keywords `NumberOfElectronSubbands`, `NumberOfHeavyHoleSubbands`, and `NumberOfLightHoleSubbands`, respectively.

> **NOTE** To use the quantum-well quantization model, you must use the `HeteroInterface` or the `Thermionic` keyword. Furthermore, each quantum-well region must be adjacent to at least one semiconductor barrier region.

> **NOTE** To use the quantum-well quantization model in the context of the simulation of light-emitting diodes, see Localized Quantum-Well Model on page 978 and Table 250 on page 1446.

LayerThickness Command

Sentaurus Device provides models (for example, mobility and MLDA) that account for quantum-mechanical effects that occur in thin semiconducting films. These models use a parameter `LayerThickness`, which is intrinsically one-dimensional: It is well defined only in the case of an infinite sheet of fixed thickness. Sentaurus Device generalizes this parameter to arbitrary structures in two and three dimensions using the concept of the *radius of the largest sphere which fits in a material and touches the surface point nearest a given point*. Therefore, a `LayerThickness` is defined as a scalar field throughout a structure.

Sentaurus Device has two ways of computing the `LayerThickness`:

- `LayerThickness` command: `LayerThickness(<geo_parameters>)`
- `ThinLayer` subcommand: `Mobility(ThinLayer(<geo/physical_parameters>)` (see Thin-Layer Mobility Model on page 356)

As a result, there are two scalar arrays: `LayerThickness` and `LayerThicknessField`.

By default, both the `LayerThickness` and `LayerThicknessField` arrays are valid only in semiconductors. For `LayerThicknessField` only, the material group where the array is valid can be selected by the `AllowLayerThickness` keyword in the global `Math` section. Possible values are `Semiconductor` (default), `Insulator`, `Metal`, and `Everywhere`.

> **NOTE** Use the `LayerThickness` command only in region- or material-specific `Physics` sections. In particular, if you use the command in the global `Physics` section, the layer will be composed of all regions of the allowed material types. Using the `LayerThickness` command with `AllowLayerThickness=Everywhere` will always result in an infinite layer.

Combining LayerThickness Command and ThinLayer Subcommand

To activate the LayerThickness command, you must specify the LayerThickness keyword with geometric parameters in the region, or material, or global Physics section. If the mobility model contains the ThinLayer subcommand with geometric parameters, this model uses the LayerThickness array; otherwise, the LayerThicknessField array will be used. For all other ThinLayer-dependent models, an external LayerThickness command must be set.

Example 1

```
Physics (Material= Silicon) {
   # LayerThickness command: computation LayerThicknessField array
   LayerThickness(<geo_params>)

# ThinLayer without <geo_params>: mobility uses LayerThicknessField array
   Mobility(ThinLayer(<physical_params>))
   MultiValley( ThinLayer )      # MultiValley uses LayerThicknessField array
}
```

Example 2

```
Physics (Material= Silicon) {
   # LayerThickness command: computation LayerThicknessField array
   LayerThickness(<geo_params>)

# ThinLayer with <geo-params>: mobility uses LayerThickness array
   Mobility( ThinLayer(<geo_params> <physical_params>) )

   MultiValley( ThinLayer )      # MultiValley uses LayerThicknessField array
}
```

Example 3

```
Physics (Material= Silicon) {      # without external LayerThickness command
   # mobility uses LayerThickness array
   Mobility( ThinLayer(<geo_params> <physical_params>) )
   MultiValley( ThinLayer )        # error: LayerThickness command must be set
}
```

Geometric Parameters of LayerThickness Command

The `LayerThickness` command has the following optional parameters: `Thickness`, `ChordWeight`, `MinAngle`, and `MaxFitWeight`.

> **NOTE** The `ThinLayer` subcommand has the same `<geo_params>` as well as the optional `<physical_params>` (see Using the Thin-Layer Mobility Model on page 358).

The parameter `Thickness` explicitly specifies the thickness of a layer (in micrometers). If it is not present, Sentaurus Device extracts the thickness automatically. For the extraction, it assumes that all regions where `ThinLayer` is specified (regardless of carrier type) belong to the thin layer.

> **NOTE** The external boundary is not considered to be a boundary of the thin layer. However, each interface between a region that specifies `ThinLayer` and a region that does not is considered to be a boundary of the thin layer, even if these two regions are both semiconductor regions.

For example:

```
Physics(Region="A") { LayerThickness() }
Physics(Region="B") { LayerThickness(Thickness=0.005) }
```

activates the computation of the `LayerThicknessField` array in regions A and B. Its thickness is extracted in region A and is assumed to be 5 nm in region B.

If the structure is a part of a larger symmetric structure and the full structure can be obtained by mirroring the simulated structure at a symmetry plane, the option `Mirror` must be activated in the global `Math` section.

`Mirror` is a vector that has the dimension of the device. Each component of the vector denotes the mirroring property for the corresponding axis and can have one of the values:

- `None` (no symmetry plane perpendicular to the axis).
- `Max` (symmetry plane at the largest coordinate of the axis).
- `Min` (symmetry plane at smallest coordinate).
- `Both` (symmetry planes at largest and smallest coordinates).

For example:

```
Math {
   ThinLayer ( Mirror = (None Max Both) )
}
```

means that there is a symmetry plane at the largest y-coordinate, as well as the smallest and largest z-coordinates. The full structure is six times as big as the simulated one.

You can verify the proper thickness extraction using the plot variables `LayerThickness` and `LayerThicknessField`. Note that the layer thickness is defined in such a way that it becomes zero in concave corners of the layer. In addition, due to interpolation, `LayerThickness` can deviate by approximately half of the local mesh spacing from the thickness actually used for computation. For more information on thickness extraction and the options to control it, see Thickness Extraction on page 313.

Thickness Extraction

The definition of the *thickness* of a layer in a general geometry is not self-evident. This section describes how Sentaurus Device defines thickness.

To determine the thickness of a layer at a given point P, Sentaurus Device first finds the closest point C_1 on the surface of the layer. Then, a sphere is constructed that touches the surface in C_1 and has its midpoint within the layer, on the line passing through C_1 and P.

Then, the diameter of this sphere is increased, until it touches the surface at a second point, C_2, and the surface normal at this point encloses an angle with the vector pointing from C_1 to P of at least β. By default, $\beta = 0$, so any second touch point C_2 is accepted, and the construction results in a sphere that is completely within the layer.

The thickness is a linear combination of the diameter of the final sphere, d, and the distance c_{12} between C_1 and C_2 (the chord length):

$$t = \alpha c_{12} + (1 - \alpha)d \tag{241}$$

The parameter α can be set with the keyword `ChordWeight`, which is an option of `ThinLayer`. The default value is zero.

The value of angle β can be changed with the keyword `MinAngle`, an option to `ThinLayer`. `MinAngle` expects two values: The first value sets β, and the second value sets an angle γ that must be larger than β.

If the angle of the surface normal at C_2 and the vector pointing from C_1 to P is between β and γ, the value of the diameter d is multiplied by a factor that is very large if the angle is close to β, and by a factor that approaches one when the angle approaches γ. The purpose of the transition region between β and γ is to smooth the transition between touch points that fulfill the angle criterion and points that do not.

The following example sets α to 0.5, β to 89°, and γ to 90°:

```
LayerThickness(
    MinAngle=(89,90)
    ChordWeight=0.5
)
```

The default value for β is zero, which causes the extracted layer thickness to go to zero in concave corners of the layer, even when the corners have a wide opening angle. This can be unwanted, and choosing a larger value for β can resolve this issue. However, there can be situations where a larger β can make the thickness extraction ambiguous, for example, when the choice of C_1 is not unique.
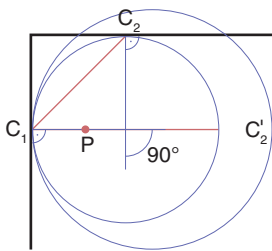
Figure 18   Thickness extraction

To illustrate the thickness extraction, consider the example in Figure 18. The thick black line is the boundary of the thin layer, and the red dot P indicates the position at which the thickness is extracted. First, the closest boundary point C_1 is found, which is to the left of P. Then, with the default $\beta = 0$, the largest circle touching at C_1 is inscribed into the layer. This is the smaller circle, with a second touch point C_2. From this circle, the layer thickness is obtained by a linear combination of the chord length (diagonal red line) and the diameter (horizontal red line).

The angle between the normal vectors C_1 and C_2 is 90°. Therefore, if the value of β is greater than 90° but smaller than 180°, the smaller circle is not considered. Instead, the larger circle (with a second touch point C_2') determines the layer thickness; for this circle, the angle between the normal vectors is 180°.

There is another option to compute the layer thickness, which also is based on considered spheres (or circles in Figure 18 for the 2D case), but with some of the following modifications. The above algorithm for each point P (that is, for each mesh element center) constructs a sphere that satisfies the described conditions. As a result, you have a set of spheres that cover the region where the thickness should be computed. After that, for each mesh element (the point P), you check whether this point is inside some subset of spheres, and you take the maximum sphere diameter d_m from this subset as the thickness for the point P. This way might be useful for spherical, circular, or nonplanar boundaries.

The user-defined keyword `MaxFitWeight` controls this option as follows:

$$t_m = \alpha_m d_m + (1 - \alpha_m)t \tag{242}$$

where t is the thickness from Eq. 241, and α_m is defined by the keyword `MaxFitWeight` and is equal to zero by default.

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[9]   O. Penzin, G. Paasch, and L. Smith, "Nonparabolic Multivalley Quantum Correction Model for InGaAs Double-Gate Structures," *IEEE Transactions on Electron Devices*, vol. 60, no. 7, pp. 2246–2250, 2013.

CHAPTER 15 Mobility Models

This chapter presents information about the different mobility models implemented in Sentaurus Device.

Sentaurus Device uses a modular approach for the description of the carrier mobilities. In the simplest case, the mobility is a function of the lattice temperature. This so-called constant mobility model described in Mobility due to Phonon Scattering on page 318 should only be used for undoped materials. For doped materials, the carriers scatter with the impurities. This leads to a degradation of the mobility. Doping-Dependent Mobility Degradation on page 318 introduces the models that describe this effect.

Models that describe the effects of carrier–carrier scattering are presented in Carrier–Carrier Scattering on page 326. The Philips unified mobility model, described in Philips Unified Mobility Model on page 328, is a well-calibrated model that accounts for both impurity and carrier–carrier scattering.

Models that describe the mobility degradation at interfaces, for example, the silicon–oxide interface in the channel region of a MOSFET, are introduced in Mobility Degradation at Interfaces on page 332. These models account for the scattering with surface phonons and surface roughness.

Finally, the models that describe mobility degradation in high electric fields are discussed in High-Field Saturation on page 361. A flexible model for hydrodynamic simulations is described in Energy-Dependent Mobility on page 772.

How Mobility Models Combine

The mobility models are selected in the `Physics` section as options to `Mobility`, `eMobility`, or `hMobility`:

```
Physics{ Mobility( <arguments> ) ... }
```

Specifications with `eMobility` apply to electrons; specifications with `hMobility` apply to holes; and specifications with `Mobility` apply to both carrier types.

If more than one mobility model is activated for a carrier type, the different mobility contributions ($\mu_1, \mu_2, \ldots$) for bulk, surface mobility, and thin layers are combined by Matthiessen's rule:

$$\frac{1}{\mu} = \frac{1}{\mu_1} + \frac{1}{\mu_2} + \ldots \tag{243}$$

If the high-field saturation model is activated, the final mobility is computed in two steps. First, the low field mobility μ_{low} is determined according to Eq. 243. Second, the final mobility is computed from a (model-dependent) formula as a function of a driving force F_{hfs}:

$$\mu = f(\mu_{\text{low}}, F_{\text{hfs}}) \tag{244}$$

Mobility due to Phonon Scattering

The constant mobility model [1] is active by default. It accounts only for phonon scattering and, therefore, it is dependent only on the lattice temperature:

$$\mu_{\text{const}} = \mu_L \left(\frac{T}{300\text{K}} \right)^{-\zeta} \tag{245}$$

where μ_L is the mobility due to bulk phonon scattering. The default values of μ_L and the exponent ζ are listed in Table 46. The constant mobility model parameters are accessible in the `ConstantMobility` parameter set.

Table 46   Constant mobility model: Default coefficients for silicon

Symbol	Parameter name	Electrons	Holes	Unit
μ_L	`mumax`	1417	470.5	cm^2/Vs
ζ	`exponent`	2.5	2.2	1

In some special cases, it may be necessary to deactivate the default constant mobility. This can be accomplished by specifying the `-ConstantMobility` option to `Mobility`:

```
Physics { Mobility ( -ConstantMobility ... ) ... }
```

Doping-Dependent Mobility Degradation

In doped semiconductors, scattering of the carriers by charged impurity ions leads to degradation of the carrier mobility. Sentaurus Device supports several built-in models (see Masetti Model on page 320, Arora Model on page 321, and University of Bologna Bulk Mobility Model on page 322), one multistate configuration–dependent model (see The

The Philips unified mobility model is also available to account for doping-dependent scattering. This model accounts for other effects as well (such as electron–hole scattering and screening of impurities by carriers) (see Philips Unified Mobility Model on page 328).

For very-short channel devices, it has been found that an additional contribution to low-field mobility is sometimes needed to match measured device characteristics. For this purpose, a ballistic mobility model is provided (see Low-Field Ballistic Mobility Model on page 325) that can be specified in addition to one of the doping-dependent mobility models described in this section.

Using Doping-Dependent Mobility

Mobility degradation due to impurity scattering is activated by specifying the `DopingDependence` option to `Mobility`. The different model choices are selected as options to `DopingDependence`:

```
Physics {
   Mobility(
      DopingDependence (
         [ Masetti | Arora | UniBo | PhuMob | PhuMob2 |
           PMIModel(Name = "<msc-dependent-bulk-model>" ...) |
           BalMob( [Lch=<float>] ) |
           <doping-dependent-pmi-model>
         ]
      )
   )
}
```

If `DopingDependence` is specified without options, Sentaurus Device uses a material-dependent default. For example, in silicon, the default is the `Masetti` model; for GaAs, the default is the `Arora` model. The default model (`Masetti` or `Arora`) for each material can be specified by using the parameter `formula`, which is accessible in the `DopingDependence` parameter set in the parameter file:

```
DopingDependence: {
   formula= 1 , 1    # [1]
}
```

If `formula` is set to 1, the `Masetti` model is the default. To use the `Arora` model as the default, use `formula=2`.

The `UniBo` option selects the University of Bologna bulk mobility model. The options `PhuMob` and `PhuMob2` select the Philips unified mobility model and an alternative version of this model, respectively (see Philips Unified Mobility Model on page 328).

Using More Than One Doping-Dependent Mobility Model

In most cases, only one doping-dependent mobility model should be specified to avoid double-counting mobility effects. However, Sentaurus Device allows more than one model to be used in a simulation. It may be useful, for example, to include additional degradation components that are created as PMI models into the bulk mobility calculation. When more than one model is specified as an option to `DopingDependence`, they are combined using Matthiessen's rule. For example, the specification:

```
Physics { Mobility( DopingDependence( Masetti pmi_model1 pmi_model2) ...) ...}
```

calculates the total bulk mobility using:

$$\frac{1}{\mu_b} = \frac{1}{\mu_{Masetti}} + \frac{1}{\mu_{pmi\_model1}} + \frac{1}{\mu_{pmi\_model2}} \tag{246}$$

Masetti Model

The default model used by Sentaurus Device to simulate doping-dependent mobility in silicon was proposed by Masetti *et al.* [2]:

$$\mu_{dop} = \mu_{min1} \exp\left(-\frac{P_c}{N_{A,0} + N_{D,0}}\right) + \frac{\mu_{const} - \mu_{min2}}{1 + ((N_{A,0} + N_{D,0})/C_r)^\alpha} - \frac{\mu_1}{1 + (C_s/(N_{A,0} + N_{D,0}))^\beta} \tag{247}$$

The reference mobilities μ_{min1}, μ_{min2}, and μ_1, the reference doping concentrations P_c, C_r, and C_s, and the exponents α and β are accessible in the parameter set `DopingDependence` in the parameter file. The corresponding values for silicon are given in Table 47.

Table 47   Masetti model: Default coefficients

Symbol	Parameter name	Electrons	Holes	Unit
μ_{min1}	`mumin1`	52.2	44.9	cm^2/Vs
μ_{min2}	`mumin2`	52.2	0	cm^2/Vs
μ_1	`mu1`	43.4	29.0	cm^2/Vs
P_c	`Pc`	0	9.23×10^{16}	cm^{-3}
C_r	`Cr`	9.68×10^{16}	2.23×10^{17}	cm^{-3}
C_s	`Cs`	3.43×10^{20}	6.10×10^{20}	cm^{-3}

Table 47   Masetti model: Default coefficients (Continued)

Symbol	Parameter name	Electrons	Holes	Unit
α	`alpha`	0.680	0.719	1
β	`beta`	2.0	2.0	1

The low-doping reference mobility μ_{const} is determined by the constant mobility model (see Mobility due to Phonon Scattering on page 318).

Arora Model

The Arora model [3] reads:

$$\mu_{\mathrm{dop}} = \mu_{\mathrm{min}} + \frac{\mu_{\mathrm{d}}}{1 + ((N_{\mathrm{A},0} + N_{\mathrm{D},0})/N_0)^{A^*}} \qquad (248)$$

with:

$$\mu_{\mathrm{min}} = A_{\mathrm{min}} \cdot \left(\frac{T}{300\,\mathrm{K}}\right)^{\alpha_{\mathrm{m}}} , \ \ \mu_{\mathrm{d}} = A_{\mathrm{d}} \cdot \left(\frac{T}{300\,\mathrm{K}}\right)^{\alpha_{\mathrm{d}}} \qquad (249)$$

and:

$$N_0 = A_N \cdot \left(\frac{T}{300\,\mathrm{K}}\right)^{\alpha_N} , \ \ A^* = A_{\mathrm{a}} \cdot \left(\frac{T}{300\,\mathrm{K}}\right)^{\alpha_{\mathrm{a}}} \qquad (250)$$

The parameters are accessible in the `DopingDependence` parameter set in the parameter file.

Table 48   Arora model: Default coefficients for silicon

Symbol	Parameter name	Electrons	Holes	Unit
A_{min}	`Ar_mumin`	88	54.3	$\mathrm{cm}^2/\mathrm{Vs}$
α_{m}	`Ar_alm`	-0.57	-0.57	1
A_{d}	`Ar_mud`	1252	407	$\mathrm{cm}^2/\mathrm{Vs}$
α_{d}	`Ar_ald`	-2.33	-2.23	1
A_N	`Ar_N0`	1.25×10^{17}	2.35×10^{17}	cm^{-3}
α_N	`Ar_alN`	2.4	2.4	1
A_{a}	`Ar_a`	0.88	0.88	1
α_{a}	`Ar_ala`	-0.146	-0.146	1

University of Bologna Bulk Mobility Model

The University of Bologna bulk mobility model was developed for an extended temperature range between $25°C$ and $973°C$. It should be used together with the University of Bologna inversion layer mobility model (see University of Bologna Surface Mobility Model on page 345). The model [4][5] is based on the Masetti approach with two major extensions. First, attractive and repulsive scattering are separately accounted for, therefore, leading to a function of both donor and acceptor concentrations. This automatically accounts for different mobility values for majority and minority carriers, and ensures continuity at the junctions as long as the impurity concentrations are continuous functions. Second, a suitable temperature dependence for most model parameters is introduced to predict correctly the temperature dependence of carrier mobility in a wider range of temperatures, with respect to other models. The temperature dependence of lattice mobility is reworked, with respect to the default temperature.

The model for lattice mobility is:

$$\mu_L(T) = \mu_{max}\left(\frac{T}{300 \text{ K}}\right)^{-\gamma + c\left(\frac{T}{300 \text{ K}}\right)} \tag{251}$$

where μ_{max} denotes the lattice mobility at room temperature, and c gives a correction to the lattice mobility at higher temperatures. The maximum mobility μ_{max} and the exponents γ and c are accessible in the `UniBoDopingDependence` parameter set in the parameter file.

The model for bulk mobility reads:

$$\mu_{dop}(T) = \mu_0(T) + \frac{\mu_L(T) - \mu_0(T)}{1 + \left(\frac{N_{D,0}}{C_{r1}(T)}\right)^{\alpha} + \left(\frac{N_{A,0}}{C_{r2}(T)}\right)^{\beta}} - \frac{\mu_1(N_{D,0}, N_{A,0}, T)}{1 + \left(\frac{N_{D,0}}{C_{s1}(T)} + \frac{N_{A,0}}{C_{s2}(T)}\right)^{-2}} \tag{252}$$

In turn, μ_0 and μ_1 are expressed as weighted averages of the corresponding limiting values for pure acceptor-doping and pure donor-doping densities:

$$\mu_0(T) = \frac{\mu_{0d}N_{D,0} + \mu_{0a}N_{A,0}}{N_{A,0} + N_{D,0}} \tag{253}$$

$$\mu_1(T) = \frac{\mu_{1d}N_{D,0} + \mu_{1a}N_{A,0}}{N_{A,0} + N_{D,0}} \tag{254}$$

The reference mobilities μ_{0d}, μ_{0a}, μ_{1d}, and μ_{1a}, and the reference doping concentrations C_{r1}, C_{r2}, C_{s1}, and C_{s2} are accessible in the `UniBoDopingDependence` parameter set in the parameter file.

Table 49 lists the corresponding values of silicon for arsenic, phosphorus, and boron; $T_n = T/300 \text{ K}$.

Table 49 Parameters of University of Bologna bulk mobility model

Symbol	Parameter name	Electrons (As)	Electrons (P)	Holes (B)	Unit
μ_{max}	mumax	1441	1441	470.5	cm^2/Vs
c	Exponent2	–0.11	–0.11	0	1
γ	Exponent	2.45	2.45	2.16	1
μ_{0d}	mumin1	$55.0 T_n^{-\gamma_{0d}}$	$62.2 T_n^{-\gamma_{0d}}$	$90.0 T_n^{-\gamma_{0d}}$	cm^2/Vs
γ_{0d}	mumin1_exp	0.6	0.7	1.3	1
μ_{0a}	mumin2	$132.0 T_n^{-\gamma_{0a}}$	$132.0 T_n^{-\gamma_{0a}}$	$44.0 T_n^{-\gamma_{0a}}$	cm^2/Vs
γ_{0a}	mumin2_exp	1.3	1.3	0.7	1
μ_{1d}	mu1	$42.4 T_n^{-\gamma_{1d}}$	$48.6 T_n^{-\gamma_{1d}}$	$28.2 T_n^{-\gamma_{1d}}$	cm^2/Vs
γ_{1d}	mu1_exp	0.5	0.7	2.0	1
μ_{1a}	mu2	$73.5 T_n^{-\gamma_{1a}}$	$73.5 T_n^{-\gamma_{1a}}$	$28.2 T_n^{-\gamma_{1a}}$	cm^2/Vs
γ_{1a}	mu2_exp	1.25	1.25	0.8	1
C_{r1}	Cr	$8.9 \times 10^{16} T_n^{\gamma_{r1}}$	$8.5 \times 10^{16} T_n^{\gamma_{r1}}$	$1.3 \times 10^{18} T_n^{\gamma_{r1}}$	cm^{-3}
γ_{r1}	Cr_exp	3.65	3.65	2.2	1
C_{r2}	Cr2	$1.22 \times 10^{17} T_n^{\gamma_{r2}}$	$1.22 \times 10^{17} T_n^{\gamma_{r2}}$	$2.45 \times 10^{17} T_n^{\gamma_{r2}}$	cm^{-3}
γ_{r2}	Cr2_exp	2.65	2.65	3.1	1
C_{s1}	Cs	$2.9 \times 10^{20} T_n^{\gamma_{s1}}$	$4.0 \times 10^{20} T_n^{\gamma_{s1}}$	$1.1 \times 10^{18} T_n^{\gamma_{s1}}$	cm^{-3}
γ_{s1}	Cs_exp	0	0	6.2	1
C_{s2}	Cs2	7.0×10^{20}	7.0×10^{20}	6.1×10^{20}	cm^{-3}
α	alpha	0.68	0.68	0.77	1
β	beta	0.72	0.72	0.719	1

The default parameters of Sentaurus Device for electrons are those for arsenic. The bulk mobility model was calibrated with experiments [5] in the temperature range from 300 K to 700 K. It is suitable for isothermal simulations at large temperatures or nonisothermal simulations.

The pmi_msc_mobility Model

The mobility model `pmi_msc_mobility` depends on the lattice temperature and the occupation probabilities of the states of a multistate configuration (MSC). The model averages the mobilities of all MSC states according to:

$$\mu = \sum_i \mu_i(T)s_i \tag{255}$$

where the sum is taken over all MSC states, μ_i are the state mobilities, and s_i are the state occupation probabilities. Each state mobility can be temperature dependent according to:

$$\mu_i = \begin{cases} \mu_{i,\,\text{ref}} & \text{if} \quad T < T_{\text{ref}} \\ \dfrac{1}{T_{\text{g}} - T_{\text{ref}}}[(T_{\text{g}} - T)\mu_{i,\,\text{ref}} + (T - T_{\text{ref}})\mu_{i,\,\text{g}}] & \text{if} \quad T_{\text{ref}} \le T < T_{\text{g}} \\ \mu_{i,\,\text{g}} & \text{if} \quad T_{\text{g}} \le T \end{cases} \tag{256}$$

where:

- The index i refers to the state.

- T_{ref} and T_{g} are the reference and glass temperatures (terminology is borrowed from and the model is used for phase transition dynamics).

- $\mu_{i,\,\text{ref}}$ and $\mu_{i,\,\text{g}}$ are the (state-specific) mobilities for the corresponding temperatures.

The model is activated (here, for MSC "m0" and model string "e") by:

```
PMIModel ( Name="pmi_msc_mobility" MSConfig="m0" String="e" )
```

The given `String` is used to determine the names of parameters in the parameter file.

Table 50   Global and model-string parameters of pmi_msc_mobility

Name	Symbol	Default	Unit	Range	Description
plot	–	0	–	{0,1}	Plot parameter to screen
Tref	T_{ref}	300.	K	>=0.	Reference temperature
Tg	T_{g}	-1.	K	>=T_{ref} or equal -1.	Glass temperature
mu_ref	–	1.	cm/Vs	>0.	Value at reference temperature
mu_g	–	1.	cm/Vs	>0.	Value at glass temperature

Table 51   State parameters of pmi_msc_mobility

Name	Symbol	Default	Unit	Range	Description
mu_ref	$\mu_{i,\,\mathrm{ref}}$	–	cm^2/Vs	>0.	Value at reference temperature
mu_g	$\mu_{i,\,g}$	–	cm^2/Vs	>0.	Value at glass temperature

The model uses a three-level hierarchy of sets of parameters to define the parameters for each state, namely, the global, the model-string, and the state parameters. The global parameters of the model are given in Table 50. They serve as defaults for the model-string parameters, which are the global parameters with the prefix:

```
<model_string>_
```

where `<model_string>` is the `String` parameter given in the command file. The model-string parameters, in turn, serve as defaults for the state parameters (see Table 51), which are prefixed by:

```
<model_string>_<state_name>_
```

where `<state_name>` is the name of the MSC state.

PMIs for Bulk Mobility

The PMIs for bulk mobility are described in Doping-Dependent Mobility on page 1107 and Multistate Configuration–Dependent Bulk Mobility on page 1113.

Low-Field Ballistic Mobility Model

The low-field ballistic mobility model [6] is given by the simple expression:

$$\mu_{\mathrm{bal}} = k \cdot L_{\mathrm{ch}} \tag{257}$$

where both k and L_{ch} are parameters. In most cases, you will specify a value for L_{ch} (in nm) that corresponds to the actual channel length for the device being simulated. The parameter k can be adjusted to match measured device characteristics.

To use the low-field ballistic mobility model, specify `BalMob` as an argument to `DopingDependence`, for example,

```
Physics {
    Mobility (
        DopingDependence ( PhuMob BalMob(Lch = 5.0) )
```

```
      )
   }
```

In this case, μ_{bal} is combined with the mobility from `PhuMob` using Matthiessen's rule. If `Lch` is not specified, the default value of 10^7 nm is used, which effectively disables the model.

The k parameter is accessible in the `BalMob` parameter set in the parameter file.

Table 52   BalMob model: Default coefficients for silicon

Symbol	Parameter name	Electrons	Holes	Unit
k	k	20.0	20.0	$cm^2/Vs\ nm$

Carrier–Carrier Scattering

Two models are supported for the description of carrier–carrier scattering. One model is based on Choo [7] and Fletcher [8], and uses the Conwell–Weisskopf theory. As an alternative to the Conwell–Weisskopf model, Sentaurus Device supports a model based on the Brooks–Herring screening theory [9]. The carrier–carrier contribution to the overall mobility degradation is captured in the mobility term μ_{eh}. This is combined with the mobility contributions from other degradation models (μ_{other}) according to Matthiessen's rule:

$$\frac{1}{\mu} = \frac{1}{\mu_{other}} + \frac{1}{\mu_{eh}} \tag{258}$$

Using Carrier–Carrier Scattering

The carrier–carrier scattering models are activated by specifying the `CarrierCarrierScattering` option to `Mobility`. Either of the two different models are selected by an additional flag:

```
Physics { Mobility (
   CarrierCarrierScattering( [ ConwellWeisskopf | BrooksHerring ] )
   ...)...}
```

The Conwell–Weisskopf model is the default in Sentaurus Device for carrier–carrier scattering and is activated when `CarrierCarrierScattering` is specified without an option.

Conwell–Weisskopf Model

$$\mu_{eh} = \frac{D(T/300\,\text{K})^{3/2}}{\sqrt{np}}\left[\ln\left(1 + F\left(\frac{T}{300\,\text{K}}\right)^2 (pn)^{-1/3}\right)\right]^{-1} \tag{259}$$

The parameters D and F are accessible in the parameter file. The default values appropriate for silicon are given in Table 53 on page 327.

Brooks–Herring Model

$$\mu_{eh} = \frac{c_1(T/300\,\text{K})^{3/2}}{\sqrt{np}}\frac{1}{\phi(\eta_0)} \tag{260}$$

where $\phi(\eta_0) = \ln(1 + \eta_0) - \eta_0/(1 + \eta_0)$ and:

$$\eta_0(T) = \frac{c_2}{N_C F_{-1/2}(n/N_C) + N_V F_{-1/2}(p/N_V)}\left(\frac{T}{300\,\text{K}}\right)^2 \tag{261}$$

Table 54 lists the silicon default values for c_1 and c_2.

Physical Model Parameters

Parameters for the carrier–carrier scattering models are accessible in the parameter set `CarrierCarrierScattering`.

Table 53   Conwell–Weisskopf model: Default parameters

Symbol	Parameter name	Value	Unit
D	D	1.04×10^{21}	$\text{cm}^{-1}\text{V}^{-1}\text{s}^{-1}$
F	F	7.452×10^{13}	cm^{-2}

Table 54   Brooks-Herring model: Default parameters

Symbol	Parameter name	Value	Unit
c_1	c1	1.56×10^{21}	$\text{cm}^{-1}\text{V}^{-1}\text{s}^{-1}$
c_2	c2	7.63×10^{19}	cm^{-3}

Philips Unified Mobility Model

The Philips unified mobility model, proposed by Klaassen [10], unifies the description of majority and minority carrier bulk mobilities. In addition to describing the temperature dependence of the mobility, the model takes into account electron–hole scattering, screening of ionized impurities by charge carriers, and clustering of impurities.

The Philips unified mobility model is well calibrated. Though it was initially used primarily for bipolar devices, it is widely used for MOS devices.

Using the Philips Model

There are different methods for activating the Philips unified mobility model.

As described in Using Doping-Dependent Mobility on page 319, you can activate the model by specifying `PhuMob` as an option to `DopingDependence`. This method is required if you want to combine `PhuMob` with an additional doping-dependent model (for example, a doping-dependent PMI model to account for other degradation effects).

Alternatively, you can activate the Philips unified mobility model by specifying the `PhuMob` option to `Mobility` directly:

```
Physics{ Mobility ( PhuMob ... ) ... }
```

Specifying `PhuMob` in this way causes Sentaurus Device to completely ignore any specification made with `DopingDependence`, if present, to avoid accidental double-counting of mobility effects.

The `PhuMob` model also can be activated with an additional option:

```
Physics{ Mobility ( PhuMob[(Arsenic | Phosphorus)] ...) ... }
```

The option `Arsenic` or `Phosphorus` specifies which parameters (see Table 56 on page 332) are used. These parameters reflect the different electron mobility degradation that is observed in the presence of these donor species.

> **NOTE** The Philips unified mobility model describes mobility degradation due to both impurity scattering and carrier–carrier scattering mechanisms. Therefore, the keyword `PhuMob` must not be combined with the keyword `DopingDependence` or `CarrierCarrierScattering`. If a combination of these keywords is specified, Sentaurus Device uses only the Philips unified mobility model.

Using an Alternative Philips Model

Sentaurus Device provides an extended PMI reimplementation of the Philips unified mobility model (see Doping-Dependent Mobility on page 1107). To use it, specify `PhuMob2` as the option for `DopingDependence`:

```
Physics { Mobility (DopingDependence(PhuMob2)...)...}
```

The reimplementation uses the `PhuMob2` parameter set. The parameter `FACT_G` has a default value of 1. It modifies the function $G(P_i)$ shown in Eq. 274 by a factor $G(P_i)$ = `FACT_G` (right-hand side in Eq. 274). Otherwise, the reimplementation fully agrees with the model described below.

Philips Model Description

According to the Philips unified mobility model, there are two contributions to carrier mobilities. The first, $\mu_{i,\,L}$, represents phonon (lattice) scattering and the second, $\mu_{i,\,DAeh}$, accounts for all other bulk scattering mechanisms (due to free carriers, and ionized donors and acceptors). These partial mobilities are combined to give the bulk mobility $\mu_{i,\,b}$ for each carrier according to Matthiessen's rule:

$$\frac{1}{\mu_{i,\,b}} = \frac{1}{\mu_{i,\,L}} + \frac{1}{\mu_{i,\,DAeh}} \tag{262}$$

In Eq. 262 and all of the following model equations, the index i takes the value 'e' for electrons and 'h' for holes. The first contribution due to lattice scattering takes the form:

$$\mu_{i,\,L} = \mu_{i,\,max}\left(\frac{T}{300\,K}\right)^{-\theta_i} \tag{263}$$

The second contribution has the form:

$$\mu_{i,\,DAeh} = \mu_{i,\,N}\left(\frac{N_{i,\,sc}}{N_{i,\,sc,eff}}\right)\left(\frac{N_{i,\,ref}}{N_{i,\,sc}}\right)^{\alpha_i} + \mu_{i,\,c}\left(\frac{n+p}{N_{i,\,sc,eff}}\right) \tag{264}$$

with:

$$\mu_{i,\,N} = \frac{\mu_{i,\,max}^2}{\mu_{i,\,max} - \mu_{i,\,min}}\left(\frac{T}{300\,K}\right)^{3\alpha_i - 1.5} \tag{265}$$

$$\mu_{i,\,c} = \frac{\mu_{i,\,max}\mu_{i,\,min}}{\mu_{i,\,max} - \mu_{i,\,min}}\left(\frac{300\,K}{T}\right)^{0.5} \tag{266}$$

for electrons:

$$N_{e,sc} = N_D^* + N_A^* + p \tag{267}$$

$$N_{e,sc,eff} = N_D^* + G(P_e)N_A^* + f_e \frac{p}{F(P_e)} \tag{268}$$

and for holes:

$$N_{h,sc} = N_A^* + N_D^* + n \tag{269}$$

$$N_{h,sc,eff} = N_A^* + G(P_h)N_D^* + f_h \frac{n}{F(P_h)} \tag{270}$$

The effects of clustering of donors (N_D^*) and acceptors (N_A^*) at ultrahigh concentrations are described by 'clustering' functions Z_D and Z_A, which are defined as:

$$N_D^* = N_{D,0}Z_D = N_{D,0}\left[1 + \frac{N_{D,0}^2}{c_D N_{D,0}^2 + N_{D,ref}^2}\right] \tag{271}$$

$$N_A^* = N_{A,0}Z_A = N_{A,0}\left[1 + \frac{N_{A,0}^2}{c_A N_{A,0}^2 + N_{A,ref}^2}\right] \tag{272}$$

The analytic functions $G(P_i)$ and $F(P_i)$ in Eq. 268 and Eq. 270 describe minority impurity and electron–hole scattering. They are given by:

$$F(P_i) = \frac{0.7643 P_i^{0.6478} + 2.2999 + 6.5502(m^*_i/m^*_j)}{P_i^{0.6478} + 2.3670 - 0.8552(m^*_i/m^*_j)} \tag{273}$$

and:

$$G(P_i) = 1 - a_g\left[b_g + P_i\left(\frac{m_0}{m^*_i}\frac{T}{300\,\text{K}}\right)^{\alpha_g}\right]^{-\beta_g} + c_g\left[P_i\left(\frac{m^*_i}{m_0}\frac{300K}{T}\right)^{\alpha'_g}\right]^{-\gamma_g} \tag{274}$$

where m^*_i denotes a fit parameter for carrier i (which is related to the effective carrier mass) and m^*_j denotes a fit parameter for the other carrier.

Screening Parameter

The screening parameter P_i is given by a weighted harmonic mean of the Brooks–Herring approach and Conwell–Weisskopf approach:

$$P_i = \left[\frac{f_{CW}}{3.97 \times 10^{13}\,\text{cm}^{-2} N_{i,\,\text{sc}}^{-2/3}} + f_{BH} \frac{(n+p)}{1.36 \times 10^{20}\,\text{cm}^{-3}} \frac{m_0}{m^*_i} \right]^{-1} \left(\frac{T}{300\,\text{K}} \right)^2 \tag{275}$$

The evaluation of $G(P_i)$ depends on the value of the screening parameter P_i. For values of $P_i < P_{i,\,\text{min}}$, $G(P_{i,\,\text{min}})$ is used instead of $G(P_i)$, where $P_{i,\,\text{min}}$ is the value at which $G(P_i)$ reaches its minimum.

Philips Model Parameters

Table 55 lists the built-in values for the parameters a_g, b_g, c_g, α_g, α'_g, β_g, and γ_g in Eq. 274.

Table 55   Philips unified mobility model parameters

Symbol	Value	Unit
a_g	0.89233	1
b_g	0.41372	1
c_g	0.005978	1
α_g	0.28227	1
α'_g	0.72169	1
β_g	0.19778	1
γ_g	1.80618	1

Other parameters for the Philips unified mobility model are accessible in the parameter set `PhuMob`.

Table 56 and Table 57 on page 332 list the silicon defaults for other parameters. Sentaurus Device supports different parameters for electron mobility, which are optimized for situations where the dominant donor species in the silicon is either arsenic or phosphorus. The arsenic parameters are used by default.

Table 56   Philips unified mobility model: Electron and hole parameters (silicon)

Symbol	Parameter name	Electrons (arsenic)	Electrons (phosphorus)	Holes (boron)	Unit
μ_{max}	`mumax_*`	1417	1414	470.5	cm^2/Vs
μ_{min}	`mumin_*`	52.2	68.5	44.9	cm^2/Vs
θ	`theta_*`	2.285	2.285	2.247	1
$N_{\{e,h\},ref}$	`n_ref_*`	9.68×10^{16}	9.2×10^{16}	2.23×10^{17}	cm^{-3}
α	`alpha_*`	0.68	0.711	0.719	1

The original Philips unified mobility model uses four fit parameters: the weight factors f_{CW} and f_{BH}, and the 'effective masses' m^*_e and m^*_h. The optimal parameter set, determined by accurate fitting to experimental data [10] is shown in Table 57. The Philips unified mobility model can be slightly modified by setting parameters $f_e = 0$ and $f_h = 0$ as required for the Lucent mobility model (see Lucent Model on page 368).

Table 57   Philips unified mobility model: Other fitting parameters (silicon)

Symbol	Parameter name	Value	Unit
m^*_e/m_0	`me_over_m0`	1	1
m^*_h/m_0	`mh_over_m0`	1.258	1
f_{CW}	`f_CW`	2.459	1
f_{BH}	`f_BH`	3.828	1
f_e	`f_e`	1.0	1
f_h	`f_h`	1.0	1

Mobility Degradation at Interfaces

In the channel region of a MOSFET, the high transverse electric field forces carriers to interact strongly with the semiconductor–insulator interface. Carriers are subjected to scattering by acoustic surface phonons and surface roughness. The models in this section describe mobility degradation caused by these effects.

Using Mobility Degradation at Interfaces

To activate mobility degradation at interfaces, select a method to compute the transverse field $F_\perp$ (see Computing Transverse Field on page 354).

To select the calculation of field perpendicular to the semiconductor–insulator interface, specify the `Enormal` option to `Mobility`:

```
Physics { Mobility ( Enormal ...) ...}
```

Alternatively, to select calculation of $F_\perp$ perpendicular to current flow, specify:

```
Physics { Mobility ( ToCurrentEnormal ...) ...}
```

To select a mobility degradation model, specify an option to `Enormal` or `ToCurrentEnormal`. Valid options are `Lombardi`, `IALMob`, `UniBo`, or a PMI model provided by users. In addition, one or more mobility degradation components can be specified. These include `NegInterfaceCharge`, `PosInterfaceCharge`, `Coulomb2D`, `RCS`, and `RPS`. For example:

```
Physics { Mobility ( Enormal(UniBo) ...) ...}
```

selects the University of Bologna model (see University of Bologna Surface Mobility Model on page 345). The default model is `Lombardi` (see Enhanced Lombardi Model on page 334).

> **NOTE** The mobility degradation models discussed in this section are very sensitive to mesh spacing. It is recommended that the vertical mesh spacing be reduced to 0.1 nm in the silicon at the oxide interface underneath the gate. For the extensions of the `Lombardi` model (see Eq. 280, p. 334), even smaller spacing of 0.05 nm is appropriate. This fine spacing is only required in the two uppermost rows of mesh and can be increased progressively moving away from the interface.

Sentaurus Device allows more than one interface degradation mobility model to be used in a simulation. For example, it may be useful to include additional degradation components that are created as PMI models into the `Enormal` mobility calculation. When more than one model is specified as an option to `Enormal`, they are combined using Matthiessen's rule. For example, the specification:

```
Physics { Mobility ( Enormal( Lombardi pmi_model1 pmi_model2) ...) ...}
```

calculates the total `Enormal` mobility using:

$$\frac{1}{\mu_{Enormal}} = \frac{1}{\mu_{Lombardi}} + \frac{1}{\mu_{pmi\_model1}} + \frac{1}{\mu_{pmi\_model2}} \tag{276}$$

Enhanced Lombardi Model

The surface contribution due to acoustic phonon scattering has the form:

$$\mu_{ac} = \frac{B}{F_\perp} + \frac{C((N_{A,0} + N_{D,0} + N_2)/N_0)^\lambda}{F_\perp^{1/3}(T/300\,\text{K})^k} \tag{277}$$

and the contribution attributed to surface roughness scattering is given by:

$$\mu_{sr} = \left(\frac{(F_\perp/F_{ref})^{A^*}}{\delta} + \frac{F_\perp^3}{\eta}\right)^{-1} \tag{278}$$

These surface contributions to the mobility (μ_{ac} and μ_{sr}) are then combined with the bulk mobility μ_b according to Matthiessen's rule (see [Mobility due to Phonon Scattering on page 318](#) and [Doping-Dependent Mobility Degradation on page 318](#)):

$$\frac{1}{\mu} = \frac{1}{\mu_b} + \frac{D}{\mu_{ac}} + \frac{D}{\mu_{sr}} \tag{279}$$

The reference field $F_{ref} = 1\,\text{V/cm}$ ensures a unitless numerator in [Eq. 278](#). $F_\perp$ is the transverse electric field normal to the semiconductor–insulator interface, see [Computing Transverse Field on page 354](#). $D = \exp(-x/l_{crit})$ (where x is the distance from the interface and l_{crit} a fit parameter) is a damping that switches off the inversion layer terms far away from the interface. All other parameters are accessible in the parameter file.

In the Lombardi model [1], the exponent A^* in [Eq. 278](#) is equal to 2. According to another study [11], an improved fit to measured data is achieved if A^* is given by:

$$A^* = A + \frac{(\alpha_{\perp,n}n + \alpha_{\perp,p}p)N_{ref}^\nu}{(N_{A,0} + N_{D,0} + N_1)^\nu} \tag{280}$$

where n and p denote the electron and hole concentrations, respectively. For electron mobility, $\alpha_{\perp,n} = \alpha_\perp$ and $\alpha_{\perp,p} = \alpha_\perp a_{other}$; for hole mobility, $\alpha_{\perp,n} = \alpha_\perp a_{other}$ and $\alpha_{\perp,p} = \alpha_\perp$.

The reference doping concentration $N_{ref} = 1\,\text{cm}^{-3}$ cancels the unit of the term raised to the power ν in the denominator of [Eq. 280](#). The Lombardi model parameters are accessible in the parameter set `EnormalDependence`.

The respective default parameters that are appropriate for silicon are given in [Table 58 on page 335](#). The parameters B, C, N_0, and λ were fitted at SGS Thomson and are not contained in the literature [1].

Table 58   Lombardi model: Default coefficients for silicon

Symbol	Parameter name	Electrons	Holes	Unit
B	B	4.75×10^7	9.925×10^6	cm/s
C	C	5.80×10^2	2.947×10^3	$cm^{5/3}V^{-2/3}s^{-1}$
N_0	N0	1	1	cm^{-3}
N_2	N2	1	1	cm^{-3}
λ	lambda	0.1250	0.0317	1
k	k	1	1	1
δ	delta	5.82×10^{14}	2.0546×10^{14}	cm^2/Vs
A	A	2	2	1
$\alpha_\perp$	alpha	0	0	cm^3
N_1	N1	1	1	cm^{-3}
ν	nu	1	1	1
η	eta	5.82×10^{30}	2.0546×10^{30}	$V^2cm^{-1}s^{-1}$
a_{other}	aother	0	0	1
l_{crit}	l_crit	1×10^{-6}	1×10^{-6}	cm
a_{ac}	a_ac	1.0	1.0	1
a_{sr}	a_sr	1.0	1.0	1

The modifications of the Lombardi model suggested in [11] can be activated by setting $\alpha_\perp$ to a nonzero value.

Table 59 lists a consistent set of parameters for the modified model.

Table 59   Lombardi model: Lucent coefficients for silicon

Symbol	Parameter name	Electrons	Holes	Unit
B	B	3.61×10^7	1.51×10^7	cm/s
C	C	1.70×10^4	4.18×10^3	$cm^{5/3}V^{-2/3}s^{-1}$
N_0	N0	1	1	cm^{-3}
N_2	N2	1	1	cm^{-3}
λ	lambda	0.0233	0.0119	1
k	k	1.7	0.9	1

Table 59   Lombardi model: Lucent coefficients for silicon (Continued)

Symbol	Parameter name	Electrons	Holes	Unit
δ	delta	3.58×10^{18}	4.10×10^{15}	cm^2/Vs
A	A	2.58	2.18	1
$\alpha_\perp$	alpha	6.85×10^{-21}	7.82×10^{-21}	cm^3
N_1	N1	1	1	cm^{-3}
ν	nu	0.0767	0.123	1
η	eta	1×10^{50}	1×10^{50}	$V^2cm^{-1}s^{-1}$
a_{other}	aother	1	1	1
l_{crit}	l_crit	1	1	cm
a_{ac}	a_ac	1.0	1.0	1
a_{sr}	a_sr	1.0	1.0	1

Stress Factors for Mobility Components

If isotropic stress-dependent mobility enhancement factors are applied to mobility components (see Factor Models Applied to Mobility Components on page 876), the `Lombardi` mobility components become:

$$\mu'_{ac} = \gamma_{ac}\mu_{ac} \quad , \quad \gamma_{ac} = 1 + a_{ac}(\gamma - 1)$$
$$\mu'_{sr} = \gamma_{sr}\mu_{sr} \quad , \quad \gamma_{sr} = 1 + a_{sr}(\gamma - 1)$$

(281)

where a_{ac} and a_{sr} are stress scaling parameters that can be specified in the `EnormalDependence` parameter set, and γ is an isotropic enhancement factor calculated from a stress-dependent `Factor` model (see Isotropic Factor Models on page 870).

Named Parameter Sets for Lombardi Model

The `EnormalDependence` parameter set can be named. For example, in the parameter file, you can write:

```
EnormalDependence "myset" { ... }
```

to declare a parameter set with the name `myset`. To use a named parameter set, specify its name with `ParameterSetName` as an option to `Lombardi` in the command file, for example:

```
Mobility (
   Enormal( Lombardi( ParameterSetName = "myset" ...) ...)
)
```

By default, the unnamed parameter set is used.

Auto-Orientation for Lombardi Model

The `Lombardi` model supports the auto-orientation framework (see Auto-Orientation Framework on page 37) that switches between different-named parameter sets based on the orientation of the nearest interface. This can be activated by specifying the `Lombardi` command file parameter `AutoOrientation`:

```
Mobility (
   Enormal( Lombardi( AutoOrientation ...) ...)
)
```

Inversion and Accumulation Layer Mobility Model

The inversion and accumulation layer mobility model (`IALMob`) is based on the *unified* portion of the model described in [12]. This model includes doping and transverse-field dependencies and is similar to the Lucent (Darwish) model [11] but it contains additional terms that account for 'two-dimensional' Coulomb impurity scattering. The implementation of the `IALMob` model is based on modified versions of the Philips Unified Mobility Model on page 328 and the Enhanced Lombardi Model on page 334, but it is completely self-contained and all parameters associated with this model are specified independently of those models. A complete description is given here.

The expressions that follow apply to both electron mobility and hole mobility when the following substitutions are made:

$$\text{Electron Mobility: } c = n, c_{\text{other}} = p, \ N_{\text{inv}} = N_{\text{A},0}, N_{\text{acc}} = N_{\text{D},0}, P = P_{\text{e}}, m^* = m_{\text{e}}^*, m_{\text{other}}^* = m_{\text{h}}^*$$
$$\text{Hole Mobility: } \quad c = p, c_{\text{other}} = n, \ N_{\text{inv}} = N_{\text{D},0}, N_{\text{acc}} = N_{\text{A},0}, P = P_{\text{h}}, m^* = m_{\text{h}}^*, m_{\text{other}}^* = m_{\text{e}}^*$$

(282)

The model has contributions from Coulomb impurity scattering, phonon scattering, and surface roughness scattering:

$$\frac{1}{\mu} = \frac{1}{\mu_C} + \frac{1}{\mu_{\text{ph}}} + \frac{D}{\mu_{\text{sr}}}$$

(283)

where $D = \exp(-x/l_{\text{crit}})$ (x is the distance from the interface).

Coulomb Scattering

The Coulomb impurity scattering term has '2D' and '3D' contributions. The 2D contribution is primarily due to effects occurring near the interface and the 3D contribution is primarily due

to effects occurring in the bulk. These contributions are combined using a field-dependent function $f(F_\perp, t, T)$ and a distance factor D_C:

$$\mu_C = \mu_{C,3D}(1 - D_C) + D_C[f(F_\perp, t, T)\mu_{C,3D} + (1 - f(F_\perp, t, T))\mu_{C,2D}] \tag{284}$$

where:

$$f(F_\perp, t, T) = \cfrac{1}{1 + \exp\left(\cfrac{SF_\perp^{2/3}}{T} + \cfrac{S_t}{(t + t_0)^2 T} - p\right)} \tag{285}$$

and $D_C = \exp(-x/l_{crit,C})$. In Eq. 285, t is the local layer thickness (see Thickness Extraction on page 313), which is calculated automatically when using the `ThinLayer` mobility model (see Thin-Layer Mobility Model on page 356) or if the `LayerThickness` command in the `Physics` section is used to request a layer thickness calculation.

The 2D Coulomb scattering has both inversion and accumulation layer contributions, and also includes a dependency on the local layer thickness:

$$\frac{1}{\mu_{C,2D}} = \text{erf}\left(\frac{t + t_1}{t_{Coulomb}}\right)\left(\frac{1}{\mu_{C,2D,inv}} + \frac{1}{\mu_{C,2D,acc}}\right) \tag{286}$$

where:

$$\mu_{C,2D,inv} = \left[\left(\frac{D_{1,inv}(T/300K)^{\alpha_{1,inv}}(c/10^{18}\ \text{cm}^{-3})^{\nu_{0,inv}}}{(N_{inv}/10^{18}\ \text{cm}^{-3})^{\nu_{1,inv}}}\right)^2 + \left(\frac{D_{2,inv}(T/300K)^{\alpha_{2,inv}}}{(N_{inv}/10^{18}\ \text{cm}^{-3})^{\nu_{2,inv}}}\right)^2\right]^{1/2} \tag{287}$$

$$\mu_{C,2D,acc} = \left[\left(\frac{D_{1,acc}(T/300K)^{\alpha_{1,acc}}(c/10^{18}\ \text{cm}^{-3})^{\nu_{0,acc}}}{(N_{acc}/10^{18}\ \text{cm}^{-3})^{\nu_{1,acc}}}\right)^2 + \left(\frac{D_{2,acc}(T/300K)^{\alpha_{2,acc}}}{(N_{acc}/10^{18}\ \text{cm}^{-3})^{\nu_{2,acc}}}\right)^2\right]^{1/2} G(P) \tag{288}$$

The 3D Coulomb scattering part of Eq. 284 is taken from the Philips unified mobility model (`PhuMob`) and is given by:

$$\mu_{C,3D} = \mu_N\left(\frac{N_{sc}}{N_{sc,eff}}\right)\left(\frac{N_{ref}}{N_{sc}}\right)^\alpha + \mu_c\left(\frac{c + c_{other}}{N_{sc,eff}}\right) \tag{289}$$

where:

$$\mu_N = \frac{\mu_{max}^2}{\mu_{max} - \mu_{min}}\left(\frac{T}{300K}\right)^{3\alpha - 1.5} \tag{290}$$

$$\mu_c = \frac{\mu_{max}\mu_{min}}{\mu_{max} - \mu_{min}} \left(\frac{300\text{K}}{T}\right)^{1/2} \tag{291}$$

$$N_{sc} = N_D^* + N_A^* + c_{other} \tag{292}$$

$$N_{sc,eff} = N_{acc}^* + G(P)N_{inv}^* + \frac{c_{other}}{F(P)} \tag{293}$$

In the previous expressions, quantities marked with an asterisk (*) indicate that the clustering formulas from the Philips unified mobility model are invoked:

$$N_D^* = N_{D,0}\left[1 + \frac{N_{D,0}^2}{c_D N_{D,0}^2 + N_{D,ref}^2}\right] \tag{294}$$

$$N_A^* = N_{A,0}\left[1 + \frac{N_{A,0}^2}{c_A N_{A,0}^2 + N_{A,ref}^2}\right] \tag{295}$$

As an option, the clustering formulas can be used for all occurrences of N_A and N_D in the model by specifying the `IALMob` command file parameter `ClusteringEverywhere`.

The functions $F(P)$ and $G(P)$ describe electron–hole and minority impurity scattering, respectively, and P is a screening parameter:

$$F(P) = \frac{0.7643 P^{0.6478} + 2.2999 + 6.5502(m^*/m^*_{other})}{P^{0.6478} + 2.3670 - 0.8552(m^*/m^*_{other})} \tag{296}$$

$$G(P) = 1 - \frac{0.89233}{\left[0.41372 + P\left(\frac{m_0}{m^*}\frac{T}{300\text{K}}\right)^{0.28227}\right]^{0.19778}} + \frac{0.005978}{\left[P\left(\frac{m^*}{m_0}\frac{300\text{K}}{T}\right)^{0.72169}\right]^{1.80618}} \tag{297}$$

$$P = \left[\frac{2.459}{3.97 \times 10^{13} \text{ cm}^{-2} N_{sc}^{-2/3}} + \frac{3.828(c + c_{other})(m_0/m^*)}{1.36 \times 10^{20} \text{ cm}^{-3}}\right]^{-1}\left(\frac{T}{300\text{K}}\right)^2 \tag{298}$$

By default, the full `PhuMob` model described by the previous expressions is used (`FullPhuMob`). However, the 'other' carrier in these expressions can be ignored ($c_{other} = 0$) by specifying `-FullPhuMob` in the command file. This specification also ignores the standard `PhuMob` modification of the $G(P)$ function, which invokes $G = G(P_{min})$ for $P < P_{min}$, where P_{min} is the value where $G(P)$ reaches its minimum.

Phonon Scattering

The phonon-scattering portion of Eq. 283 also has 2D and 3D parts. The way in which these parts are combined depends on the value of the `IALMob` command file parameter `PhononCombination`:

$$
\mu_{ph} = \begin{cases}
\min\left\{ \dfrac{\mu_{ph,2D}}{D}, \mu_{ph,3D} \right\} & , \texttt{PhononCombination=0} \\[2ex]
\left[\dfrac{D}{\mu_{ph,2D}} + \dfrac{1}{\mu_{ph,3D}} \right]^{-1} & , \texttt{PhononCombination=1 (default)} \\[2ex]
\left[\dfrac{D}{\mu_{ph,2D}} + \dfrac{f(F_\perp, t, T)}{\mu_{ph,3D}} \right]^{-1} & , \texttt{PhononCombination=2}
\end{cases}
\tag{299}
$$

where:

$$
\mu_{ph,2D} = \frac{B}{F_\perp} + \frac{C\left(\alpha_{ph,2D,A}((N_{A,0} + N_2/2)/1\ \text{cm}^{-3})^{\lambda_{ph,2D,A}} + \alpha_{ph,2D,D}((N_{D,0} + N_2/2)/1\ \text{cm}^{-3})^{\lambda_{ph,2D,D}} \right)^{\lambda}}{F_\perp^{1/3}(T/300\,\text{K})^k}
\tag{300}
$$

$$
\mu_{ph,3D} = \mu_{max}\left(\frac{T}{300\,\text{K}} \right)^{-\theta}
\tag{301}
$$

Surface Roughness Scattering

Surface roughness scattering is given by:

$$
\mu_{sr} = \frac{\left(\alpha_{sr,A}((N_{A,0} + N_2/2)/1\ \text{cm}^{-3})^{\lambda_{sr,A}} + \alpha_{sr,D}((N_{D,0} + N_2/2)/1\ \text{cm}^{-3})^{\lambda_{sr,D}} \right)^{\lambda_{sr}}}{\left(\dfrac{(F_\perp/1\ \text{V/cm})^{A^*}}{\delta} + \dfrac{F_\perp^3}{\eta} \right)}
\tag{302}
$$

where:

$$
A^* = A + \frac{\alpha_\perp(n + p)}{((N_{A,0} + N_{D,0} + N_1)/1\ \text{cm}^{-3})^{\nu}}
\tag{303}
$$

Parameters

Parameters associated with the model are accessible in the `IALMob` parameter set. Their values for silicon are shown in Table 60 and Table 61.

Table 60   IALMob parameters (part 1): Default coefficients for silicon

Symbol	Parameter name	Value	Unit
–	EnormMinimum	0.0	V/cm
$N_{D,ref}$	nref_D	4×10^{20}	cm^{-3}
$N_{A,ref}$	nref_A	7.2×10^{20}	cm^{-3}
c_D	cref_D	0.21	1
c_A	cref_A	0.5	1
m_e^*/m_0	me_over_m0	1.0	1
m_h^*/m_0	mh_over_m0	1.258	1

Table 61   IALMob parameters (part 2): Default coefficients for silicon

Symbol	Parameter name	Electron value	Hole value	Unit
μ_{max}	mumax	1417.0	470.5	$cm^2/(Vs)$
μ_{min}	mumin	52.2	44.9	$cm^2/(Vs)$
θ	theta	2.285	2.247	1
N_{ref}	n_ref	9.68×10^{16}	2.23×10^{17}	cm^{-3}
α	alpha	0.68	0.719	1
S	S	0.3042	0.3042	$K(cm/V)^{2/3}$
S_t	S_t	0.0	0.0	$K(\mu m)^2$
t_0	t0	0.0005	0.0005	μm
p	p	4.0	4.0	1
$l_{crit,C}$	l_crit_c	10^3	10^3	cm
B	B	9.0×10^5	9.0×10^5	cm/s
C	C	4400.0	4400.0	$cm^{5/3}/V^{2/3}/s$
λ	lambda	0.057	0.057	1
k	k	1.0	1.0	1
$\alpha_{ph,2D,A}$	alpha_ph2d_A	1.0	1.0	1

Table 61   IALMob parameters (part 2): Default coefficients for silicon (Continued)

Symbol	Parameter name	Electron value	Hole value	Unit
$\alpha_{\text{ph,2D,D}}$	alpha_ph2d_D	1.0	1.0	1
$\lambda_{\text{ph,2D,A}}$	lambda_ph2d_A	1.0	1.0	1
$\lambda_{\text{ph,2D,D}}$	lambda_ph2d_D	1.0	1.0	1
δ	delta	3.97×10^{13}	3.97×10^{13}	$cm^2/(Vs)$
λ_{sr}	lambda_sr	0.057	0.057	1
A	A	2.0	2.0	1
$\alpha_\perp$	alpha_sr	0.0	0.0	cm^3
ν	nu	0.0	0.0	1
η	eta	1.0×10^{50}	1.0×10^{50}	$V^2/cm/s$
N_1	N1	1.0	1.0	cm^{-3}
N_2	N2	1.0	1.0	cm^{-3}
$\alpha_{\text{sr,A}}$	alpha_sr_A	1.0	1.0	1
$\alpha_{\text{sr,D}}$	alpha_sr_D	1.0	1.0	1
$\lambda_{\text{sr,A}}$	lambda_sr_A	1.0	1.0	1
$\lambda_{\text{sr,D}}$	lambda_sr_D	1.0	1.0	1
l_{crit}	l_crit	10^3	10^3	cm
$D_{1,\text{inv}}$	D1_inv	135.0	135.0	$cm^2/(Vs)$
$D_{2,\text{inv}}$	D2_inv	40.0	40.0	$cm^2/(Vs)$
$\nu_{0,\text{inv}}$	nu0_inv	1.5	1.5	1
$\nu_{1,\text{inv}}$	nu1_inv	2.0	2.0	1
$\nu_{2,\text{inv}}$	nu2_inv	0.5	0.5	1
$\alpha_{1,\text{inv}}$	alpha1_inv	0.0	0.0	1
$\alpha_{2,\text{inv}}$	alpha2_inv	0.0	0.0	1
$D_{1,\text{acc}}$	D1_acc	135.0	135.0	$cm^2/(Vs)$
$D_{2,\text{acc}}$	D2_acc	40.0	40.0	$cm^2/(Vs)$
$\nu_{0,\text{acc}}$	nu0_acc	1.5	1.5	1
$\nu_{1,\text{acc}}$	nu1_acc	2.0	2.0	1

Table 61   IALMob parameters (part 2): Default coefficients for silicon (Continued)

Symbol	Parameter name	Electron value	Hole value	Unit
$\nu_{2,\text{acc}}$	nu2_acc	0.5	0.5	1
$\alpha_{1,\text{acc}}$	alpha1_acc	0.0	0.0	1
$\alpha_{2,\text{acc}}$	alpha2_acc	0.0	0.0	1
t_{Coulomb}	tcoulomb	0.0	0.0	μm
t_1	t1	0.0003	0.0003	μm
$a_{\text{ph,2D}}$	a_ph2d	1.0	1.0	1
$a_{\text{ph,3D}}$	a_ph3d	1.0	1.0	1
$a_{\text{C,2D}}$	a_c2d	1.0	1.0	1
$a_{\text{C,3D}}$	a_c3d	1.0	1.0	1
a_{sr}	a_sr	1.0	1.0	1

Stress Factors for Mobility Components

If isotropic stress-dependent mobility enhancement factors are applied to mobility components (see Factor Models Applied to Mobility Components on page 876), the IALMob mobility components become:

$$
\begin{aligned}
\mu'_{\text{ph,2D}} &= \gamma_{\text{ph,2D}}\mu_{\text{ph,2D}} \; , \; \gamma_{\text{ph,2D}} = 1 + a_{\text{ph,2D}}(\gamma - 1) \\
\mu'_{\text{ph,3D}} &= \gamma_{\text{ph,3D}}\mu_{\text{ph,3D}} \; , \; \gamma_{\text{ph,3D}} = 1 + a_{\text{ph,3D}}(\gamma - 1) \\
\mu'_{\text{C,2D}} &= \gamma_{\text{C,2D}}\mu_{\text{C,2D}} \; , \; \gamma_{\text{C,2D}} = 1 + a_{\text{C,2D}}(\gamma - 1) \\
\mu'_{\text{C,3D}} &= \gamma_{\text{C,3D}}\mu_{\text{C,3D}} \; , \; \gamma_{\text{C,3D}} = 1 + a_{\text{C,3D}}(\gamma - 1) \\
\mu'_{\text{sr}} &= \gamma_{\text{sr}}\mu_{\text{sr}} \; , \; \gamma_{\text{sr}} = 1 + a_{\text{sr}}(\gamma - 1)
\end{aligned}
\tag{304}
$$

where $a_{\text{ph,2D}}$, $a_{\text{ph,3D}}$, $a_{\text{C,2D}}$, $a_{\text{C,3D}}$, and a_{sr} are stress scaling parameters that can be specified in the IALMob parameter set, and γ is an isotropic enhancement factor calculated from a stress-dependent Factor model (see Isotropic Factor Models on page 870).

Using Inversion and Accumulation Layer Mobility Model

The inversion and accumulation layer mobility model is selected by specifying the IALMob keyword as an argument to Enormal in the command file. No mobility DopingDependence should be specified, as this is already included in the model. It is also not necessary to specify -ConstantMobility, as this will be invoked automatically with IALMob.

For small values of $F_\perp$, the acoustic phonon and surface roughness components of `IALMob` make an insignificant contribution to the total mobility. If required, the parameter `EnormMinimum` can be specified (in the parameter file) to suppress the calculation of acoustic phonon scattering and surface roughness for $F_\perp <$ `EnormMinimum`.

The complete model described in [12] is obtained by combining `IALMob` with the Hänsch model [13] for high-field saturation (see Extended Canali Model on page 363), for example:

```
Physics {
   Mobility (
      Enormal(IALMob)
      HighFieldSaturation
   )
}
```

To select the Hänsch model, specify the parameter $\alpha = 1$ in the `HighFieldDependence` section. In addition, the β exponent in the Hänsch model is equal to 2, which can be specified by setting $\beta_0 = 2$ and $\beta_{exp} = 0$:

```
HighFieldDependence {
   alpha   = 1.0, 1.0    # [1]
   beta0   = 2.0, 2.0    # [1]
   betaexp = 0.0, 0.0
}
```

Named Parameter Sets for IALMob

The `IALMob` parameter set can be named. For example, in the parameter file, you can write:

```
IALMob "myset" { ... }
```

to declare a parameter set with the name `myset`. To use a named parameter set, specify its name with `ParameterSetName` as an option to `IALMob` in the command file, for example:

```
Mobility (
   Enormal( IALMob( ParameterSetName = "myset" ...) ...)
)
```

By default, the unnamed parameter set is used.

Auto-Orientation for IALMob

The `IALMob` model supports the auto-orientation framework (see Auto-Orientation Framework on page 37) that switches between different named parameter sets based on the orientation of the nearest interface. This can be activated by specifying the `IALMob` command file parameter `AutoOrientation`:

```
Mobility (
    Enormal( IALMob( AutoOrientation ...) ...)
)
```

University of Bologna Surface Mobility Model

The University of Bologna surface mobility model was developed for an extended temperature range between $25°C$ and $648°C$. It should be used together with the University of Bologna bulk mobility model (see University of Bologna Bulk Mobility Model on page 322). The inversion layer mobility in MOSFETs is degraded by Coulomb scattering at low normal fields and by surface phonons and surface roughness scattering at large normal fields.

In the University of Bologna model [4], all these effects are combined by using Matthiessen's rule:

$$\frac{1}{\mu} = \frac{1}{\mu_{bsc}} + \frac{D}{\mu_{ac}} + \frac{D}{\mu_{sr}} \tag{305}$$

where $1/\mu_{bsc}$ is the contribution of Coulomb scattering, and $1/\mu_{ac}$, $1/\mu_{sr}$ are those of surface phonons and surface roughness scattering, respectively. $D = \exp(-x/l_{crit})$ (where x is the distance from the interface and l_{crit} a fit parameter) is a damping that switches off the inversion layer terms far away from the interface.

The term μ_{bsc} is associated with substrate impurity and carrier concentration. It is decomposed in an unscreened part (due to the impurities) and a screened part (due to local excess carrier concentration):

$$\mu_{bsc}^{-1} = \mu_b^{-1}[D(1+f_{sc}^{\tau})^{-1/\tau} + (1-D)] \tag{306}$$

where μ_b is given by the bulk mobility model, and τ is a fit parameter. The screening function is given by:

$$f_{sc} = \left(\frac{N_1}{N_{A,0}+N_{D,0}}\right)^{\eta} \frac{N_{min}}{N_{A,0}+N_{D,0}} \tag{307}$$

where N_{min} is the minority carrier concentration.

If surface mobility is plotted against the effective normal field, mobility data converges toward a universal curve. Deviations from this curve appear at the onset of weak inversion, and the threshold field changes with the impurity concentration at the semiconductor surface [14]. The term μ_{bsc} models these deviations, in that, it is the roll-off in the effective mobility characteristics. As the effective field increases, the mobilities become independent of the channel doping and approach the universal curve.

The main scattering mechanisms are, in this case, surface phonons and surface roughness scattering, which are expressed by:

$$\mu_{ac} = C(T)\left(\frac{N_{A,0} + N_{D,0}}{N_2}\right)^a \frac{1}{F_\perp{}^\delta} \tag{308}$$

$$\mu_{sr} = B(T)\left(\frac{N_{A,0} + N_{D,0} + N_3}{N_4}\right)^b \frac{1}{F_\perp{}^\lambda} \tag{309}$$

$F_\perp$ is the electric field normal to semiconductor–insulator interface, see Computing Transverse Field on page 354.

The parameters for the model are accessible in the parameter set `UniBoEnormalDependence`. Table 62 lists the silicon default parameters. The reported parameters are detailed in the literature [15]. The model was calibrated with experiments [14][15] in the temperature range from $300\,\text{K}$ to $700\,\text{K}$.

Table 62   Parameters of University of Bologna surface mobility model ($T_n = T/300$ K)

Symbol	Parameter name	Electrons	Holes	Unit
N_1	N1	2.34×10^{16}	2.02×10^{16}	cm^{-3}
N_2	N2	4.0×10^{15}	7.8×10^{15}	cm^{-3}
N_3	N3	1.0×10^{17}	2.0×10^{15}	cm^{-3}
N_4	N4	2.4×10^{18}	6.6×10^{17}	cm^{-3}
B	B	$5.8 \times 10^{18}\ T_n^{\gamma_B}$	$7.82 \times 10^{15}\ T_n^{\gamma_B}$	cm^2/Vs
γ_B	B_exp	0	1.4	1
C	C	$1.86{\times}10^4 T_n^{-\gamma_C}$	$5.726{\times}10^3 T_n^{-\gamma_C}$	cm^2/Vs
γ_C	C_exp	2.1	1.3	1
τ	tau	1	3	1
η	eta	0.3	0.5	1
a	ac_exp	0.026	–0.02	1

Table 62   Parameters of University of Bologna surface mobility model ($T_n = T/300$ K) (Continued)

Symbol	Parameter name	Electrons	Holes	Unit
b	sr_exp	0.11	0.08	1
l_{crit}	l_crit	1×10^{-6}	1×10^{-6}	cm
δ	delta	0.29	0.3	1
λ	lambda	2.64	2.24	1

Mobility Degradation Components due to Coulomb Scattering

Three mobility degradation components due to Coulomb scattering are available in Sentaurus Device that can be combined with other interface mobility degradation models:

- `NegInterfaceCharge`: Accounts for mobility degradation due to a negative interface charge (from charged traps and fixed charge).
- `PosInterfaceCharge`: Accounts for mobility degradation due to a positive interface charge (from charged traps and fixed charge).
- `Coulomb2D`: Accounts for mobility degradation due to ionized impurities near the interface.

These degradation components can be specified separately or in combination with each other. If specified, they will be combined using Matthiessen's rule:

$$\frac{1}{\mu} = \frac{1}{\mu_{other}} + \frac{1}{\mu_{nic}} + \frac{1}{\mu_{pic}} + \frac{1}{\mu_{C2D}}$$

(310)

where:

- μ_{other} represents the other `DopingDependence` and `Enormal` models specified for the simulation.
- μ_{nic} represents the `NegInterfaceCharge` mobility degradation component.
- μ_{pic} represents the `PosInterfaceCharge` mobility degradation component.
- μ_{C2D} represents the `Coulomb2D` mobility degradation component.

The general form of the mobility degradation components due to Coulomb scattering is given by:

$$\mu_C = \frac{\mu_1 \left(\dfrac{T}{300\,\text{K}}\right)^k \left\{ 1 + \left[c \Big/ \left(c_{\text{trans}} \left(\dfrac{N_{\text{A,D}} + N_1}{10^{18}\,\text{cm}^{-3}}\right)^{\gamma_1} \left(\dfrac{N_{\text{coulomb}}}{N_0}\right)^{\eta_1} \right) \right]^{\nu} \right\}}{\left(\dfrac{N_{\text{A,D}} + N_2}{10^{18}\,\text{cm}^{-3}}\right)^{\gamma_2} \left(\dfrac{N_{\text{coulomb}}}{N_0}\right)^{\eta_2} \cdot D \cdot f(F_\perp)} \tag{311}$$

where:

- $N_{\text{coulomb}} = \begin{cases} \text{negative interface charge density,} & \text{for the NegInterfaceCharge component} \\ \text{positive interface charge density,} & \text{for the PosInterfaceCharge component} \\ \text{local } N_{\text{A,D}}, & \text{for the Coulomb2D component} \end{cases}$

- $N_0 = \begin{cases} 10^{11}\,\text{cm}^{-2}, & \text{for the Neg/PosInterfaceCharge components} \\ 10^{18}\,\text{cm}^{-3}, & \text{for the Coulomb2D component} \end{cases}$

- $c = n$ (electron mobility) or p (hole mobility)

- $N_{\text{A,D}} = N_{\text{A,0}}$ (electron mobility) or $N_{\text{D,0}}$ (hole mobility)

and:

$$f(F_\perp) = 1 - \exp[-(F_\perp/E_0)^\gamma] \tag{312}$$

$$D = \exp(-x/l_{\text{crit}}) \tag{313}$$

In Eq. 313, x is the distance from the interface.

Parameters associated with the components are accessible in the parameter sets `NegInterfaceChargeMobility`, `PosInterfaceChargeMobility`, and `Coulomb2DMobility`. Table 63 lists their default values.

Table 63   Parameters for mobility degradation components due to Coulomb scattering

Symbol	Parameter name	μ_{nic} Electron	μ_{nic} Hole	μ_{pic} Electron	μ_{pic} Hole	μ_{C2D} Electron	μ_{C2D} Hole	Unit
μ_1	mu1	40.0	40.0	40.0	40.0	40.0	40.0	$\text{cm}^2\text{V}^{-1}\text{s}^{-1}$
k	T_exp	1.0	1.0	1.0	1.0	1.0	1.0	1
c_{trans}	c_trans	10^{18}	10^{18}	10^{18}	10^{18}	10^{18}	10^{18}	cm^{-3}

Table 63   Parameters for mobility degradation components due to Coulomb scattering
(Continued)

Symbol	Parameter name	μ_{nic} **Electron**	μ_{nic} **Hole**	μ_{pic} **Electron**	μ_{pic} **Hole**	μ_{C2D} **Electron**	μ_{C2D} **Hole**	Unit
ν	c_exp	1.5	1.5	1.5	1.5	1.5	1.5	1
η_1	Nc_exp1	1.0	1.0	1.0	1.0	1.0	1.0	1
η_2	Nc_exp2	0.5	0.5	0.5	0.5	0.5	0.5	1
N_1	N1	1.0	1.0	1.0	1.0	1.0	1.0	cm^{-3}
N_2	N2	1.0	1.0	1.0	1.0	1.0	1.0	cm^{-3}
γ_1	N_exp1	0.0	0.0	0.0	0.0	0.0	0.0	1
γ_2	N_exp2	0.0	0.0	0.0	0.0	0.0	0.0	1
l_{crit}	l_crit	10^{-6}	10^{-6}	10^{-6}	10^{-6}	10^{-6}	10^{-6}	cm
E_0	E0	$2.0{\times}10^5$	$2.0{\times}10^5$	$2.0{\times}10^5$	$2.0{\times}10^5$	$2.0{\times}10^5$	$2.0{\times}10^5$	V/cm
γ	En_exp	2.0	2.0	2.0	2.0	2.0	2.0	1
a_C	a_c	1.0	1.0	1.0	1.0	1.0	1.0	1

Stress Factors for Mobility Components

If isotropic stress-dependent mobility enhancement factors are applied to mobility components (see Factor Models Applied to Mobility Components on page 876), the Coulomb degradation component becomes:

$$\mu'_C = \gamma_C \mu_C \, , \; \gamma_C = 1 + a_C(\gamma - 1) \tag{314}$$

where a_C is a stress scaling parameter that can be specified in the NegInterfaceChargeMobility, PosInterfaceChargeMobility, or Coulomb2DMobility parameter set, and γ is an isotropic enhancement factor calculated from a stress-dependent Factor model (see Isotropic Factor Models on page 870).

Using Mobility Degradation Components

The Coulomb2D model is a local model that uses local values of N_A and N_D. To use this model, specify Coulomb2D in addition to the standard Enormal model, for example:

```
Physics {
   Mobility (
      PhuMob HighFieldSaturation
      Enormal (Lombardi Coulomb2D)
```

```
      )
   }
```

The `NegInterfaceCharge` and `PosInterfaceCharge` models are nonlocal models because N_C used in these models is a charge density at a location that may be different from the point where mobility is being calculated.

If `Math{-GeometricDistances}` is not specified, $N_{coulomb}$ is the charge density at the point on the interface that is the closest distance to the point where mobility is being calculated. If there is not a vertex at this interface point, $N_{coulomb}$ is interpolated from the charge density at the surrounding vertices.

If `Math{-GeometricDistances}` is specified, $N_{coulomb}$ is the charge density at the vertex on the interface that is the closest distance to the point where mobility is being calculated.

To use these models, specify `NegInterfaceCharge`, or `PosInterfaceCharge`, or both in addition to a standard `Enormal` model. For convenience, both models can be specified with the single keyword `InterfaceCharge`, for example:

```
Physics {
   Mobility (
      PhuMob HighFieldSaturation
      Enormal (Lombardi InterfaceCharge)
   )
}
```

> **NOTE** When using mobility degradation components, a standard `Enormal` model (such as `Lombardi`) must be specified explicitly in addition to the mobility degradation component. Sentaurus Device will not include the `Lombardi` model by default (this only occurs when `Enormal` is specified with no arguments).

By default, the `NegInterfaceCharge` and `PosInterfaceCharge` models use the charge density $N_{coulomb}$ located at the nearest semiconductor–insulator interface. Alternatively, these models can use the charge density at the nearest user-defined surface by specifying the surface name as an argument to the interface charge model. For example:

```
Physics {
   Mobility (
      PhuMob  HighFieldSaturation
      Enormal (Lombardi
        NegInterfaceCharge(SurfaceName="S1")
        PosInterfaceCharge(SurfaceName="S2")
        ...
      )
   )
}
```

Surfaces are defined in the global `Math` section and represent the union of an arbitrary number of interfaces. The following example specifies a surface named `S1` that consists of all the HfO$_2$–oxide interfaces, as well as the `region_1–region_2` interface:

```
Math {
    Surface "S1" (
        MaterialInterface="HfO2/Oxide"
        RegionInterface="region_1/region_2"
    )
}
```

Remote Coulomb Scattering Model

High-k gate dielectrics are being considered as an alternative to SiO$_2$ to reduce unacceptable leakage currents as transistor dimensions decrease. One obstacle when using high-k gate dielectrics is that a degraded carrier mobility is often observed for such devices. Although the causes of high-k mobility degradation are not completely understood, a possible contributor is remote Coulomb scattering (RCS).

Sentaurus Device provides an empirical model for RCS degradation that can be combined with other `Enormal` models using Matthiessen's rule:

$$\frac{1}{\mu_{Enormal}} = \frac{1}{\mu_{Enormal_1}} + \frac{1}{\mu_{Enormal_2}} + ... + \frac{D_{rcs}D_{rcs\_highk}}{\mu_{rcs}} \tag{315}$$

The `RCS` model is taken from [16] and accounts for the mobility degradation observed with HfSiON MISFETs. This is attributed to RCS:

$$\mu_{rcs} = \mu_{rcs0}\left(\frac{N_{A,D}}{3 \times 10^{16}\,cm^{-3}}\right)^{\gamma_1}\left(\frac{T}{300\,K}\right)^{\gamma_2}(g_{screening})^{\gamma_3 + \gamma_4 \cdot \ln\left(\frac{N_{A,D}}{3 \times 10^{16}\,cm^{-3}}\right)}/f(F_\perp) \tag{316}$$

where:

- $N_{A,D} = N_{A,0}$ (electron mobility) or $N_{D,0}$ (hole mobility)

In Eq. 316, the $g_{screening}$ factor accounts for screening of the remote charge by carriers. In [16], this is expressed in terms of the inversion charge density. Here, a local expression that depends on carrier concentration is used:

$$g_{screening} = s + \frac{c}{c_0\left(\frac{N_{A,D}}{3 \times 10^{16}\,cm^{-3}}\right)^{\gamma_5}} \tag{317}$$

In Eq. 317, c is the carrier concentration (n for electron mobility and p for hole mobility), and s, c_0, and γ_5 are parameters.

In Eq. 316, $f(F_\perp)$ is a function that confines the degradation to areas of the structure where $F_\perp$ is large enough to initiate inversion:

$$f(F_\perp) = 1 - \exp(-\xi F_\perp / N_{\text{depl}})$$ (318)

In the above expression, N_{depl} is a doping- and temperature-dependent approximation for the depletion charge density $[\text{cm}^{-2}]$.

The distance factors used in Eq. 315 are given by:

$$D_{\text{rcs}} = \exp(-(\text{dist} + d_{\text{crit}})/l_{\text{crit}})$$ (319)

$$D_{\text{rcs\_highk}} = \exp(-\text{dist}_{\text{highk}}/l_{\text{crit\_highk}})$$ (320)

In these expressions, dist is the distance from the nearest semiconductor–insulator interface, and $\text{dist}_{\text{highk}}$ is the distance from the nearest high-k insulator. If no high-k insulator is found in the structure, $D_{\text{rcs\_highk}} = 1$.

Parameters used in the RCS model are accessible in the RCSMobility parameter set in the parameter file. Values for silicon are shown in Table 64.

Table 64   RCSMobility parameters: Default coefficients for silicon

Symbol	Parameter name	Electron value	Hole value	Unit
μ_{rcs0}	murcs0	149.0	149.0	cm^2/Vs
γ_1	gamma1	–0.23187	–0.23187	1
γ_2	gamma2	2.1	2.1	1
γ_3	gamma3	0.40	0.40	1
γ_4	gamma4	0.05	0.05	1
γ_5	gamma5	1.0	1.0	1
s	s	0.1	0.1	1
c_0	c0	3.0×10^{16}	3.0×10^{16}	cm^{-3}
d_{crit}	d_crit	0.0	0.0	cm
l_{crit}	l_crit	1×10^{-6}	1×10^{-6}	cm
$l_{\text{crit\_highk}}$	l_crit_highk	1×10^{6}	1×10^{6}	cm

Table 64   RCSMobility parameters: Default coefficients for silicon (Continued)

Symbol	Parameter name	Electron value	Hole value	Unit
ξ	xi	1.3042×10^7	1.3042×10^7	$V^{-1}cm^{-1}$
a_{rcs}	a_rcs	1.0	1.0	1

Stress Factors for Mobility Components

If isotropic stress-dependent mobility enhancement factors are applied to mobility components (see Factor Models Applied to Mobility Components on page 876), the RCS degradation becomes:

$$\mu'_{rcs} = \gamma_{rcs}\mu_{rcs} \quad , \quad \gamma_{rcs} = 1 + a_{rcs}(\gamma - 1) \tag{321}$$

where a_{rcs} is a stress scaling parameter that can be specified in the RCSMobility parameter set, and γ is an isotropic enhancement factor calculated from a stress-dependent Factor model (see Isotropic Factor Models on page 870).

Remote Phonon Scattering Model

Sentaurus Device also provides a simple empirical model for remote phonon scattering (RPS) degradation that can be combined with other Enormal models using Matthiessen's rule:

$$\frac{1}{\mu_{Enormal}} = \frac{1}{\mu_{Enormal_1}} + \frac{1}{\mu_{Enormal_2}} + ... + \frac{D_{rps}D_{rps\_highk}}{\mu_{rps}} \tag{322}$$

The RPS model is extracted from figures in [17] and accounts for a portion of the mobility degradation observed with HfO_2-gated MOSFETs. This term is attributed to RPS:

$$\mu_{rps} = \frac{\mu_{rps0}}{\left(\dfrac{F_\perp}{10^6 \ V/cm}\right)^{\gamma_1}\left(\dfrac{T}{300 \ K}\right)^{\gamma_2}} \tag{323}$$

The distance factors used in Eq. 322 are given by:

$$D_{rps} = \exp(-(dist + d_{crit})/l_{crit}) \tag{324}$$

$$D_{rps\_highk} = \exp(-dist_{highk}/l_{crit\_highk}) \tag{325}$$

In these expressions, dist is the distance from the nearest semiconductor–insulator interface, and $dist_{highk}$ is the distance from the nearest high-k insulator. If no high-k insulator is found in the structure, $D_{rps\_highk} = 1$.

Parameters used in the `RPS` model are accessible in the `RPSMobility` parameter set in the parameter file. Values for silicon are shown in Table 65.

Table 65   RPSMobility parameters: Default coefficients for silicon

Symbol	Parameter Name	Electron value	Hole value	Unit
μ_{rps0}	`murps0`	496.7	496.7	cm^2/Vs
γ_1	`gamma1`	0.68	0.68	1
γ_2	`gamm2`	0.34	0.34	1
d_{crit}	`d_crit`	0.0	0.0	cm
l_{crit}	`l_crit`	1×10^{-6}	1×10^{-6}	cm
l_{crit_highk}	`l_crit_highk`	1×10^{6}	1×10^{6}	cm
a_{rps}	`a_rcs`	1.0	1.0	1

Stress Factors for Mobility Components

If isotropic stress-dependent mobility enhancement factors are applied to mobility components (see Factor Models Applied to Mobility Components on page 876), the `RPS` degradation becomes:

$$\mu'_{rps} = \gamma_{rps}\mu_{rps} \quad , \quad \gamma_{rps} = 1 + a_{rps}(\gamma - 1) \tag{326}$$

where a_{rps} is a stress scaling parameter that can be specified in the `RPSMobility` parameter set, and γ is an isotropic enhancement factor calculated from a stress-dependent `Factor` model (see Isotropic Factor Models on page 870).

Computing Transverse Field

Sentaurus Device supports two different methods for computing the normal electric field $F_\perp$:

- Using the normal to the interface.
- Using the normal to the current.

Furthermore, for vertices at the interface, an optional correction F_{corr} for the field value is available.

Normal to Interface

Assume that mobility degradation occurs at an interface Γ. By default, the distance to the interface is the true geometric distance, and $\hat{n}$ is the gradient of the distance to the interface. When the -GeometricDistances option is specified in the Math section, for a given point $\vec{r}$, Sentaurus Device locates the nearest vertex $\vec{r}_i$ on the interface Γ, approximates the distance of $\vec{r}$ to the interface by the distance to $\vec{r}_i$, and determines the direction $\hat{n}$ normal to the interface at vertex $\vec{r}_i$. From $\hat{n}$, the normal electric field is:

$$F_\perp(\vec{r}) = \left| \vec{F}(\vec{r}) \cdot \hat{n} + F_{\text{corr}} \right| \tag{327}$$

To activate the Lombardi model with this method of computing $F_\perp$, specify the Enormal flag to Mobility. The keyword ToInterfaceEnormal is synonymous with Enormal.

By default, the interface Γ is a semiconductor–insulator interface. Sometimes, it is important to change this default interface definition, for example, when the insulator (oxide) is considered a wide-bandgap semiconductor. In this case, Sentaurus Device allows this interface to be specified with EnormalInterface in the Math section.

In the following example, Sentaurus Device takes as Γ the union of interfaces between materials, OxideAsSemiconductor and Silicon, and regions, regionK1 and regionL1:

```
Math {
    EnormalInterface (
        regioninterface=["regionK1/regionL1"],
        materialinterface=["OxideAsSemiconductor/Silicon"]
    )
}
```

Normal to Current Flow

Using this method, $F_\perp(\vec{r})$ is defined as the component of the electric field normal to the electron ($c = n$) or hole ($c = p$) currents $\vec{J}_c(\vec{r})$:

$$F_{c,\perp}(\vec{r}) = F(\vec{r}) \sqrt{1 - \left(\frac{\vec{F}(\vec{r}) \cdot \vec{J}_c(\vec{r})}{F(\vec{r})J_c(\vec{r})} \right)^2} + F_{\text{corr}} \tag{328}$$

where $F_{n,\perp}$ is used for the evaluation of electron mobility and $F_{p,\perp}$ is used for the evaluation of hole mobility. Through corrections of the current, $F_{n,\perp}$ and $F_{p,\perp}$ also are affected by the keyword ParallelToInterfaceInBoundaryLayer (see Field Correction Close to Interfaces on page 375).

NOTE   For very low current levels, the computation of the electric field component normal to the currents may be numerically problematic and lead to convergence problems. It is recommended to use the option `Enormal`. Besides possible numeric problems, both approaches give the same or very similar results.

Field Correction on Interface

For vertices on the interface, due to discretization, the normal electric field in inversion is underestimated systematically due to screening by the charge at the same vertex. Therefore, Sentaurus Device supports a correction of the field:

$$F_{\text{corr}}(\vec{r}) = \frac{\alpha l \rho(\vec{r})}{\varepsilon} \tag{329}$$

where α is dimensionless and is specified with `NormalFieldCorrection` in the `Math` section (reasonable values range from 0 to 1; the default is zero), ρ is the space charge, ε is the dielectric constant in the semiconductor, and l is an estimate for the depth of the box of the vertex in the normal direction.

Thin-Layer Mobility Model

The thin-layer mobility model applies to devices with silicon layers that are only a few nanometers thick. In such devices, geometric quantization leads to a mobility that cannot be expressed with a normal field-dependent interface model such as those described in Mobility Degradation at Interfaces on page 332, but it depends explicitly on the layer thickness. The thin-layer mobility model described here is based on the model described in the literature [18] and is used in conjunction with either the Lombardi model (see Enhanced Lombardi Model on page 334) or the `IALMob` model (see Inversion and Accumulation Layer Mobility Model on page 337).

NOTE   When using the thin-layer mobility model in conjunction with the Lombardi model, it is recommended to also use the Philips Unified Mobility Model on page 328. The Philips unified mobility model must be activated separately from the thin-layer mobility model.

The thin-layer mobility μ_{tl} consists of contributions of thickness fluctuation scattering, surface phonon scattering, bulk phonon scattering, and additional contributions from the normal field-dependent interface model used in conjunction with it:

$$\frac{1}{\mu_{tl}} = \frac{D}{\mu_{tf}} + \frac{D}{\mu_{sp}} + \frac{D}{\mu_{bp}} + \begin{cases} \dfrac{D}{\mu_{sr}} & , \text{ Lombardi} \\ \dfrac{D}{\mu_{sr}} + \dfrac{1}{\mu_{ph,3D}} + \dfrac{1}{\mu_C} & , \text{ IALMob} \end{cases} \tag{330}$$

where:

- $D = \exp(-x/l_{crit})$ (see Enhanced Lombardi Model on page 334 (`Lombardi`) or Inversion and Accumulation Layer Mobility Model on page 337 (`IALMob`)).
- μ_{sr} is given by Eq. 278, p. 334 (`Lombardi`) or Eq. 302, p. 340 (`IALMob`).
- $\mu_{ph,3D}$ is given by Eq. 301, p. 340 (`IALMob`).
- μ_C is given by Eq. 287, p. 338 (`IALMob`).

The thickness fluctuation term is given by:

$$\frac{1}{\mu_{tf}} = \frac{1}{\mu_{tf0}(t_b/1\,\text{nm})^{\eta_1}\left[1 + \left(\dfrac{F_\perp}{F_{tf0}}\right)^{\eta_2}\right]} + \frac{1}{\mu_{tfh0}(t_b/1\,\text{nm})^{\eta_1}\left(\dfrac{F_{tfh0}}{F_\perp}\right)} \tag{331}$$

The surface phonon term is given by:

$$\mu_{sp} = \mu_{sp0}\exp(t_b/t_{sp0}) \tag{332}$$

The bulk phonon term is given by:

$$\mu_{bp} = P_1\mu_{ac,1} + (1 - P_1)\mu_{ac,2} \tag{333}$$

$$P_1 = p_1 + \frac{1 - p_1}{1 + p_2\exp(-p_3\Delta E/kT)} \tag{334}$$

$$\Delta E = \frac{\hbar^2\pi^2}{2t_b^2}\left(\frac{1}{m_{z2}} - \frac{1}{m_{z1}}\right) \tag{335}$$

$$\mu_{ac,v} = \frac{\mu_{ac0,v}}{[1 + (W_{Tv}/W_{Fv})^\beta]^{1/\beta}}\left(\frac{W_{Tv}}{1\,\text{nm}}\right) \tag{336}$$

$$W_{Tv} = \frac{2}{3}t_b + W_{T0v}\left(\frac{t_b}{1\,\text{nm}}\right)^4\left(\frac{F_\perp}{1\,\text{MV/cm}}\right) \tag{337}$$

$$\frac{W_{Fv}}{1\,\text{nm}} = \zeta^{v-1}\frac{\mu_{ac}}{P_{bulk}\mu_{ac0,1} + \zeta(1-P_{bulk})\mu_{ac0,2}} \tag{338}$$

where:

- μ_{ac} is given by [Eq. 277, p. 334](#) (`Lombardi`) or by $\mu_{ph,2D}$ [Eq. 300, p. 340](#) (`IALMob`).
- $P_{bulk} = p_1 + (1-p_1)/(1+p2)$.
- The thickness t_b is the larger of the local layer thickness and t_{min}.
- t_{min}, μ_{tf0}, F_{tf0}, μ_{tfh0}, F_{tfh0}, η_1, η_2, μ_{sp0}, t_{sp0}, $\mu_{ac0,v}$, p_1, p_2, p_3, m_{z1}, m_{z2}, β, W_{T0v}, and ζ are model parameters.

Using the Thin-Layer Mobility Model

To activate the thin-layer mobility model, specify `ThinLayer(<parameters>)` as an option to `eMobility`, `hMobility`, or `Mobility`. The optional parameters are `<geo_parameters>` and `<physical_parameters>`.

The `ThinLayer` subcommand has the same `<geo_parameters>` as the `LayerThickness` command (see [LayerThickness Command on page 310](#)).

Physical Parameters

Specify `Lombardi` or `IALMob` (including any optional arguments for these models) as an option to `ThinLayer` to indicate which normal field-dependent interface model is used in conjunction with the thin-layer mobility calculations (`Lombardi` is the default). For example:

```
Physics {
   Mobility (
      PhuMob
      ThinLayer (Lombardi(...))
   )
}
```

or:

```
Physics {
   Mobility (
      ThinLayer (IALMob(...))
   )
}
```

NOTE When using `ThinLayer(Lombardi)` or `ThinLayer(IALMob)`, do not specify `Enormal(Lombardi)` or `Enormal(IALMob)` in addition. This would result in double-counting the scattering mechanisms that are already accounted for (see Eq. 330). However, `Enormal` must still be used to include other required degradation terms, for example:

```
Physics {
  Mobility (
     ThinLayer (IALMob(...))
     Enormal (InterfaceCharge)
  )
}
```

When `ThinLayer(Lombardi(...))` is specified, the parameters to compute D, μ_{sr}, and μ_{ac} are the same as used for the Lombardi model (see Table 58 on page 335 and Table 59 on page 335). Synopsys considers the parameters in Table 59 to be more suitable for the thin-layer mobility model; however, the defaults are still given in Table 58.

When `ThinLayer(IALMob(...))` is specified, the parameters to compute D, μ_{sr}, $\mu_{ph,3D}$, μ_C, and $\mu_{ph,2D}$ are the same as used for the `IALMob` model (see Table 60 through Table 61 on page 341).

The other parameters are specified as electron–hole pairs in the `ThinLayerMobility` parameter set. Table 66 summarizes the parameters.

Table 66   Parameters for thin-layer mobility model

Symbol	Parameter name	Electron	Hole	Unit
t_{min}	tmin	0.002	0.002	μm
μ_{tf0}	mutf0	0.15	0.28	$cm^2V^{-1}s^{-1}$
F_{tf0}	ftf0	6250	10^{100}	Vcm^{-1}
μ_{tfh0}	mutfh0	10^6	10^6	$cm^2V^{-1}s^{-1}$
F_{tfh0}	ftfh0	10^{100}	10^{100}	Vcm^{-1}
η_1	eta1	6	6	1
η_2	eta2	1	1	1
μ_{sp0}	musp0	1.145×10^{-8}	1.6×10^{-10}	$cm^2V^{-1}s^{-1}$
t_{sp0}	tsp0	10^{-4}	10^{-4}	μm
$\mu_{ac0,\,1}$	muac01	315	30.2	$cm^2V^{-1}s^{-1}$
$\mu_{ac0,\,2}$	muac02	6.4	69	$cm^2V^{-1}s^{-1}$
p_1	p1	0.55	0	1

Table 66   Parameters for thin-layer mobility model (Continued)

Symbol	Parameter name	Electron	Hole	Unit
p_2	p2	400	0.66	1
p_3	p3	1.44	1	1
m_{z1}	mz1	0.916	0.29	m_0
m_{z2}	mz2	0.19	0.25	m_0
β	beta	4	4	1
W_{T01}	wt01	3×10^{-6}	0	μm
W_{T02}	wt02	3.5×10^{-7}	0	μm
ζ	zeta	2.88	1.05	1
a_{tf}	a_tf	1.0	1.0	1
a_{sp}	a_sp	1.0	1.0	1
a_{bp}	a_bp	1.0	1.0	1

Stress Factors for Mobility Components

If isotropic stress-dependent mobility enhancement factors are applied to mobility components (see Factor Models Applied to Mobility Components on page 876), the `ThinLayer` mobility components become:

$$\mu'_{tf} = \gamma_{tf}\mu_{tf} \; , \; \gamma_{tf} = 1 + a_{tf}(\gamma - 1)$$
$$\mu'_{sp} = \gamma_{sp}\mu_{sp} \; , \; \gamma_{sp} = 1 + a_{sp}(\gamma - 1) \tag{339}$$
$$\mu'_{bp} = \gamma_{bp}\mu_{bp} \; , \; \gamma_{bp} = 1 + a_{bp}(\gamma - 1)$$

where a_{tf}, a_{sp}, and a_{bp} are stress scaling parameters that can be specified in the `ThinLayerMobility` parameter set, and γ is an isotropic enhancement factor calculated from a stress-dependent `Factor` model (see Isotropic Factor Models on page 870).

Auto-Orientation and Named Parameter Sets

The thin-layer mobility model implicitly supports the auto-orientation framework (see Auto-Orientation Framework on page 37) and named parameter sets (see Named Parameter Sets on page 36). That is, auto-orientation or named parameter sets for the `ThinLayerMobility` parameters will be used (and required) if these options are invoked for the normal field–dependent interface model used in conjunction with the thin-layer mobility model.

For example, this specification:

```
Physics {
   Mobility (
      PhuMob
      ThinLayer (Lombardi(AutoOrientation))
   )
}
```

invokes auto-orientation for both the Lombardi-specific calculations *and* the thin layer–specific calculations. In this case, Sentaurus Device requires orientation-dependent parameter sets for both the `EnormalDependence` parameters (for Lombardi) and the `ThinLayerMobility` parameters.

As another example, this specification:

```
Physics {
   Mobility (
      ThinLayer (IALMob(ParameterSetName="110"))
   )
}
```

uses both the `IALMob` `"110"` parameter set and the `ThinLayerMobility` `"110"` parameter set.

Geometric Parameters

The `ThinLayer` subcommand has the same `<geo parameters>` as the `LayerThickness` command (see Geometric Parameters of LayerThickness Command on page 312).

High-Field Saturation

In high electric fields, the carrier drift velocity is no longer proportional to the electric field, instead, the velocity saturates to a finite speed v_{sat}. Sentaurus Device supports different models for the description of this effect:

- The Canali model, two transferred electron models, and two PMIs are available for all transport models.
- The basic model and the Meinerzhagen–Engl model both require hydrodynamic simulations.
- Another flexible model for hydrodynamic simulation is described in Energy-Dependent Mobility on page 772.

Using High-Field Saturation

The high-field saturation models comprise three submodels: the actual mobility model, the velocity saturation model, and the driving force model. With a some restrictions, these models can be freely combined.

The actual mobility model is selected by flags to `eHighFieldSaturation` or `hHighFieldSaturation`. The default is the Canali model (see Extended Canali Model on page 363).

The flag `TransferredElectronEffect` selects the transferred electron model (see Transferred Electron Model on page 364). Similarly, an alternative transferred electron model is activated by the flag `TransferredElectronEffect2` (see Transferred Electron Model 2 on page 365).

The flags `CarrierTempDriveBasic` and `CarrierTempDriveME` activate the 'basic' and the Meinerzhagen–Engl model, respectively (see Basic Model on page 367 and Meinerzhagen–Engl Model on page 367). These two models require hydrodynamic simulations.

For the Canali model, the two transferred electron models, and the `PMI_HighFieldMobility` PMI, the driving force model is selected by a flag to `eHighFieldSaturation` or `hHighFieldSaturation`. Available flags are `GradQuasiFermi` (the default), `Eparallel`, `EparallelToInterface`, and `CarrierTempDrive` (see Driving Force Models on page 369). The latter is only available in hydrodynamic simulations. The `PMI_HighFieldMobility2` PMI supports `EparallelToInterface`, `Eparallel`, and `ElectricField` for the electric-field driving force. For the 'basic' model and the Meinerzhagen–Engl model, the driving force is part of the actual mobility model and cannot be chosen independently.

For all except the 'basic' model and the PMIs, a velocity saturation model can be selected in the `HighFieldDependence` parameter set (see Velocity Saturation Models on page 369).

Named Parameter Sets for High-Field Saturation

The `HighFieldDependence` and `HydroHighFieldDependence` parameter sets can be named. For example, in the parameter file, you can write:

```
HighFieldDependence "myset" { ... }
```

to declare a parameter set with the name `myset`.

To use a named parameter set, specify its name with `ParameterSetName` as an option to
`HighFieldSaturation`, `eHighFieldSaturation`, or `hHighFieldSaturation`. For
example:

```
eMobility (
   HighFieldSaturation( ParameterSetName = "myset" ...) ...
)
```

By default, the unnamed parameter set is used.

Auto-Orientation for High-Field Saturation

The `HighFieldSaturation` and `Diffusivity` models support the auto-orientation
framework (see Auto-Orientation Framework on page 37) that switches between different
`HighFieldDependence` named parameter sets based on the surface orientation of the nearest
interface. This feature can be activated by specifying `AutoOrientation` as an option to either
`HighFieldSaturation` or `Diffusivity` in the command file, for example:

```
Mobility (
   HighFieldSaturation( AutoOrientation ...) ...
)
```

Extended Canali Model

The Canali model [19] originates from the Caughey–Thomas formula [20], but has
temperature-dependent parameters, which were fitted up to 430 K by Canali *et al*. [19]:

$$\mu(F) = \frac{(\alpha + 1)\mu_{\text{low}}}{\alpha + \left[1 + \left(\frac{(\alpha + 1)\mu_{\text{low}} F_{\text{hfs}}}{v_{\text{sat}}} \right)^{\beta} \right]^{1/\beta}} \tag{340}$$

where μ_{low} denotes the low-field mobility. Its definition depends on which of the previously
described mobility models have been activated (see Mobility due to Phonon Scattering on
page 318 to Philips Unified Mobility Model on page 328). The exponent β is temperature
dependent according to:

$$\beta = \beta_0 \left(\frac{T}{300\,\text{K}} \right)^{\beta_{\text{exp}}} \tag{341}$$

Details about the saturation velocity v_{sat} and driving field F_{hfs} are discussed in Velocity
Saturation Models on page 369 and Driving Force Models on page 369. All other parameters
are accessible in the parameter set `HighFieldDependence`.

The silicon default values are listed in Table 67 on page 364.

A modified version of the Canali model is the Hänsch model [13]. It is activated by setting the parameter $\alpha = 1$. The Hänsch model is part of the Lucent mobility model (see Lucent Model on page 368). When using the hydrodynamic driving force Eq. 356, α must be zero.

For the hydrodynamic driving force, Eq. 356 can be substituted into Eq. 340. Solving for μ yields the hydrodynamic Canali model:

$$\mu = \frac{\mu_{low}}{\left[\sqrt{1 + \gamma^2 \max(w_c - w_0, 0)^\beta} + \gamma \max(w_c - w_0, 0)^{\beta/2} \right]^{2/\beta}} \tag{342}$$

where γ is given by:

$$\gamma = \frac{1}{2} \left(\frac{\mu_{low}}{q\tau_{e,c} v_{sat}^2} \right)^{\beta/2} \tag{343}$$

In this form, the model has a discontinuous derivative at $w_0 = w_c$, which can lead to numeric problems. Therefore, Sentaurus Device applies a smoothing algorithm in the carrier temperature region $T < T_c < (1 + K_{dT})T$ to create a smooth transition between the low-field mobility μ_{low} and the mobility given in Eq. 342. K_{dT} defaults to 0.2 and can be accessed in the parameter set `HighFieldDependence`.

Table 67   Canali model parameters (default values for silicon)

Symbol	Parameter name	Electrons	Holes	Unit
β_0	`beta0`	1.109	1.213	1
β_{exp}	`betaexp`	0.66	0.17	1
α	`alpha`	0	0	1

Transferred Electron Model

For GaAs and other materials with a similar band structure, a negative differential mobility can be observed for high driving fields. This effect is caused by a transfer of electrons into a energetically higher side valley with a much larger effective mass. Sentaurus Device includes a transferred electron model for the description of this effect, as given by [21]:

$$\mu = \frac{\mu_{low} + \left(\dfrac{v_{sat}}{F_{hfs}} \right) \left(\dfrac{F_{hfs}}{E_0} \right)^4}{1 + \left(\dfrac{F_{hfs}}{E_0} \right)^4} \tag{344}$$

Details of the saturation velocity v_{sat} and the driving field F_{hfs} are discussed in Velocity Saturation Models on page 369 and Driving Force Models on page 369. The reference field strength E_0 can be set in the parameter set `HighFieldDependence`.

The `HighFieldDependence` parameter set also includes a variable K_{smooth}, which is equal to 1 by default. If $K_{smooth} > 1$, a smoothing algorithm is applied to the formula for mobility in the driving force interval $F_{vmax} < F < K_{smooth}F_{vmax}$, where F_{vmax} is the field strength at which the velocity is at its maximum, $v_{max} = \mu F_{vmax}$. In this interval, Eq. 344 is replaced by a polynomial that produces the same values and derivatives at the points F_{vmax} and $K_{smooth}F_{vmax}$. It is sometimes numerically advantageous to set $K_{smooth} \approx 20$.

Table 68   Transferred electron model: Default parameters

Symbol	Parameter	Electrons	Holes	Unit
E_0	E0_TrEf	4000	4000	Vcm^{-1}
K_{smooth}	Ksmooth_TrEf	1	1	1

Transferred Electron Model 2

Sentaurus Device provides an alternative high-field saturation mobility model for III–nitride materials:

$$\mu = \frac{\mu_{low} + \mu_1\left(\dfrac{F_{hfs}}{E_0}\right)^{\alpha} + v_{sat}\dfrac{F_{hfs}^{\beta-1}}{E_1^{\beta}}}{1 + \gamma\left(\dfrac{F_{hfs}}{E_0}\right)^{\alpha} + \left(\dfrac{F_{hfs}}{E_1}\right)^{\beta}} \tag{345}$$

This model is a unification of the two models proposed in [22] and [23]. The model in [22] can be obtained by setting $\mu_1 = 0$ and $E_0 = E_1$. Similarly, the model in [23] can be obtained by setting $\gamma = 1$.

The model parameters are specified in the `TransferredElectronEffect2` section of the parameter file:

```
TransferredElectronEffect2 (
   mu1 = 0, 0
   E0 = 220893.6, 4000
   E1 = 220893.6, 4000
   alpha = 0.7857, 0
   beta = 7.2044, 4
   gamma = 6.1973, 0
)
```

The default electron parameters for $Al_xGa_{1-x}N$ and $In_xGa_{1-x}N$ are taken from [22] and are shown in Table 69 and Table 70.

Table 69   Transferred electron effect 2 model parameters in $Al_xGa_{1-x}N$

Material	μ_1 [cm²V⁻¹s⁻¹]	$E_0 = E_1$ [Vcm⁻¹]	α [1]	β [1]	γ [1]
GaN	0	220893.6	0.7857	7.2044	6.1973
$Al_{0.2}Ga_{0.8}N$	0	245579.4	0.7897	7.8138	6.9502
$Al_{0.5}Ga_{0.5}N$	0	304554.1	0.8080	9.4438	8.0022
$Al_{0.8}Ga_{0.2}N$	0	386244.0	0.8324	12.5795	8.6037
AlN	0	447033.9	0.8554	17.3681	8.7253

Table 70   Transferred electron effect 2 model parameters in $In_xGa_{1-x}N$

Material	μ_1 [cm²V⁻¹s⁻¹]	$E_0 = E_1$ [Vcm⁻¹]	α [1]	β [1]	γ [1]
GaN	0	220893.6	0.7857	7.2044	6.1973
$In_{0.2}Ga_{0.8}N$	0	151887.0	0.7670	6.0373	5.1797
$In_{0.5}Ga_{0.5}N$	0	93815.1	0.7395	4.8807	3.7387
$In_{0.8}Ga_{0.2}N$	0	63430.5	0.6725	4.1330	2.7321
InN	0	52424.2	0.6078	3.8501	2.2623

For other materials, as well as for hole mobility, the parameters in Table 71 are used.

Table 71   Default transferred electron effect 2 model parameters

μ_1 [cm²V⁻¹s⁻¹]	$E_0 = E_1$ [Vcm⁻¹]	α [1]	β [1]	γ [1]
0	4000	0	4	0

With these parameters, the model reverts to the standard transferred electron model (see Transferred Electron Model on page 364).

Sometimes, convergence problems are observed when the derivative of the velocity $v = \mu F_{hfs}$ with respect to the driving force F_{hfs} becomes negative. As a potential solution, Sentaurus Device provides an option to specify a lower bound for this derivative:

```
Math {
    TransferredElectronEffect2_MinDerivativePerField = 0
}
```

If required, individual bounds can be specified for electrons and holes:

```
Math {
   TransferredElectronEffect2_eMinDerivativePerField = -1e-3
   TransferredElectronEffect2_hMinDerivativePerField = -1e-2
}
```

By default, Sentaurus Device applies the lower bound $\partial v / \partial F_{\text{hfs}} \geq -10^{100} \text{cm}^2 \text{V}^{-1} \text{s}^{-1}$. Note that this lower bound cannot be applied to the hydrodynamic driving force (`CarrierTempDrive`).

Basic Model

According to this very simple model, the mobility decays inversely with the carrier temperature:

$$\mu = \mu_{\text{low}} \left(\frac{300\,\text{K}}{T_c} \right) \tag{346}$$

where μ_{low} is the low-field mobility and T_c is the carrier temperature.

Meinerzhagen–Engl Model

According to the Meinerzhagen–Engl model [24], the high field mobility degradation is given by:

$$\mu = \frac{\mu_{\text{low}}}{\left[1 + \left(\mu_{\text{low}} \frac{3k}{2q} \frac{(T_c - T)}{\tau_{e,c} v_{\text{sat}}^2} \right)^{\beta} \right]^{1/\beta}} \tag{347}$$

where $\tau_{e,c}$ is the energy relaxation time. The coefficients of the saturation velocity v_{sat} (see Eq. 348) and the exponent β (see Eq. 341) are accessible in the parameter file:

```
HighFieldDependence {
   vsat0  = <value for electrons> <value for holes>
   vsatexp = <value for electrons> <value for holes>
}

HydroHighFieldDependence {
   beta0  = <value for electrons> <value for holes>
   betaexp = <value for electrons> <value for holes>
}
```

The silicon default values are given in Table 72 and Table 73 on page 369.

Table 72   Meinerzhagen–Engl model: Default parameters

Silicon	Electrons	Holes	Unit
β_0	0.6	0.6	1
β_{exp}	0.01	0.01	1

Physical Model Interface

Sentaurus Device offers two physical model interfaces (PMIs) for high-field mobility saturation.

The first PMI is activated by specifying the name of the model as an option of `HighFieldSaturation`, `eHighFieldSaturation`, or `hHighFieldSaturation`. For more details about this model, see High-Field Saturation Model on page 1125.

The second PMI allows you to implement models that depend on two driving forces. It is specified by `PMIModel` as the option to `HighFieldSaturation`, `eHighFieldSaturation`, or `hHighFieldSaturation`. For details, see High-Field Saturation With Two Driving Forces on page 1134.

Lucent Model

The Lucent model has been developed by Darwish *et al.* [11]. Sentaurus Device implements this model as a combination of:

- An extended Philips unified mobility model (see Philips Unified Mobility Model on page 328) with the parameters $f_e = 0$ and $f_h = 0$ (see Table 57 on page 332). The Lucent model described in [11] also does not include clustering. To disable clustering in the Philips unified mobility model, set the parameters $N_{ref,A}$ and $N_{ref,D}$ to very large numbers.
- The enhanced Lombardi model (see Enhanced Lombardi Model on page 334) with the parameters from Table 59 on page 335.
- The Hänsch model (see Extended Canali Model on page 363) with the parameter $\alpha = 1$ (see Table 67 on page 364). In addition, the β exponent in the Hänsch model is equal to 2, which can be accomplished by setting $\beta_0 = 2$ and $\beta_{exp} = 0$.

Velocity Saturation Models

Sentaurus Device supports two velocity saturation models. Model 1 is part of the Canali model and is given by:

$$v_{\text{sat}} = v_{\text{sat},0}\left(\frac{300\,\text{K}}{T}\right)^{v_{\text{sat,exp}}} \tag{348}$$

This model is recommended for silicon.

Model 2 is recommended for GaAs. Here, v_{sat} is given by:

$$v_{\text{sat}} = \begin{cases} A_{\text{vsat}} - B_{\text{vsat}}\left(\dfrac{T}{300\,\text{K}}\right) & v_{\text{vsat}} > v_{\text{sat,min}} \\ v_{\text{sat,min}} & \text{otherwise} \end{cases} \tag{349}$$

The parameters of both models are accessible in the `HighFieldDependence` parameter set.

Selecting Velocity Saturation Models

The variable `Vsat_formula` in the `HighFieldDependence` parameter set selects the velocity saturation model. If `Vsat_formula` is set to 1, Eq. 348 is used. If `Vsat_formula` is set to 2, Eq. 349 is selected. The default value of `Vsat_formula` depends on the semiconductor material, for example, for silicon the default is 1; for GaAs, it is 2.

Table 73   Velocity saturation parameters

Symbol	Parameter	Electrons	Holes	Unit
$v_{\text{sat},0}$	vsat0	1.07×10^{7}	8.37×10^{6}	cm/s
$v_{\text{sat,exp}}$	vsatexp	0.87	0.52	1
A_{vsat}	A_vsat	1.07×10^{7}	8.37×10^{6}	cm/s
B_{vsat}	B_vsat	3.6×10^{6}	3.6×10^{6}	cm/s
$v_{\text{sat,min}}$	vsat_min	5.0×10^{5}	5.0×10^{5}	cm/s

Driving Force Models

Sentaurus Device supports five different models for the driving force F_{hfs}, the first two of which also are affected by the `ParallelToInterfaceInBoundaryLayer` keyword (see Field Correction Close to Interfaces on page 375). See Table 273 on page 1461 for a summary of keywords.

Electric Field Parallel to the Current

For the first model (flag `Eparallel`), the driving field for electrons is the electric field parallel to the electron current density:

$$F_{\text{hfs},\,n} = \vec{F} \cdot \frac{\vec{J}_n}{J_n} \tag{350}$$

To avoid numeric noise in the calculation of the `Eparallel` driving force, Sentaurus Device provides an option of setting $F_{\text{hfs},\,n}$ to zero for very small current densities, defined as:

$$\frac{J_n}{\mu_n} < \frac{c_{\min}}{\mu_{\text{ref}}} \tag{351}$$

Here, $\mu_{\text{ref}} = 1000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ is an arbitrary reference mobility, and $c_{\min}$ is specified (in Acm^{-2}) by `CDensityMin` in the `Math` section (default is `0`).

The driving field for holes is analogous.

The electric field parallel to the current is the physically correct driving force for high-field saturation mobility models as well as for avalanche generation. Unfortunately, this driving force suffers from numeric instabilities for small currents because the direction of the current is not well defined and fluctuates easily. Therefore, the radius of convergence can be very small. The following driving forces are provided as alternatives with improved numeric stability.

Gradient of Quasi-Fermi Potential

For the second model (flag `GradQuasiFermi`), the driving field for electrons is:

$$F_{\text{hfs},\,n} = \left| \nabla \Phi_n \right| \tag{352}$$

By default, the electric field replaces the gradient of the quasi-Fermi potential within mesh elements touching a contact:

$$F_{\text{hfs},\,n} = \left| \vec{F} \right| \tag{353}$$

In the `Math` section, you can request that Eq. 352 is used for all elements:

```
Math {
    ComputeGradQuasiFermiAtContacts = UseQuasiFermi
}
```

The driving field for holes is analogous.

NOTE Usually, Eq. 350 and Eq. 352 give the same or very similar results. However, numerically, one model may prove to be more stable. For example, in regions with small current, the evaluation of the parallel electric field can be numerically problematic.

This is the default driving force for drift-diffusion simulations.

Electric Field Parallel to the Interface

The third model (keyword `EparallelToInterface`) computes the driving force as the electric field parallel to the closest semiconductor–insulator interface:

$$F_{\text{hfs}} = \left| (I - \hat{n}\hat{n}^{\text{T}})\vec{F} \right| \tag{354}$$

The vector $\hat{n}$ is a unit vector pointing to the closest semiconductor–insulator interface. It is determined in the same way as for the mobility degradation at interfaces. To select explicitly a semiconductor–insulator interface, use the `EnormalInterface` specification in the `Math` section (see Normal to Interface on page 355).

The driving force of `EparallelToInterface` is the same for electrons and holes. It is numerically stable because it does not depend on the direction of the current. However, this model will only give valid results if the current flows predominantly parallel to the interface (such as in the channel of MOSFET devices).

In certain situations, for example, in the channel of a FinFET, the direction of the current is known. In this case, you can specify a constant direction vector $\vec{d}$ in the `Math` section:

```
Math {
   EparallelToInterface (
      Direction = (1 0 0)
   )
}
```

Then, the driving force is computed as the electric field $\vec{F}$ parallel to the direction vector $\vec{d}$:

$$F_{\text{hfs}} = \frac{\max(\vec{d}\vec{F},0)}{|\vec{d}|} \tag{355}$$

NOTE Eq. 355 ensures a nonnegative driving force $F_{\text{hfs},n}$. If the scalar product between the direction vector $\vec{d}$ and the electric field $\vec{F}$ becomes negative, the driving force will be set to zero. This effectively switches off high-field saturation.
Therefore, it is crucial that the direction of vector $\vec{d}$ is aligned with the direction of the current flow. Otherwise, you may inadvertently disable the high-field saturation mobility model.

An `EparallelToInterface` specification can appear in the global `Math` section, as well as in materialwise or regionwise `Math` sections. If no direction vector, or a zero direction vector, has been specified, the driving force will revert to Eq. 354.

It also may be required to restrict the validity of the direction vector $\vec{d}$ to only a part of a device. This can be accomplished by specifying a list of boxes together with the required direction vector:

```
Math {
   EparallelToInterface (     # 2D example
      Direction = (1 0)
      Box = ((1 1) (3 4))
      Box = ((3 3) (5 4))
   )

   EparallelToInterface (     # 3D example
      Direction = (0 0 1)
      Box = ((1 1 0) (3 4 1))
      Box = ((3 3 0) (5 4 1))
   )
}
```

Boxes are specified by the coordinates of the corners of a diagonal (units of µm). The driving force in Eq. 355 is then only applied to mesh vertices that are contained in at least one of the boxes. On all other vertices, the driving force in Eq. 354 is used. You can specify different direction vectors $\vec{d}$ in different parts of a device by using multiple `EparallelToInterface` statements in the `Math` section.

You also can plot the normalized direction vector $\vec{d}/|\vec{d}|$ in the `Plot` section:

```
Plot {
   EP2I_Direction/Vector
}
```

This can be useful to visualize the areas where the driving force in Eq. 355 applies.

Hydrodynamic Driving Force

The fourth model (keyword `CarrierTempDrive`) requires hydrodynamic simulation. The driving field for electrons is:

$$F_{\text{hfs},\,n} = \sqrt{\frac{\max(w_n - w_0,\,0)}{\tau_{\text{e},\,n}q\mu_n}} \tag{356}$$

where $w_n = 3kT_n/2$ is the average electron thermal energy, $w_0 = 3kT/2$ is the equilibrium thermal energy, and $\tau_{e,n}$ is the energy relaxation time. The driving fields for holes are analogous.

This is the default driving force for hydrodynamic simulations.

Electric Field

The fifth model (keyword `ElectricField`) uses the electric field as an approximation for F_{hfs}.

Interpolation of Driving Forces to Zero Field

For numeric reasons, Sentaurus Device actually implements the following generalizations of Eq. 350 and Eq. 352:

$$F_{\text{hfs},n} = \frac{n}{n+n_0}\vec{F}\cdot\frac{\vec{J}_n}{J_n} \tag{357}$$

$$F_{\text{hfs},n} = \frac{n}{n+n_0}|\nabla\Phi_n| \tag{358}$$

Here, n_0 is a numeric damping parameter. The values for electrons and holes default to zero, and are set (in cm^{-3}) with the parameters `RefDens_eGradQuasiFermi_Zero` and `RefDens_hGradQuasiFermi_Zero` in the `Math` section. Using positive values for n_0 can improve convergence for problems where strong generation–recombination occurs in regions with small density.

Instead of `RefDens_eGradQuasiFermi_Zero` and `RefDens_hGradQuasiFermi_Zero`, the old aliases `eDrForceRefDens` and `hDrForceRefDens` can be used as well.

Interpolation of the GradQuasiFermi Driving Force

Occasionally, convergence problems can be attributed to the `GradQuasiFermi` driving force, particularly when $\nabla\Phi_n$ changes rapidly for small changes in the electron density n. In such cases, you can use the gradient of a modified quasi-Fermi potential Φ_n instead. In the case of Boltzmann statistics, the modified quasi-Fermi potentials are given by:

$$\tilde{\Phi}_n = \phi - \phi_{\text{ref}} + \frac{\chi}{q} - \frac{kT}{q}\log\frac{n+n_0}{N_C} \tag{359}$$

$$\tilde{\Phi}_p = \phi - \phi_{\text{ref}} + \frac{\chi}{q} + \frac{E_{g,\text{eff}}}{q} + \frac{kT}{q}\log\frac{p+p_0}{N_V} \tag{360}$$

The equivalent expressions for Fermi statistics are:

$$\tilde{\Phi}_n \;=\; \phi - \phi_{\text{ref}} + \frac{\chi}{q} - \frac{kT}{q}F_{1/2}^{-1}\Big(\frac{n + n_0}{N_C}\Big) \tag{361}$$

$$\tilde{\Phi}_p \;=\; \phi - \phi_{\text{ref}} + \frac{\chi}{q} + \frac{E_{g,\,\text{eff}}}{q} + \frac{kT}{q}F_{1/2}^{-1}\Big(\frac{p + p_0}{N_V}\Big) \tag{362}$$

The values of n_0 and p_0 can be specified with the following parameters in the `Math` section:

- `RefDens_eGradQuasiFermi_ElectricField_HFS`
- `RefDens_hGradQuasiFermi_ElectricField_HFS`

For $n_0 = 0$, you have $\nabla\tilde{\Phi}_n = \nabla\Phi_n$ and, for $n_0 \rightarrow \infty$, you have $\nabla\tilde{\Phi}_n \rightarrow \vec{F}$ as a limit (in the isothermal case). Therefore, this approach represents an interpolation between the gradient of the quasi-Fermi potential $\nabla\Phi_n$ and the electric field $\vec{F}$.

These interpolation parameters affect only the computation of the `GradQuasiFermi` driving force for high-field saturation mobility. If you want the driving force for both high-field saturation mobility *and* avalanche generation to use interpolation to the electric field, you can use the following keywords (see Interpolation of Avalanche Driving Forces on page 426):

- `RefDens_eGradQuasiFermi_ElectricField`
- `RefDens_hGradQuasiFermi_ElectricField`

As an alternative, Sentaurus Device also provides an interpolation between the gradient of the quasi-Fermi potential and the electric field parallel to the interface:

$$F_{\text{hfs},\,n} \;=\; \frac{n}{n + n_0}\big|\nabla\Phi_n\big| + \frac{n_0}{n + n_0}\big|(I - \hat{n}\hat{n}^T)\vec{F}\big| \tag{363}$$

The reference densities for electrons and holes can be specified in the `Math` section by the following parameters:

- `RefDens_eGradQuasiFermi_EparallelToInterface_HFS`
- `RefDens_hGradQuasiFermi_EparallelToInterface_HFS`

Interpolation of the Eparallel Driving Force

As with the `GradQuasiFermi` driving force, convergence problems associated with the `Eparallel` driving force can sometimes be alleviated with an interpolation to the electric field $\vec{F}$ at low carrier concentrations:

$$F_{\text{hfs},\,n} \;=\; \frac{n}{n + n_0}\bigg(\vec{F} \cdot \frac{\vec{J}_n}{J_n}\bigg) + \frac{n_0}{n + n_0}\big|\vec{F}\big| \tag{364}$$

In this case, the reference densities for electrons and holes can be specified in the `Math` section by the following parameters:

- `RefDens_eEparallel_ElectricField_HFS`
- `RefDens_hEparallel_ElectricField_HFS`

Interpolation of the `Eparallel` driving force to the electric field for avalanche generation can be specified with separate parameters (see Interpolation of Avalanche Driving Forces on page 426).

Field Correction Close to Interfaces

`ParallelToInterfaceInBoundaryLayer` in the `Math` section controls the computation of driving forces for mobility and avalanche models along interfaces. With this switch, the avalanche and mobility computations in boundary elements along interfaces use only the component parallel to the interface of the following vectors:

- Current vector
- Gradient of the quasi-Fermi potential

In this context, an interface is either a semiconductor–insulator region interface or an external boundary interface of the device.

This switch can be useful to avoid nonphysical breakdowns along an interface with a coarse mesh. It may be specified regionwise, in which case it only applies to boundary elements in a given region.

The switch `ParallelToInterfaceInBoundaryLayer` supports two "layer" options:

```
Math {
   ParallelToInterfaceInBoundaryLayer (PartialLayer)
   ParallelToInterfaceInBoundaryLayer (FullLayer)
}
```

If `PartialLayer` is specified, parallel fields are only used in elements that are connected to the interface by an edge (in 2D) or a face (in 3D). This is the default. The option `FullLayer` uses parallel fields in all elements that touch the interface by either a face, an edge, or a vertex.

The switch `ParallelToInterfaceInBoundaryLayer` is enabled by default. It can be disabled by specifying `-ParallelToInterfaceInBoundaryLayer`. Additional options are available for `ParallelToInterfaceInBoundaryLayer` to disable it only on portions of the interface. Specifying `-ExternalBoundary` disables it on all external boundaries; whereas, `-ExternalXPlane`, `-ExternalYPlane`, and `-ExternalZPlane` disables it only on external boundaries perpendicular to the x-axis, y-axis, and z-axis, respectively. Specifying `-Interface` disables it on semiconductor–insulator region interfaces.

Non-Einstein Diffusivity

By default, in the drift-diffusion equation (see Drift-Diffusion Model on page 182), Sentaurus Device assumes that the Einstein relation holds, and the diffusivity is related to the mobility by $D_n = kT\mu_n$ and $D_p = kT\mu_p$. For short-channel devices with steep doping gradients, this relation is no longer valid. Therefore, Sentaurus Device allows you to compute the diffusivities independently from the mobilities.

To be able to reuse existing mobility models, Sentaurus Device expresses the diffusivities in terms of *diffusivity mobilities*, $D_n = kT\mu_{n,\,\mathrm{diff}}$ and $D_p = kT\mu_{p,\,\mathrm{diff}}$, and you can specify models and parameters for $\mu_{n,\,\mathrm{diff}}$ and $\mu_{p,\,\mathrm{diff}}$, which are different from μ_n and μ_p.

To compute the diffusivity mobilities, specify the keyword `Diffusivity`, `eDiffusivity`, or `hDiffusivity` as an option to `eMobility`, `hMobility`, or `Mobility`. The options for `eDiffusivity` and `hDiffusivity` are the same as for `HighFieldSaturation`. The low-field mobility that enters the diffusivity mobility is the same as for the high-field mobility.

The simplest way to obtain diffusivity mobilities different from the mobilities is to use named parameters sets to achieve a different parameterization (see Named Parameter Sets for High-Field Saturation on page 362). For example:

```
eMobility (
   HighFieldSaturation(ParameterSetName = "mymobpara")
   Diffusivity(ParameterSetName = "mydiffpara")
   DopingDependence              * applies to both diffusivity and mobility
)
```

It is also possible to use entirely different models for high-field mobilities and diffusivity mobilities.

The diffusivity mobilities can be plotted. The names of the datasets are `eDiffusivityMobility` and `hDiffusivityMobility`.

The current implementation of non-Einstein diffusivities has several restrictions. In particular, the following models use a current density that assumes the Einstein relation still holds:

- The models to compute the driving fields for mobility (Driving Force Models on page 369) and avalanche generation (see Driving Force on page 426).
- The J-model for trap cross sections (see J-Model Cross Sections on page 458).
- The current densities that appear in Eq. 76 and Eq. 77, p. 196.

Transport in magnetic fields is not supported. Support for anisotropy is restricted to the tensor grid method with current-independent anisotropy. The hydrodynamic model is supported, but it is not recommended for use with non-Einstein diffusivity.

High-Field Saturation Mobility Scaling

Sentaurus Device allows the mobility calculated by the `HighFieldSaturation` models to be scaled. The parameters `ku` and `kv` are used to scale low-field mobility (μ_{low}) and saturation velocity (v_{sat}), respectively, which appear in the formulas presented in this section:

$$\mu_{\text{low}} \rightarrow \text{ku} \cdot \mu_{\text{low}} \tag{365}$$

$$v_{\text{sat}} \rightarrow \text{kv} \cdot \mu_{\text{sat}} \tag{366}$$

The parameters `ku` and `kv` are specified in the `HighFieldDependence` parameter set in the parameter file and have default values of 1.0.

Ballistic Mobility Model

To account for the ballistic effect in drift-diffusion transport, a ballistic mobility model can be combined with the total drift-diffusion mobility using Matthiessen's rule:

$$\frac{1}{\mu} = \frac{1}{\mu_{\text{dd}}} + \frac{1}{\mu_{\text{bal}}} \tag{367}$$

where μ_{bal} represents the ballistic mobility. Sentaurus Device provides two models for μ_{bal} that are described in the following sections:

- Channel Length–Dependent Model
- Kinetic Velocity Model

Channel Length–Dependent Model

The simplest channel length–dependent ballistic mobility model [6] is given by the following expression:

$$\mu_{\text{bal}}(T) = k(T) \cdot L_{\text{ch}} \tag{368}$$

where L_{ch} is a user-defined parameter. In most cases, you will specify a value for L_{ch} (in nm) that corresponds to the actual channel length for the device being simulated.

According to [6], $k(T)$ is expressed as:

$$k(T) = \frac{q v_T}{2 k_{\text{B}} T} \qquad v_T = \sqrt{\frac{2 k_{\text{B}} T}{\pi m^*}} \tag{369}$$

where q is the electron charge, T is the lattice temperature, k_B is the Boltzmann constant, and v_T is the thermal velocity with the effective mass m^* in the transport direction. If you define the parameter $k_{300} = k(300\ \text{K})$, then the effective mass m^* from Eq. 369 can be expressed as:

$$m^* = \frac{q^2}{600\pi k_B k_{300}^2} \tag{370}$$

Using k_{300}, Eq. 368 can be rewritten as:

$$\mu_{\text{bal}}(T) = k_{300}\sqrt{\frac{300}{T}} \cdot L_{\text{ch}} \tag{371}$$

where k_{300} is a user-defined parameter specified in the parameter file. This parameter can be adjusted to match measured device characteristics.

Kinetic Velocity Model

To avoid using the explicit channel length dependency in Eq. 371, the authors of [25] developed a kinetic velocity model (KVM) with the following terms: thermionic emission and free carrier acceleration. The thermionic emission term in the ballistic mobility is given by:

$$\mu^T{}_{\text{bal}} = \frac{\sqrt{\frac{k_B T}{m^*}} y_T\left(\frac{q\psi}{k_B T}\right)}{|\nabla\psi|} \qquad y_T(x) = e^x\sqrt{\alpha_0 + 2(1 - e^{-x})} \tag{372}$$

where ψ is the quasi-Fermi potential with reference to the source contact and with a negative sign for holes, m^* is from Eq. 370 and can be adjusted using the parameter k_{300}, and α_0 is a factor to an initial kinetic velocity near source.

The free carrier acceleration term in the ballistic mobility is given by:

$$\mu^B{}_{\text{bal}} = \frac{\sqrt{\frac{k_B T}{m^*}} y_B\left(\frac{q\psi}{k_B T}\right)}{|\nabla\psi|} \qquad y_B(x) = \sqrt{\alpha_0 + 2x} \tag{373}$$

The total KVM ballistic mobility is expressed as follows:

$$\frac{1}{\mu_{\text{bal}}} = \frac{\alpha_T}{\mu^T{}_{\text{bal}}} + \frac{\alpha_B}{\mu^B{}_{\text{bal}}} \tag{374}$$

where α_T is the thermionic emission constant, which according to the theory of [26] should equal 1.52, and α_B is the distribution function factor of the free carrier acceleration term, which should be effective mass (semiconductor material) dependent.

NOTE   The free carrier acceleration term (Eq. 373) is required if pure ballistic transport should be modeled using the drift-diffusion model. However, for typical MOSFET applications where carrier mobility is affected by carrier scattering in the channel, the thermionic emission term alone (Eq. 372 and Eq. 374) should be sufficient.

Fermi–Dirac Statistics

Both Eq. 371 and Eq. 374 are written for the Boltzmann statistics, but for the strong inversion regime in MOSFET applications, accounting for Fermi–Dirac statistics might be essential (especially for III–V materials). To account for that, the following correction is suggested in [25]:

$$\mu_{\text{bal}} = \tilde{\mu}_{\text{bal}} \sqrt{\frac{k_B T}{q} \frac{\partial \ln n}{\partial \psi}} \tag{375}$$

where $\tilde{\mu}_{\text{bal}}$ is from Eq. 371 or Eq. 374, and n is the carrier concentration.

Frensley Rule

Typically, the ballistic mobility is combined with the total drift-diffusion mobility μ_{dd} using Matthiessen's rule (Eq. 367), but [25] and [26] suggest the following Frensley rule to compute the final mobility μ:

$$\frac{\mu}{\mu_{\text{dd}}} + \left(\frac{\mu}{\mu_{\text{bal}}}\right)^2 = 1 \tag{376}$$

Using the Ballistic Mobility Model

To activate the channel length–dependent ballistic mobility (Eq. 371) with available options, you can specify the following in the `Physics` section of the command file:

```
Mobility (
    BalMob(Lch = 5.0 Fermi Frensley TempDep)
)
```

Here, `Lch` is the channel length (in nm), the `Fermi` option activates the Fermi–Dirac correction (Eq. 375), the `Frensley` option activates Eq. 376 for the final mobility μ (if not specified, Matthiessen's rule is used), and the `TempDep` option activates the temperature dependency in Eq. 371. If `Lch` is not specified, the default value of 10^7 nm is used, which effectively disables the model.

The model has one user-defined fitting parameter k_{300} that is accessible in the `BalMob` parameter set in the parameter file.

Table 74   BalMob model: Default coefficients for silicon

Symbol	Parameter name	Electrons	Holes	Unit
k_{300}	k	20.0	20.0	$cm^2/Vs\ nm$

To activate only the thermionic emission term of the KVM (Eq. 372 and Eq. 374) with available options, you can specify the following in the `Physics` section of the command file:

```
Mobility (
    BalMob(KVM Fermi Frensley)
)
```

where the `KVM` option must be used and activates the model, the `Fermi` option activates the Fermi–Dirac correction (Eq. 375), and the `Frensley` option activates Eq. 376 for the final mobility μ (if not specified, Matthiessen's rule is used). To activate the total KVM with the free carrier acceleration term (Eq. 372, Eq. 373, and Eq. 374) the `KVM(Full)` option must be used.

The KVM also has the same fitting parameter k_{300} that must be specified in the parameter file (see Table 74) and defines the effective mass m^* needed in Eq. 372 and Eq. 373. In addition, Table 75 lists the KVM-specific parameters that are accessible in the `BalMob` parameter set in the parameter file.

Table 75   BalMob model: KVM default coefficients for silicon

Symbol	Parameter name	Electrons	Holes	Unit
α_T	Tfactor	2	2	1
α_B	Bfactor	0.3	0.3	1
α_0	V0factor	1	1	1

Monte Carlo–Computed Mobility for Strained Silicon

Based on Monte Carlo simulations [27], the parameter file `StrainedSilicon.par` has been created, which is shipped with Sentaurus Device (see Default Parameters on page 35). This file contains in-plane transport parameters at $300\,K$ for silicon under biaxial tensile strain that is present when a thin silicon film is grown on top of a relaxed `SiliconGermanium` substrate. (*In-plane* refers to charge transport that is parallel to the interface to `SiliconGermanium`, as is the case in MOSFETs.)

In the `Physics` section of the command file, the germanium content (`XFraction`) of the `SiliconGermanium` substrate at the interface to the `StrainedSilicon` channel must be specified (this value determines the strain in the top silicon film) according to:

```
MoleFraction (RegionName=["TopLayer"] XFraction = 0.2 Grading = 0.0)
```

where the material of `TopLayer` is `StrainedSilicon`.

Band offsets and bulk mobility data are obtained from the model-solid theory of Van de Walle and descriptions of Monte Carlo simulations [27].

A parameterization of the surface mobility model as a function of strain is not yet possible. The present values for the parameters `B` and `C` of the surface mobility were extracted in a $1 \, \mu m$ bulk MOSFET at a high effective field (where the silicon control measurements of the references [28][29] were in good agreement with the universal mobility curve of silicon, and where the neglected effect of the SiGe substrate is minimal) of approximately $0.7 \, MV/cm$ to reproduce reported experimental data [28][29], for the typical germanium content in the `SiliconGermanium` substrate of 30%. The values for other germanium contents are given as comments.

Monte Carlo–Computed Mobility for Strained SiGe in npn-SiGe HBTs

Based on Monte Carlo simulations [30], the parameter file `SiGeHBT.par` has been created, which is shipped with Sentaurus Device (see Default Parameters on page 35). This file contains transport parameters at $300 \, K$ for silicon germanium under biaxial compressive strain present when a thin SiGe film is grown on top of a relaxed silicon substrate, which occurs in the base of npn-SiGe heterojunction bipolar transistors (HBTs).

The electron parameters refer to the out-of-plane direction (that is, perpendicular to the SiGe–silicon interface) and the hole parameters to the in-plane direction (that is, parallel to the SiGe–silicon interface). The profile of the germanium content can either originate from a process simulation or be specified in the command file of Sentaurus Device (see Abrupt and Graded Heterojunctions on page 10).

The transport parameters have been obtained from the full-band Monte Carlo simulations [30].

The band gap in relaxed SiGe alloys has been extracted from the measurements in [31] and the values in strained SiGe calculated according to the model solid theory of C. G. Van de Walle.

Consistent limiting values for silicon (and polysilicon) are also provided.

Incomplete Ionization–Dependent Mobility Models

Sentaurus Device supports incomplete ionization–dependent mobility models. This dependence is activated by specifying the keyword `IncompleteIonization` in `Mobility` sections. The incomplete ionization model (see Chapter 13 on page 277) must be activated also. The `Physics` sections for this case can be as follows:

```
Physics {
   IncompleteIonization
   Mobility ( Enormal IncompleteIonization )
}
```

In this case, for all equations that contain $N_{A,0}, N_{D,0}, N_{tot}$, Sentaurus Device will use N_A, N_D, N_i.

The following mobility models depend on incomplete ionization:

- Masetti model, see Eq. 247
- Arora model, see Eq. 248
- University of Bologna bulk model, see Eq. 252–Eq. 254
- Philips unified model, see Eq. 271 and Eq. 272
- Lombardi model, see Eq. 277 and Eq. 280
- IALMob model, see Eq. 282, Eq. 294, Eq. 295, Eq. 300, Eq. 302, and Eq. 303
- University of Bologna inversion layer model, see Eq. 307–Eq. 309
- Coulomb degradation components, see Eq. 311
- RCS model, see Eq. 316 and Eq. 317

Poole–Frenkel Mobility (Organic Material Mobility)

Most organic semiconductors have mobilities dependent on the electric field. Sentaurus Device supports mobilities having a square-root dependence on the electric field, which is a typical mobility dependence for organic semiconductors. The mobility as a function of the electric field is given by:

$$\mu = \mu_0 \exp\left(-\frac{E_0}{kT}\right) \exp\left(\sqrt{F}\left(\frac{\beta}{T} - \gamma\right)\right) \tag{377}$$

where μ_0 is the low-field mobility, β and γ are fitting parameters, E_0 is the effective activation energy, and F is the driving force (electric field).

The parameters E_0, β, and γ can be adjusted in the `PFMob` section of the parameter file:

```
Material = "pentacene"
...
PFMob {
   beta_e = 1.1
   beta_h = 1.1
   E0_e = 0.0
   E0_h = 0.0
   gamma_e = 0.1
   gamma_h = 0.2
}
...
}
```

with their default parameters: `beta_e=beta_h=0.1`, `E0_e=E0_h=0` (in eV), and `gamma_e=gamma_h=0.0`.

Since the derivative of mobility with respect to the driving force is infinite at zero fields, the evaluation of this derivative is performed by replacing the square root of the driving force with an equivalent approximation having a finite derivative for zero field. The approximation of the square root with the regular square root can be adjusted by specifying the parameter `delta_sqrtReg` in the `PFMob` section of the parameter file. Typical values are in the range 0.1–0.0001; its default value is 0.1.

The model can be activated for both electrons and holes by specifying the keyword `PFMob` as a model for `HighFieldSaturation` in the `Mobility` section and the driving force as a parameter:

```
Physics(Region="pentacene") {
   ...
   Mobility (
      HighFieldSaturation(PFMob Eparallel)
   )
   ...
}
```

The model can also be selected for electrons or holes separately:

```
Physics { Mobility ( [eHighFieldSaturation(PFMob Eparallel)]
                      [hHighFieldSaturation(PFMob Eparallel)]) ...}
```

NOTE Because the Poole–Frenkel mobility model is implemented through the high-field saturation framework, all the parameters specified for driving forces (see Driving Force Models on page 369) also apply to this model.

Mobility Averaging

Sentaurus Device computes separate values of the mobility for each vertex of each semiconductor element of the mesh. To guarantee current conservation, these mobilities are then averaged to obtain either one value for each semiconductor element of the mesh or one value for each edge of each semiconductor element.

Element averaging is used by default and requires less memory than element–edge averaging. Element–edge averaging results in a smaller discretization error than element averaging, in particular, when the enhanced Lombardi model (see Enhanced Lombardi Model on page 334) with $\alpha_\perp \neq 0$ is used. The time to compute the mobility is nearly identical for both approaches.

To select the mobility averaging approach, specify `eMobilityAveraging` and `hMobilityAveraging` in the `Math` section. The value is `Element` for element averaging, and `ElementEdge` for element–edge averaging.

Mobility Doping File

The `Grid` parameter in the `File` section of a command file can be used to read a TDR file that contains the device geometry, mesh, and doping.

By default, the doping read from this file is used in the mobility calculations previously described.

As an alternative, Sentaurus Device allows the donor and acceptor concentrations *for mobility calculations only* to be read from a separate TDR file. This is accomplished using the `MobilityDoping` parameter:

```
File {
   Grid          = "mosfet.tdr"
   MobilityDoping = "mosfet_mobility.tdr"
}
```

Notes:

- The geometry and mesh in the `MobilityDoping` file must match the `Grid` file.

- If a `MobilityDoping` file is specified, it disables the mobility dependency on `IncompleteIonization` if this mobility option is specified.

- The donor and acceptor concentrations read from a `MobilityDoping` file can be specified in the `Plot` section of the command file with `MobilityDonorConcentration` and `MobilityAcceptorConcentration`, respectively.

■ For PMI models, the `MobilityDoping` file concentrations can be read using:

```
double Nd = ReadDoping("MobilityDonorConcentration")
double Na = ReadDoping("MobilityAcceptorConcentration")
```

Effective Mobility

It is often useful to know the effective channel mobility seen by carriers as well as other effective or averaged quantities in the channel. To simplify the task of obtaining such quantities, Sentaurus Device provides an `EffectiveMobility` current plot PMI that extracts several quantities of interest for both electrons and holes. Table 76 lists the electron quantities extracted by the `EffectiveMobility` PMI. The extracted hole quantities are analogous.

Table 76   Electron quantities extracted with the EffectiveMobility PMI; hole quantities are analogous ($\tilde{n} = n$ or n_{SHE} if UseSHEDensity = 0 or 1, respectively)

Name	Symbol	Start Point or Start Box method	Volume Box method	Unit
eSheetDensity	n_{sheet}	$\displaystyle\int_0^{s_{\max}} n(s)ds$	$\displaystyle\frac{\int n(\boldsymbol{r})d\Omega}{\int dS}$	cm^{-2}
eAverageDensity	n_{avg}	$\displaystyle\frac{1}{s_{\max}}\int_0^{s_{\max}} n(s)ds$	$\displaystyle\frac{\int n(\boldsymbol{r})d\Omega}{\int d\Omega}$	cm^{-3}
eSHESheetDensity	$n_{\mathrm{SHE,sheet}}$	$\displaystyle\int_0^{s_{\max}} n_{\mathrm{SHE}}(s)ds$	$\displaystyle\frac{\int n_{\mathrm{SHE}}(\boldsymbol{r})d\Omega}{\int dS}$	cm^{-2}
eSHEAverageDensity	$n_{\mathrm{SHE,avg}}$	$\displaystyle\frac{1}{s_{\max}}\int_0^{s_{\max}} n_{\mathrm{SHE}}(s)ds$	$\displaystyle\frac{\int n_{\mathrm{SHE}}(\boldsymbol{r})d\Omega}{\int d\Omega}$	cm^{-3}
eAverageField	$E_{\mathrm{avg,n}}$	$\displaystyle\frac{1}{\tilde{n}_{\mathrm{sheet}}}\int_0^{s_{\max}} E_\perp(s)\tilde{n}(s)ds$	$\displaystyle\frac{\int |E(\boldsymbol{r})|\tilde{n}(\boldsymbol{r})d\Omega}{\int \tilde{n}(\boldsymbol{r})d\Omega}$	V/cm
eEffectiveField	$E_{\mathrm{eff,n}}$	$E_{\mathrm{avg,n}} + \left(\eta_{\mathrm{e}} - \frac{1}{2}\right)\frac{q}{\varepsilon_{\mathrm{s}}}\tilde{n}_{\mathrm{sheet}}$	$E_{\mathrm{avg,n}} + \left(\eta_{\mathrm{e}} - \frac{1}{2}\right)\frac{q}{\varepsilon_{\mathrm{s}}}\tilde{n}_{\mathrm{sheet}}$	V/cm
eChargeEffField	$E_{\mathrm{eff,ch,n}}$	$\displaystyle\frac{q}{\varepsilon_{\mathrm{s}}}\left(\int_0^{s_{\max}}(N_{\mathrm{A}} - N_{\mathrm{D}} - p)ds + \eta_{\mathrm{e}}\tilde{n}_{\mathrm{sheet}}\right)$	$\displaystyle\frac{q}{\varepsilon_{\mathrm{s}}}\left(\frac{\int(N_{\mathrm{A}} - N_{\mathrm{D}} - p)d\Omega}{\int dS} + \eta_{\mathrm{e}}\tilde{n}_{\mathrm{sheet}}\right)$	V/cm

Table 76   Electron quantities extracted with the EffectiveMobility PMI; hole quantities are analogous ($\tilde{n} = n$ or n_{SHE} if UseSHEDensity = 0 or 1, respectively) (Continued)

Name	Symbol	Start Point or Start Box method	Volume Box method	Unit
eMobility	$\mu_{\text{eff,n}}$	$\dfrac{1}{\tilde{n}_{\text{sheet}}} \displaystyle\int_0^{s_{\max}} \mu_{\text{n}}(s)\tilde{n}(s)\,ds$	$\dfrac{\displaystyle\int \mu_{\text{n}}(\boldsymbol{r})\tilde{n}(\boldsymbol{r})\,d\Omega}{\displaystyle\int \tilde{n}(\boldsymbol{r})\,d\Omega}$	cm^2/Vs
eStressFactorXX	$\left(\dfrac{\mu_{\text{n,xx}}}{\mu_{\text{n0}}}\right)_{\text{eff}}$	$\dfrac{1}{\tilde{n}_{\text{sheet}}\mu_{\text{eff,n}}} \displaystyle\int_0^{s_{\max}} \left(\dfrac{\mu_{\text{n,xx}}}{\mu_{\text{n0}}}\right)\mu_{\text{n}}(s)\tilde{n}(s)\,ds$	$\dfrac{\displaystyle\int (\mu_{\text{n,xx}}/\mu_{\text{n0}})\mu_{\text{n}}(\boldsymbol{r})\tilde{n}(\boldsymbol{r})\,d\Omega}{\displaystyle\int \mu_{\text{n}}(\boldsymbol{r})\tilde{n}(\boldsymbol{r})\,d\Omega}$	1
eStressFactorYY	$\left(\dfrac{\mu_{\text{n,yy}}}{\mu_{\text{n0}}}\right)_{\text{eff}}$	$\dfrac{1}{\tilde{n}_{\text{sheet}}\mu_{\text{eff,n}}} \displaystyle\int_0^{s_{\max}} \left(\dfrac{\mu_{\text{n,yy}}}{\mu_{\text{n0}}}\right)\mu_{\text{n}}(s)\tilde{n}(s)\,ds$	$\dfrac{\displaystyle\int (\mu_{\text{n,yy}}/\mu_{\text{n0}})\mu_{\text{n}}(\boldsymbol{r})\tilde{n}(\boldsymbol{r})\,d\Omega}{\displaystyle\int \mu_{\text{n}}(\boldsymbol{r})\tilde{n}(\boldsymbol{r})\,d\Omega}$	1
eStressFactorZZ	$\left(\dfrac{\mu_{\text{n,zz}}}{\mu_{\text{n0}}}\right)_{\text{eff}}$	$\dfrac{1}{\tilde{n}_{\text{sheet}}\mu_{\text{eff,n}}} \displaystyle\int_0^{s_{\max}} \left(\dfrac{\mu_{\text{n,zz}}}{\mu_{\text{n0}}}\right)\mu_{\text{n}}(s)\tilde{n}(s)\,ds$	$\dfrac{\displaystyle\int (\mu_{\text{n,zz}}/\mu_{\text{n0}})\mu_{\text{n}}(\boldsymbol{r})\tilde{n}(\boldsymbol{r})\,d\Omega}{\displaystyle\int \mu_{\text{n}}(\boldsymbol{r})\tilde{n}(\boldsymbol{r})\,d\Omega}$	1

EffectiveMobility PMI Methods

The `EffectiveMobility` PMI provides different methods for extracting quantities from the device:

- The *Start Point method* extracts quantities at a single point in the channel. The method is invoked by specifying the `Start` parameter (see Using the EffectiveMobility PMI) to identify the starting location for a line that will pass through the structure. The extracted quantities will be obtained from integrals along this line. By default, the selected `Start` location will snap to the nearest semiconductor–insulator interface vertex, and the line will be normal to the interface.

- The *Start Box method* is an extension of the Start Point method and is used to extract quantities over an extended region of the channel. The method is invoked by specifying the `StartBoxMin` and `StartBoxMax` parameters to surround the portion of the semiconductor–insulator interface where the extraction will occur. All interface vertices enclosed in the start box will be used as starting locations for line integrals through the device. The reported extracted quantities will be an interface-area weighted average of all the calculated line integrals.

- In contrast to the previous method, the quantities extracted with the *Volume Box method* will be obtained by performing volume integrals over a selected portion of the device. The method is invoked by specifying the `BoxMin` and `BoxMax` parameters to identify where the integration should occur. The specified box should surround both the interface and volume

of interest. The size of the semiconductor–insulator interface area enclosed in the box will be extracted and used in the calculations whenever a sheet density ($\#/cm^2$) is required.

Using the EffectiveMobility PMI

To include the quantities listed in Table 76 on page 385 in the current plot file, specify one or more instances of the `EffectiveMobility` PMI in the `CurrentPlot` section of the command file. The syntax and options for the `EffectiveMobility` PMI are:

```
CurrentPlot {
   PMIModel (
      Name = "EffectiveMobility"
      [GroupName = <string>]
      [ [ Start = (x₀, y₀, z₀) [SnapToNode = 0 | 1] ] |
        [ StartBoxMin = (xₘᵢₙ, yₘᵢₙ, zₘᵢₙ) StartBoxMax = (xₘₐₓ, yₘₐₓ, zₘₐₓ) ]
        [Direction = (dx, dy, dz)] [Depth = sₘₐₓ] ] |
      [BoxMin = (xₘᵢₙ, yₘᵢₙ, zₘᵢₙ) BoxMax = (xₘₐₓ, yₘₐₓ, zₘₐₓ) [Width = <float>] ]
      [Region = (<string1>, <string2>, ...)]
      [ChannelType = -1 | 1 | 0]
      [eta_e = η_e] [eta_h = η_h] [epsilon = ε_s/ε₀]
      [UseSHEDensity = 0 | 1]
   )
}
```

The parameters are described here:

- `GroupName` is the name of the data group for the extracted quantities. A data group with this name will appear in Sentaurus Visual or Inspect when a current plot file (`*.plt` file) is loaded. The default group name is `"Channel"`. If there is more than one `EffectiveMobility` PMI used in a `CurrentPlot` section, `GroupName` must be used to distinguish between different sets of results.

- `Start` specifies the starting location used in the Start Point method. All coordinates must be specified in μm. Only the coordinates corresponding to the dimensionality of the structure are required (for example, only x_0 and y_0 in two dimensions).

- `SnapToNode` is used to snap the `Start` location to the nearest semiconductor–insulator interface vertex. Specify `SnapToNode=1` to snap (default). Specify `SnapToNode=0` to not snap.

- `Direction` is used to specify a direction vector for the line along which the line integrals will be performed. By default, the direction for lines initiated at a semiconductor–insulator interface vertex will be taken as normal to the interface. If `Direction` is specified, the units are arbitrary, as the specified direction vector will be normalized.

- `Depth` is the line integration distance in μm. The default is $0.5 \, \mu m$. The actual integration distance may be shorter if the line encounters a structure boundary, a non-semiconductor

material, or a region not included in the Region list (see below). Depth is usually chosen so that contributions to the integral beyond a distance of Depth are negligible.

- StartBoxMin and StartBoxMax specify the minimum and maximum coordinates for a box that surrounds the semiconductor–insulator interface starting points used in the Start Box method. All coordinates are specified in μm.

- BoxMin and BoxMax specify the minimum and maximum coordinates for a box that surrounds the semiconductor volume and interface used in the Volume Box method. All coordinates are specified in μm.

- Width represents an interface length in two dimensions or an interface area in three dimensions, and is used when sheet densities are required for the extracted quantities. Width must be specified in μm for 2D structures and μm^2 for 3D structures. If Width is not specified, the interface length or area is extracted automatically from the portion of the interface enclosed within the user-specified box. A default value of Width $= 0.04\,\mu m$ in two dimensions or $0.0016\,\mu m^2$ in three dimensions will be used if an interface length or area cannot be found.

- Region can optionally be used to specify a list of region names where the extraction calculations will be confined. If Region is not specified, all semiconductor regions will be considered.

- ChannelType specifies which quantities are extracted. Specify ChannelType=-1 to extract electron quantities. Specify ChannelType=1 to extract hole quantities. Specify ChannelType=0 to extract both quantities.

- eta_e, eta_h, and epsilon are parameters used in the calculation of effective fields. Their default values are eta_e=0.5, eta_h=0.333333, and epsilon=11.7.

- UseSHEDensity specifies whether the standard carrier densities (UseSHEDensity=0) or the SHE carrier densities (UseSHEDensity=1) are used as the weighting functions in the integral calculations. The default is UseSHEDensity=0.

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CHAPTER 16 Generation–Recombination

This chapter describes the generation–recombination processes that can be modeled in Sentaurus Device.

Generation–recombination processes are processes that exchange carriers between the conduction band and the valence band. They are very important in device physics, in particular, for bipolar devices. This chapter describes the generation–recombination models available in Sentaurus Device. Most models are local in the sense that their implementation (sometimes in contrast to reality) does not involve spatial transport of charge. For each individual generation or recombination process, the electrons and holes involved appear or vanish at the same location. The only exceptions are one of the trap-assisted tunneling models and one of the band-to-band tunneling models (see Dynamic Nonlocal Path Trap-Assisted Tunneling on page 400 and Dynamic Nonlocal Path Band-to-Band Tunneling Model on page 436). For other models that couple the conduction and valence bands and account for spatial transport of charge, see Tunneling and Traps on page 463 and Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722.

Shockley–Read–Hall Recombination

Recombination through deep defect levels in the gap is usually labeled Shockley–Read–Hall (SRH) recombination. In Sentaurus Device, the following form is implemented:

$$R_{\text{net}}^{\text{SRH}} = \frac{np - n_{\text{i,eff}}^2}{\tau_p(n + n_1) + \tau_n(p + p_1)} \tag{378}$$

with:

$$n_1 = n_{\text{i,eff}} \exp\left(\frac{E_{\text{trap}}}{kT}\right) \tag{379}$$

and:

$$p_1 = n_{\text{i,eff}} \exp\left(\frac{-E_{\text{trap}}}{kT}\right) \tag{380}$$

where E_{trap} is the difference between the defect level and intrinsic level. The variable E_{trap} is accessible in the parameter file. The silicon default value is $E_{\text{trap}} = 0$.

The lifetimes τ_n and τ_p are modeled as a product of a doping-dependent (see SRH Doping Dependence on page 393), field-dependent (see SRH Field Enhancement on page 396), and temperature-dependent (see SRH Temperature Dependence on page 394) factor:

$$\tau_c = \tau_{\text{dop}} \frac{f(T)}{1 + g_c(F)} \tag{381}$$

where $c = n$ or $c = p$. For an additional density dependency of the lifetimes, see Trap-Assisted Auger Recombination on page 403.

For simulations that use Fermi statistics (see Fermi Statistics on page 176) or quantization (see Chapter 14 on page 283), Eq. 378 needs to be generalized. The modified equation reads:

$$R_{\text{net}}^{\text{SRH}} = \frac{np - \gamma_n \gamma_p n_{\text{i,eff}}^2}{\tau_p(n + \gamma_n n_1) + \tau_n(p + \gamma_p p_1)} \tag{382}$$

where γ_n and γ_p are given by Eq. 47 and Eq. 48, p. 177.

Using SRH Recombination

The generation–recombination models are selected in the `Physics` section as an argument to the `Recombination` keyword:

```
Physics{ Recombination( <arguments> ) ...}
```

The SRH model is activated by specifying the `SRH` argument:

```
Physics{ Recombination( SRH ...) ...}
```

The keyword for plotting the SRH recombination rate is:

```
Plot{ ...
   SRHRecombination
}
```

SRH Doping Dependence

The doping dependence of the SRH lifetimes is modeled in Sentaurus Device with the Scharfetter relation:

$$\tau_{dop}(N_{A,\,0} + N_{D,\,0}) \ = \ \tau_{min} + \frac{\tau_{max} - \tau_{min}}{1 + \left(\dfrac{N_{A,\,0} + N_{D,\,0}}{N_{ref}}\right)^{\gamma}} \tag{383}$$

Such a dependence arises from experimental data [1] and the theoretical conclusion that the solubility of a fundamental, acceptor-type defect (probably a divacancy (E5) or a vacancy complex) is strongly correlated to the doping density [2][3][4]. Default values are listed in Table 77 on page 395. The Scharfetter relation is used when the argument `DopingDependence` is specified for the SRH recombination. Otherwise, $\tau = \tau_{max}$ is used.

The evaluation of the SRH lifetimes according to the Scharfetter model is activated by specifying the additional argument `DopingDependence` for the `SRH` keyword in the `Recombination` statement:

```
Physics{ Recombination( SRH( DopingDependence ... ) ...) ...}
```

Lifetime Profiles From Files

Sentaurus Device can use spatial lifetime profiles provided by a file. Such profiles can be precomputed or generated manually by an editor such as Sentaurus Structure Editor (refer to the *Sentaurus™ Structure Editor User Guide*).

The names of the datasets for the electron and hole lifetimes must be `eLifetime` and `hLifetime`, respectively. They are loaded from a file named by the keyword `LifeTime` in the `File` section:

```
File {
   Grid    = "MyDev_msh.tdr"
   LifeTime = "MyDev_msh.tdr"
   ...
}
```

For each grid point, the values defined by the lifetime profile are used as τ_{max} in Eq. 383.

The lifetime data can be in a separate file from the doping, but must correspond to the same grid.

Improved Nakagawa Model

The Scharfetter relation can be expanded to be:

$$\tau_{dop}(N_{A,0} + N_{D,0}) = \frac{\tau_{max} + \tau_{min}\left(\dfrac{N_{A,0} + N_{D,0}}{N_{ref}}\right)^{\gamma}}{1 + \dfrac{\tau_{max}}{\tau_0}\left(\dfrac{N_{A,0} + N_{D,0}}{N_{ref}}\right)^{\gamma}} \tag{384}$$

Here, τ_0 is an additional fitting parameter. By default, $\tau_0 = \tau_{max}$, and Eq. 384 is simplified as:

$$\tau_{dop}(N_{A,0} + N_{D,0}) = \frac{\tau_{max} + \tau_{min}\left(\dfrac{N_{A,0} + N_{D,0}}{N_{ref}}\right)^{\gamma}}{1 + \left(\dfrac{N_{A,0} + N_{D,0}}{N_{ref}}\right)^{\gamma}} = \tau_{min} + \frac{\tau_{max} - \tau_{min}}{1 + \left(\dfrac{N_{A,0} + N_{D,0}}{N_{ref}}\right)^{\gamma}} \tag{385}$$

This is the same as Eq. 383. By default, $\tau_{min} = 0$ and $\gamma = 1$. Eq. 385 is further simplified as:

$$\frac{1}{\tau_{dop}(N_{A,0} + N_{D,0})} = \frac{1}{\tau_{max}} + \frac{1}{\tau_{max}} \cdot \left(\frac{N_{A,0} + N_{D,0}}{N_{ref}}\right) \tag{386}$$

This is the original equation in [5]. Table 77 on page 395 lists the default values. To activate the Nakagawa model, an additional option Nakagawa is specified in the SRH(DopingDependence) statement:

```
Physics{ Recombination( SRH( DopingDependence ( Nakagawa )... ) ...) ...}
```

SRH Temperature Dependence

To date, there is no consensus on the temperature dependence of the SRH lifetimes. This appears to originate from a different understanding of lifetime. From measurements of the recombination lifetime [6][7]:

$$\tau = \delta n / R \tag{387}$$

in power devices (δn is the excess carrier density under neutral conditions, $\delta n = \delta p$), it was concluded that the lifetime increases with rising temperature. Such a dependence was modeled either by a power law [6][7]:

$$\tau(T) = \tau_0\left(\frac{T}{300\,\text{K}}\right)^{\alpha} \tag{388}$$

or an exponential expression of the form:

$$\tau(T) = \tau_0 e^{C\left(\frac{T}{300\,\mathrm{K}} - 1\right)} \tag{389}$$

A calculation using the low-temperature approximation of multiphonon theory [8] gives:

$$\tau_{\mathrm{SRH}}(T) = \tau_{\mathrm{SRH}}(300\,\mathrm{K}) \cdot f(T) \ \ \text{with} \ f(T) = \left(\frac{T}{300\,\mathrm{K}}\right)^{T_\alpha} \tag{390}$$

with $T_\alpha = -3/2$, which is the expected decrease of minority carrier lifetimes with rising temperature. Since the temperature behavior strongly depends on the nature of the recombination centers, there is no universal law $\tau_{\mathrm{SRH}}(T)$.

In Sentaurus Device, the power law model, Eq. 388, can be activated with the keyword `TempDependence` in the `SRH` statement:

```
Physics{ Recombination( SRH( TempDependence ...) ...}
```

Additionally, Sentaurus Device supports an exponential model for $f(T)$:

$$f(T) = e^{C\left(\frac{T}{300\,\mathrm{K}} - 1\right)} \tag{391}$$

This model is activated with the keyword `ExpTempDependence`:

```
Physics{ Recombination( SRH( ExpTempDependence ...) ...}
```

SRH Doping- and Temperature-Dependent Parameters

All the parameters of the doping- and temperature-dependent SRH recombination models are accessible in the parameter set `Scharfetter`.

Table 77   Default parameters for doping- and temperature-dependent SRH lifetime

Symbol	Parameter name	Electrons	Holes	Unit
$\tau_{\min}$	taumin	0	0	s
$\tau_{\max}$	taumax	1×10^{-5}	3×10^{-6}	s
τ_0	tau0	1×10^{-5}	3×10^{-6}	s
N_{ref}	Nref	1×10^{16}	1×10^{16}	cm^{-3}
γ	gamma	1	1	1
T_α	Talpha	−1.5	−1.5	1

Table 77   Default parameters for doping- and temperature-dependent SRH lifetime

Symbol	Parameter name	Electrons	Holes	Unit
C	Tcoeff	2.55	2.55	1
E_{trap}	Etrap	0	0	eV

SRH Field Enhancement

Field enhancement reduces SRH recombination lifetimes in regions of strong electric fields. It must not be neglected if the electric field exceeds a value of approximately 3×10^5 V/cm in certain regions of the device. For example, the I–V characteristics of reverse-biased p-n junctions are extremely sensitive to defect-assisted tunneling, which causes electron–hole pair generation before band-to-band tunneling or avalanche generation sets in. Therefore, it is recommended that field-enhancement is included in the simulation of drain reverse leakage and substrate currents in MOS transistors.

Sentaurus Device provides two field-enhancement models: the Schenk trap-assisted tunneling model (see Schenk Trap-Assisted Tunneling (TAT) Model on page 397) and the Hurkx trap-assisted tunneling model (see Hurkx TAT Model on page 399). The Hurkx model is also available for trap capture and emission rates (see Hurkx Model for Cross Sections on page 458).

Using Field Enhancement

The local field–dependence of the SRH lifetimes is activated by parameters in the ElectricField option of SRH:

```
SRH( ...
   ElectricField (
      Lifetime = Schenk | Hurkx | Constant
      DensityCorrection = Local | None
   )
)
```

Lifetime selects the lifetime model. The default is Constant, for field-independent lifetime. Schenk selects the Schenk lifetimes (see Schenk Trap-Assisted Tunneling (TAT) Model on page 397), and Hurkx selects the Hurkx lifetimes (see Hurkx TAT Model on page 399).

DensityCorrection defaults to None. A value of Local selects the model described in Schenk TAT Density Correction on page 398.

For backward compatibility:

- `SRH (Tunneling)` selects `Lifetime = Schenk` and `DensityCorrection = Local`.

- `SRH(Tunneling(Hurkx))` selects `Lifetime = Hurkx` and `DensityCorrection = None`.

> **NOTE** The inclusion of defect-assisted tunneling may lead to convergence problems. In such cases, it is recommended that the flag `NoSRHperPotential` is specified in the `Math` section. This causes Sentaurus Device to exclude derivatives of $g(F)$ with respect to the potential from the Jacobian matrix.

Schenk Trap-Assisted Tunneling (TAT) Model

The field dependence of the recombination rate is taken into account by the field enhancement factors:

$$[1 + g(F)]^{-1} \tag{392}$$

of the SRH lifetimes [8] (see Eq. 381).

In the case of electrons, $g(F)$ has the form:

$$g_n(F) = \left(1 + \frac{(\hbar\Theta)^{3/2}\sqrt{E_t - E_0}}{E_0\hbar\omega_0}\right)^{-\frac{1}{2}} \frac{(\hbar\Theta)^{3/4}(E_t - E_0)^{1/4}}{2\sqrt{E_t E_0}}\left(\frac{\hbar\Theta}{kT}\right)^{\frac{3}{2}} \tag{393}$$

$$\times \exp\left(-\frac{E_t - E_0}{\hbar\omega_0} + \frac{\hbar\omega_0 - kT}{2\hbar\omega_0} + \frac{2E_t + kT}{2\hbar\omega_0}\ln\frac{E_t}{\varepsilon_R} - \frac{E_0}{\hbar\omega_0}\ln\frac{E_0}{\varepsilon_R} + \frac{E_t - E_0}{kT} - \frac{4}{3}\left(\frac{E_t - E_0}{\hbar\Theta}\right)^{\frac{3}{2}}\right)$$

where E_0 denotes the energy of an optimum horizontal transition path, which depends on field strength and temperature in the following way:

$$E_0 = 2\sqrt{\varepsilon_F}[\sqrt{\varepsilon_F + E_t + \varepsilon_R} - \sqrt{\varepsilon_F}] - \varepsilon_R, \varepsilon_F = \frac{(2\varepsilon_R kT)^2}{(\hbar\Theta)^3} \tag{394}$$

In this expression, $\varepsilon_R = S\hbar\omega_0$ is the lattice relaxation energy, S is the Huang–Rhys factor, $\hbar\omega_0$ is the effective phonon energy, E_t is the energy level of the recombination center (thermal depth), and $\Theta = (q^2 F^2/2\hbar m_{\Theta, n})^{1/3}$ is the electro-optical frequency. The mass $m_{\Theta, n}$ is the electron tunneling mass in the field direction and is given in the parameter file. The expression for holes follows from Eq. 393 by replacing $m_{\Theta, n}$ with $m_{\Theta, p}$ and E_t with $E_{g,\text{eff}} - E_t$.

For electrons, E_t is related to the defect level E_{trap} of Eq. 379 and Eq. 380 by:

$$E_t = \frac{1}{2}E_{g,eff} + \frac{3}{4}kT\ln\left(\frac{m_n}{m_p}\right) - E_{trap} - (32R_C\hbar^3\Theta^3)^{1/4} \tag{395}$$

where the effective Rydberg constant R_C is:

$$R_C = m_C\left(\frac{Z^2}{\varepsilon^2}\right)Ry \tag{396}$$

where Ry is the Rydberg energy ($13.606\,\text{eV}$), ε is the relative dielectric constant, and Z is a fit parameter.

For holes, E_t is given by:

$$E_t = \frac{1}{2}E_{g,eff} - \frac{3}{4}kT\ln\left(\frac{m_n}{m_p}\right) + E_{trap} - (32R_V\hbar^3\Theta^3)^{1/4} \tag{397}$$

Note that E_{trap} is measured from the intrinsic level and not from mid gap. The zero-field lifetime τ_{SRH} is defined by Eq. 383.

Schenk TAT Density Correction

In the original Schenk model [8], the density n in Eq. 378 is replaced by:

$$\tilde{n} = n\exp\left(-\frac{\gamma_n|\nabla E_{F,n}|(E_t - E_0)}{kTF}\right) \tag{398}$$

with E_0 and E_t according to Eq. 394 and Eq. 395. p is replaced by an analogous expression.

The parameters $\gamma_n = n/(n + n_{ref})$ and $\gamma_p = p/(p + p_{ref})$ are close to one for significantly large densities and vanish for small densities, switching off the density correction and improving numeric robustness. The reference densities n_{ref} and p_{ref} are specified (in cm^{-3}) by the `DenCorRef` parameter pair in the `TrapAssistedTunneling` parameter set. They default to 10^3 cm^{-3}.

The parameters for the Schenk model are accessible in the parameter set `TrapAssistedTunneling`. The default parameters implemented in Sentaurus Device are related to the gold acceptor level: $E_{trap} = 0\,\text{eV}$, $S = 3.5$, and $\hbar\omega_0 = 0.068\,\text{eV}$. `TrapAssistedTunneling` provides a parameter `MinField` (specified in Vcm^{-1}) used for smoothing at small electric fields. A value of zero (the default) disables smoothing.

Hurkx TAT Model

The following equations apply to electrons and holes. The lifetimes and capture cross sections become functions of the trap-assisted tunneling factor $g(F) = \Gamma_{\text{tat}}$:

$$\tau = \tau_0 / (1 + \Gamma_{\text{tat}}) \ , \quad \sigma = \sigma_0 (1 + \Gamma_{\text{tat}}) \tag{399}$$

where Γ_{tat} is given by:

$$\Gamma_{\text{tat}} = \int_0^{\tilde{E}_n} \exp\left[u - \frac{2}{3}\frac{\sqrt{u^3}}{\tilde{E}}\right] du \tag{400}$$

with the approximate solutions:

$$\Gamma_{\text{tat}} \approx \begin{cases} \sqrt{\pi \tilde{E}} \cdot \exp\left[\frac{1}{3}\tilde{E}^2\right]\left(2 - \text{erfc}\left[\frac{1}{2}\left(\frac{\tilde{E}_n}{\tilde{E}} - \tilde{E}\right)\right]\right), & \tilde{E} \le \sqrt{\tilde{E}_n} \\[2em] \sqrt{\pi \tilde{E}} \cdot \tilde{E}_n^{1/4} \exp\left[-\tilde{E}_n + \tilde{E}\sqrt{\tilde{E}_n} + \frac{1}{3}\frac{\sqrt{\tilde{E}_n}^3}{\tilde{E}}\right]\text{erfc}[\tilde{E}_n^{1/4}\sqrt{\tilde{E}} - \tilde{E}_n^{3/4}/\sqrt{\tilde{E}}], & \tilde{E} > \sqrt{\tilde{E}_n} \end{cases} \tag{401}$$

where $\tilde{E}$ and $\tilde{E}_n$ are respectively defined as:

$$\tilde{E} = \frac{E}{E_0}, \text{ where } E_0 = \frac{\sqrt{8 m_0 m_{\text{t}} k^3 T^3}}{q\hbar} \tag{402}$$

$$\tilde{E}_n = \frac{E_n}{kT} = \begin{cases} 0, & kT\ln\frac{n}{n_{\text{i}}} > 0.5 E_{\text{g}} \\[1em] \dfrac{0.5 E_{\text{g}}}{kT} - \ln\dfrac{n}{n_{\text{i}}}, & E_{\text{trap}} \le kT\ln\dfrac{n}{n_{\text{i}}} \le 0.5 E_{\text{g}} \\[1em] \dfrac{0.5 E_{\text{g}}}{kT} - \dfrac{E_{\text{trap}}}{kT}, & E_{\text{trap}} > kT\ln\dfrac{n}{n_{\text{i}}} \end{cases} \tag{403}$$

where m_{t} is the carrier tunneling mass and E_{trap} is an energy of trap level that is taken from SRH recombination if the model is applied to the lifetimes (τ) or from trap equations if it is applied to cross sections (σ).

When quantization is active (see Chapter 14 on page 283), the classical density:

$$n_{\text{cl}} = n \exp\left(\frac{\Lambda}{kT}\right) \tag{404}$$

rather than the true density n enters Eq. 403.

The Hurkx model has only one parameter, m_t, the carrier tunneling mass, which can be specified in the parameter file for electrons and holes as follows:

```
HurkxTrapAssistedTunneling {
   mt = <value>, <value>
}
```

Dynamic Nonlocal Path Trap-Assisted Tunneling

The local Schenk and Hurkx TAT models described in SRH Field Enhancement on page 396 may fail to give accurate results at low temperatures or near abrupt junctions with a strong, nonuniform, electric field profile. Moreover, the local TAT models are not suitable for computing TAT in heterojunctions where the band edge is modulated by the material composition rather than the electric field. In addition to the local Schenk and Hurkx TAT models, Sentaurus Device provides dynamic nonlocal path Schenk and Hurkx TAT models. These models take into account nonlocal TAT processes with the WKB transmission coefficient based on the exact tunneling barrier. In the present models, electrons and holes are captured in or emitted from the defect level at different locations by the phonon-assisted tunneling process. As a result, the position-dependent electron and hole recombination rates as well as the recombination rate at the defect level are all different. For each location and for each carrier type, the tunneling path is determined dynamically based on the energy band profile rather than predefined by the nonlocal mesh. Therefore, the present models do not require user-specification of the nonlocal mesh.

> **NOTE** The nonlocal path TAT models are not suitable for AC or noise analysis as nonlocal derivative terms in the Jacobian matrix are not taken into account. The lack of the derivative terms can degrade convergence when the high-field saturation mobility model is switched on, or when the series resistance is defined at electrodes, or when there is a floating region.

Recombination Rate

To compute the net electron recombination rate, the model dynamically searches for the tunneling path with the following assumptions:

- The tunneling path is a straight line with its direction equal to the gradient of the conduction band at the starting position.
- The tunneling energy is equal to the conduction band energy at the starting position and is equal to the defect level ($E_T(x) = E_{trap}(x) + E_i(x)$) at the ending position.

- Electrons can be captured in or emitted from the defect level at any location between the starting position and the ending position of the tunneling path.

- When the tunneling path encounters Neumann boundaries or semiconductor–insulator interfaces, it undergoes specular reflection.

For a given tunneling path of length l that starts at $x = 0$ and ends at $x = l$, electron capture and emission between the conduction band at $x = 0$ and the defect level at any position x for $0 \leq x \leq l$ is possible. As a result, the net electron recombination rate at $x = 0$ from the conduction band due to the TAT process $R_{\text{net},\,n}^{\text{TAT}}$ involves integration along the path as follows:

$$R_{\text{net},\,n}^{\text{TAT}} = C_n \int_0^l \frac{\Gamma_C(x, E_C(0))}{\tau_n(x)} \frac{T(0) + T(x)}{2\sqrt{T(0)T(x)}} \left[\exp\left[\frac{E_{F,\,n}(0) - E_C(0)}{kT(0)}\right] f^p(x) - \exp\left[\frac{E_T(x) - E_C(0)}{kT(x)}\right] f^n(x) \right] dx \qquad (405)$$

$$C_n = |\nabla E_C(0)| \frac{N_C(0)}{kT(0)} \left(\exp\left[\frac{E_{F,\,n}(0) - E_C(0)}{kT(0)}\right] + 1 \right)^{-\alpha} \qquad (406)$$

$$\Gamma_C(x, \varepsilon) = W_C(x, \varepsilon) \exp\left(-2\int_0^x \kappa_C(x, \varepsilon)dr \right) \qquad (407)$$

where:

- τ_n is the electron lifetime.

- $\alpha = 0$ for Boltzmann statistics and $\alpha = 1$ for Fermi–Dirac statistics.

- f^n is the electron occupation probability at the defect level.

- f^p is the hole occupation probability at the defect level.

- κ_C is the magnitude of the imaginary wavevector obtained from the effective mass approximation or from the Franz two-band dispersion relation (Eq. 777, p. 730).

- $W_C(x, \varepsilon) = 1$ for the nonlocal Hurkx TAT model. For the nonlocal Schenk TAT model, $W_C(x, \varepsilon)$ is modeled as:

$$W_C(x, \varepsilon) = \frac{\hbar[E_C(x) - E_C(0)] \exp(0.5) W[\varepsilon - E_T(x)]}{4x[E_C(x) - E_T(x)]\sqrt{\pi m_C kT(x)} W[E_C(x) + kT(x)/2 - E_T(x)]} \qquad (408)$$

$$W(\varepsilon) = \frac{1}{\sqrt{\chi}} \exp\left(\frac{\varepsilon}{2kT} + \chi\right)\left(\frac{z}{l + \chi}\right)^l \qquad (409)$$

where:

- $\chi = \sqrt{l^2 + z^2}$.

- $l = \varepsilon / \hbar\omega_0$.

- $z = S / \sinh(\hbar\omega_0 / 2kT)$.

- $\hbar\omega_0$ is the phonon energy.
- S is the Huang–Rhys constant.

The net hole recombination rate can be obtained in a similar way. The quasistatic electron and hole occupation probabilities at the defect level can be determined by balancing the net electron capture rate and the net hole capture rate.

Using Dynamic Nonlocal Path TAT Model

The nonlocal path TAT model is switched on when the model is selected in the `SRH` option as follows:

```
Recombination( ...
   SRH( ...
      NonlocalPath (
         Lifetime = Schenk | Hurkx    # Hurkx model is used by default
         Fermi | -Fermi               # use alpha=1 (alpha=0 by default)
         TwoBand | -TwoBand    # use Franz two band dispersion (off by default)
      )
   )
)
```

`Lifetime=Hurkx` (default) selects the nonlocal Hurkx model, while `Lifetime=Schenk` selects the nonlocal Schenk model. The `Fermi` option sets α equal to 1 ($\alpha = 0$ by default). The `TwoBand` option activates the Franz two-band dispersion (Eq. 777, p. 730) instead of the effective mass approximation for the computation of the imaginary wavevector.

The nonlocal path TAT model introduces no additional model parameters. The same minority carrier lifetime for the SRH model is used in the nonlocal path TAT model. The doping- and temperature-dependent lifetime as well as the lifetime loaded from file can be specified together with the nonlocal path TAT model.

> **NOTE** The SRH field-enhancement model should not be used together with the nonlocal path TAT model to avoid double-counting of the TAT process.

The nonlocal Hurkx model uses the tunneling mass specified in the `HurkxTrapAssistedTunneling` parameter set. The tunneling mass, the phonon energy, and the Huang–Rhys coupling constant for the nonlocal Schenk model are specified in the `TrapAssistedTunneling` parameter set.

The maximum length of the tunneling path is determined by the parameter `MaxTunnelLength` in the `Band2BandTunneling` parameter set.

You can consider electron TAT from Schottky contacts or Schottky metal–semiconductor interfaces using the nonlocal path TAT model. To consider the electron capture and emission

from the Schottky contact, you must specify the parameter `TATNonlocalPathNC`, which represents the room temperature effective density-of-states ($N_C(300K)$) for the Schottky contact in the electrode-specific `Physics` section, for example:

```
Physics (electrode = "source") { ...
   TATNonlocalPathNC = 2.0e19
}
```

Similarly, to consider the TAT from the Schottky metal–semiconductor interface, you must specify the room temperature effective density-of-states in the corresponding interface-specific `Physics` section, for example:

```
Physics (MaterialInterface = "Gold/Silicon") { ...
   TATNonlocalPathNC = 2.0e19
}
```

Sentaurus Device assumes that the effective density-of-states at T follows:

$$N_C(T) = N_C(300K)\left(\frac{T}{300K}\right)^{\frac{3}{2}} \tag{410}$$

The electron and hole recombination rates as well as the recombination rate at the defect level can be plotted as:

```
Plot { ...
   eSRHRecombination      # electron recombination rate
   hSRHRecombination      # hole recombination rate
   tSRHRecombination      # recombination rate at the defect level
}
```

Trap-Assisted Auger Recombination

Trap-assisted Auger (TAA) recombination is a modification to the SRH recombination (see Shockley–Read–Hall Recombination on page 391) and coupled defect level (see Coupled Defect Level (CDL) Recombination on page 405) models. When TAA is active, Sentaurus Device uses the lifetimes [4]:

$$\frac{\tau_p}{1 + \tau_p / \tau_p^{\text{TAA}}} \tag{411}$$

$$\frac{\tau_n}{1 + \tau_n / \tau_n^{\text{TAT}}} \tag{412}$$

in place of the lifetimes τ_p and τ_n in Eq. 378 and Eq. 419.

The TAA lifetimes in Eq. 411 depend on the carrier densities:

$$\frac{1}{\tau_n^{\text{TAA}}} \approx C_p^{\text{TAA}}(n + p) \tag{413}$$

$$\frac{1}{\tau_p^{\text{TAA}}} \approx C_n^{\text{TAA}}(n + p) \tag{414}$$

A reasonable order of magnitude for the TAA coefficients C_n^{TAA} and C_p^{TAA} is 1×10^{-12} cm^{3}s^{-1} to 1×10^{-11} cm^{3}s^{-1}; the default values are $C_n^{\text{TAA}} = C_p^{\text{TAA}} = 1 \times 10^{-12}$ cm^{3}s^{-1}.

TAA recombination is activated by using the keyword `TrapAssistedAuger` in the `Recombination` statement in the `Physics` section (see Table 234 on page 1436):

```
Physics {
   Recombination(TrapAssistedAuger ...)
   ...
}
```

The trap-assisted Auger parameters C_n^{TAA} and C_p^{TAA} are accessible in the parameter set `TrapAssistedAuger`.

Surface SRH Recombination

The surface SRH recombination model can be activated at semiconductor–semiconductor and semiconductor–insulator interfaces (see Interface-Specific Models on page 20).

At interfaces, an additional formula is used that is structurally equivalent to the bulk expression of the SRH generation–recombination:

$$R_{\text{surf, net}}^{\text{SRH}} = \frac{np - n_{\text{i,eff}}^2}{(n + n_1)/s_p + (p + p_1)/s_n} \tag{415}$$

with:

$$n_1 = n_{\text{i,eff}} \exp\left(\frac{E_{\text{trap}}}{kT}\right) \text{ and } p_1 = n_{\text{i,eff}} \exp\left(\frac{-E_{\text{trap}}}{kT}\right) \tag{416}$$

For Fermi statistics and quantization, the equations are modified in the same manner as for bulk SRH recombination (see Eq. 382).

The recombination velocities of otherwise identically prepared surfaces depend, in general, on the concentration of dopants at the surface [9][10][11]. Particularly, in cases where the doping

concentration varies along an interface, it is desirable to include such a doping dependence. Sentaurus Device models doping dependence of surface recombination velocities according to:

$$s = s_0 \left[1 + s_{\text{ref}} \left(\frac{N_{\text{i}}}{N_{\text{ref}}} \right)^{\gamma} \right] \tag{417}$$

The results of Cuevas [11] indicate that for phosphorus-diffused silicon, $\gamma = 1$; while the results of King and Swanson [10] seem to imply that no significant doping dependence exists for the recombination velocities of boron-diffused silicon surfaces.

To activate the model, specify the option `SurfaceSRH` to the `Recombination` keyword in the `Physics` section for the respective interface. To plot the surface recombination, specify `SurfaceRecombination` in the `Plot` section. The parameters E_{trap}, s_{ref}, N_{ref}, and γ are accessible in the parameter set `SurfaceRecombination`. The corresponding values for silicon are given in Table 78.

Table 78   Surface SRH parameters

Symbol	Parameter name	Electrons	Holes	Unit
s_0	S0	1×10^3	1×10^3	cm/s
s_{ref}	Sref	1×10^{-3}		1
N_{ref}	Nref	1×10^{16}		cm^{-3}
γ	gamma	1		1
E_{trap}	Etrap	0		eV

The doping dependence of the recombination velocity can be suppressed by setting s_{ref} to zero.

NOTE   The `SurfaceSRH` keyword also is supported for metal–semiconductor interfaces, but the model it activates there is different from the one described in this section (see Electric Boundary Conditions for Metals on page 240).

Coupled Defect Level (CDL) Recombination

The steady state recombination rate for two coupled defect levels generalizes the familiar single-level SRH formula. An important feature of the model is a possibly increased field effect that may lead to large excess currents. The model is discussed in the literature [12].

Using CDL

The CDL recombination can be switched on using the keyword CDL in the Physics section:

```
Physics{ Recombination( CDL ...) ...}
```

The contributions R_1 and R_2 in Eq. 420 can be plotted by using the keywords CDL1 and CDL2 in the Plot section. For the net rate and coupling term, $R - R_1 - R_2$, the keywords CDL and CDL3 must be specified.

CDL Model

The notation of the model parameters is illustrated in Figure 19.
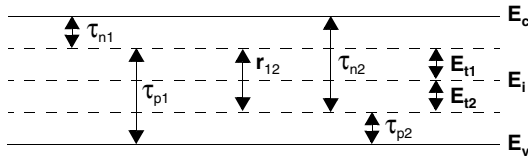
Figure 19   Notation for CDL recombination including all capture and emission processes

The CDL recombination rate is given by:

$$R = R_1 + R_2 + \left(\sqrt{R_{12}^2 - S_{12}} - R_{12} \right) \times \frac{\tau_{n1}\tau_{p2}(n + n_2)(p + p_1) - \tau_{n2}\tau_{p1}(n + n_1)(p + p_2)}{r_1 r_2} \tag{418}$$

with:

$$r_j = \tau_{nj}(p + p_j) + \tau_{pj}(n + n_j) \tag{419}$$

$$R_j = \frac{np - n_{i,\text{eff}}^2}{r_j}, \qquad j = 1, 2 \tag{420}$$

$$R_{12} = \frac{r_1 r_2}{2 r_{12}\tau_{n1}\tau_{n2}\tau_{p1}\tau_{p2}(1-\varepsilon)} + \frac{\tau_{n1}(p + p_1) + \tau_{p2}(n + n_2)}{2\tau_{n1}\tau_{p2}(1-\varepsilon)} + \frac{\varepsilon[\tau_{n2}(p + p_2) + \tau_{p1}(n + n_1)]}{2\tau_{n2}\tau_{p1}(1-\varepsilon)} \tag{421}$$

$$S_{12} = \frac{1}{\tau_{n1}\tau_{p2}(1-\varepsilon)}\left(1 - \frac{\tau_{n1}\tau_{p2}}{\tau_{n2}\tau_{p1}}\varepsilon \right)(np - n_{i,\text{eff}}^2) \tag{422}$$

$$\varepsilon = \exp\left(-\frac{|E_{t2} - E_{t1}|}{kT} \right) \tag{423}$$

where τ_{ni} and τ_{pi} denote the electron and hole lifetimes of the defect level i. The coupling parameter between the defect levels is called r_{12} (keyword `TrapTrapRate` in the parameter file). The carrier lifetimes are calculated analogously to the carrier lifetimes in the SRH model (see). The number of parameters is doubled compared to the SRH model, and they are changeable in the parameter set `CDL`.

The quantities n_2 and p_2 are the corresponding quantities of n_1 and p_1 for the second defect level. They are defined analogously to and .

For Fermi statistics and quantization, the equations are modified in the same manner as for SRH recombination (see).

Radiative Recombination

Using Radiative Recombination

The radiative recombination model is activated in the `Physics` section by the keyword `Radiative`:

```
Physics {
   Recombination (Radiative)
}
```

It can also be switched on or off by using the notation `+Radiative` or `-Radiative`:

```
Physics (Region = "gate") {
   Recombination (+Radiative)
}

Physics (Material = "AlGaAs") {
   Recombination (-Radiative)
}
```

The value of the radiative recombination rate is plotted as follows:

```
Plot {
   RadiativeRecombination
}
```

The value of the parameter C can be changed in the parameter file:

```
RadiativeRecombination {
   C = 2.5e-10
}
```

Radiative Model

The radiative (direct) recombination model expresses the recombination rate as:

$$R_{\text{net}} = C \cdot (np - n_{\text{i,eff}}^2) \tag{424}$$

By default, Sentaurus Device selects $C = 2 \times 10^{-10}$ cm^{3}s^{-1} for GaAs and $C = 0$ cm^{3}s^{-1} for other materials. For Fermi statistics and quantization, the equations are modified in the same manner than for SRH recombination (see Eq. 382, p. 392).

Auger Recombination

The rate of band-to-band Auger recombination $R_{\text{net}}^{\text{A}}$ is given by:

$$R_{\text{net}}^{\text{A}} = \left(C_n n + C_p p \right) \left(np - n_{\text{i,eff}}^2 \right) \tag{425}$$

with temperature-dependent Auger coefficients [13][14][15]:

$$C_n(T) = \left(A_{\text{A},n} + B_{\text{A},n} \left(\frac{T}{T_0} \right) + C_{\text{A},n} \left(\frac{T}{T_0} \right)^2 \right) \left[1 + H_n \exp\left(-\frac{n}{N_{0,n}} \right) \right] \tag{426}$$

$$C_p(T) = \left(A_{\text{A},p} + B_{\text{A},p} \left(\frac{T}{T_0} \right) + C_{\text{A},p} \left(\frac{T}{T_0} \right)^2 \right) \left[1 + H_p \exp\left(-\frac{p}{N_{0,p}} \right) \right] \tag{427}$$

where $T_0 = 300$ K. There is experimental evidence for a decrease of the Auger coefficients at high injection levels [15]. This effect is explained as resulting from exciton decay: at lower carrier densities, excitons, which are loosely bound electron–hole pairs, increase the probability for Auger recombination. Excitons decay at high carrier densities, resulting in a decrease of recombination. This effect is modeled by the terms $1 + H \exp(-n/N_0)$ in Eq. 426 and Eq. 427.

Auger recombination is typically important at high carrier densities. Therefore, this injection dependence will only be seen in devices where extrinsic recombination effects are extremely low, such as high-efficiency silicon solar cells. The injection dependence of the Auger coefficient can be deactivated by setting H to zero in the parameter file.

For Fermi statistics and quantization, the equations are modified in the same manner as for SRH recombination (see Eq. 382, p. 392). Default values for silicon are listed in Table 79.

Table 79   Default coefficients of Auger recombination model

Symbol	A_A [cm^{6}s^{-1}]	B_A [cm^{6}s^{-1}]	C_A [cm^{6}s^{-1}]	H [1]	N_0 [cm^{-3}]
Parameter name	A	B	C	H	N0
Electrons	6.7×10^{-32}	2.45×10^{-31}	-2.2×10^{-32}	3.46667	1×10^{18}
Holes	7.2×10^{-32}	4.5×10^{-33}	2.63×10^{-32}	8.25688	1×10^{18}

Auger recombination is activated with the argument `Auger` in the `Recombination` statement:

```
Physics{ Recombination( Auger ...) ...}
```

By default, Sentaurus Device uses Eq. 425 only if R_{net}^A is positive and replaces the value by zero if R_{net}^A is negative. To use Eq. 425 for negative values (that is, to allow for Auger generation of electron–hole pairs), use the `WithGeneration` option to the `Auger` keyword:

```
Physics { Recombination( Auger(WithGeneration) ...) ...}
```

The Auger parameters are accessible in the parameter set `Auger`.

Intrinsic Recombination Model for Silicon

With improvements in the quality of silicon bulk material, the technological progress of passivation techniques, and advanced characterization methods, an accurate description of the intrinsic recombination mechanisms of silicon became important to predict the performance of silicon-based devices. Richter *et al.* [16] developed a model to describe intrinsic recombination in crystalline silicon at 300 K covering a wide range of doping and carrier injection levels. The intrinsic recombination rate is calculated according to:

$$R_{\text{intrinsic}} = (np - n_{\text{i, eff}}^2)[C_{n0} \cdot g_{\text{eeh}}(n_0) \cdot n_0 + C_{p0} \cdot g_{\text{ehh}}(p_0) \cdot p_0 + C_{\Delta n} \cdot \Delta n^{\exp_{\Delta n}} + B_{\text{low}} \cdot B_{\text{rel}}(n, p)] \qquad (428)$$

The first two terms in the brackets stand for the common Auger expression with Coulomb enhancement factors g_{eeh} and g_{ehh}, which are dominant in the low-injection condition. n, p describe the electron and hole carrier concentrations, $n_{\text{i,eff}}$ is the effective intrinsic carrier density, and n_0, p_0 denote the electron and hole concentration at thermal equilibrium (zero voltage applied), that is, for p-type doping:

$$p_0 = N_a - N_d \qquad n_0 = \frac{n_{\text{i,eff}}^2}{p_0} \qquad (429)$$

For n-type doping:

$$n_0 = N_d - N_a \qquad p_0 = \frac{n_{i,eff}^2}{n_0} \tag{430}$$

N_a is the total acceptor doping concentration, and N_d is the total donor doping concentration.

The Coulomb enhancement factors g_{eeh} and g_{ehh} account for the enhanced probability of finding an electron and a hole in the immediate vicinity of each other:

$$g_{eeh}(n_0) = 1 + C_{geeh}\left\{ 1 - \tanh\left[\left(\frac{n_0}{N_{0,eeh}}\right)^{E_{geeh}}\right]\right\} \tag{431}$$

$$g_{ehh}(p_0) = 1 + C_{gehh}\left\{ 1 - \tanh\left[\left(\frac{p_0}{N_{0,ehh}}\right)^{E_{gehh}}\right]\right\} \tag{432}$$

The third term in the brackets of Eq. 428 is proportional to the excess carrier density Δn and describes the Auger recombination for the high-injection condition.

Finally, the last term in the brackets of Eq. 428 describes the injection-dependent radiative recombination according to Altermatt *et al.* [17][1]:

$$B_{rel}(n, p) = b_{min} + \frac{b_{max} - b_{min}}{1 + \left(\frac{n+p}{b_1}\right)^{b_2} + \left(\frac{n+p}{b_3}\right)^{b_4}} \tag{433}$$

with:

$$b_{min} = r_{max} + \frac{r_{min} - r_{max}}{1 + \left(\frac{T}{r_1}\right)^{r_2}} \tag{434}$$

$$b_1 = 2\left[s_{max} + \frac{s_{min} - s_{max}}{1 + \left(\frac{T}{s_1}\right)^{s_2}}\right] \tag{435}$$

---

1. For Eq. 433, Reference [17] notes the terms $n + p/b_1$ and $n + p/b_2$, instead of $(n + p)/b_1$ and $(n + p)/b_2$. In addition, a factor of 2 is missing in Eq. 435 and Eq. 436. This has been verified with the author and corrected in the implementation.

$$b_3 = 2\left[w_{\max} + \frac{w_{\min} - w_{\max}}{1 + \left(\frac{T}{w_1}\right)^{w_2}}\right] \tag{436}$$

T is the temperature.

This model can be switched on by specifying `intrinsicRichter` in the `Recombination` section. The model parameters can be set in the Sentaurus Device parameter file section:

```
Material = "Silicon" {
   intrinsicRichter {
       blow=4.73e-15
       rmax=0.25
       ...
   }
}
```

The parameter name and default value for each constant in Eq. 428–Eq. 436 are taken from [16] and [17], and are listed in Table 80.

Table 80   Parameter name and default value for constants

Constant	Parameter name	Default value	Unit
B_{low}	`Blow`	4.73e-15	cm^3/s
$b_{\max}$	`bmax`	1	1
b_2	`b2`	0.54	1
b_4	`b4`	1.25	1
$r_{\max}$	`rmax`	0.2	1
$r_{\min}$	`rmin`	0	1
r_1	`r1`	320	K
r_2	`r2`	2.5	1
$s_{\max}$	`smax`	1.5e18	cm^{-3}
$s_{\min}$	`smin`	1e7	cm^{-3}
s_1	`s1`	550	K
s_2	`s2`	3	1
$w_{\max}$	`wmax`	4e18	cm^{-3}
$w_{\min}$	`wmin`	1e9	cm^{-3}
w_1	`w1`	365	K

Table 80   Parameter name and default value for constants (Continued)

Constant	Parameter name	Default value	Unit
w_2	w2	3.54	1
C_{n0}	cn0	2.5e-31	cm^6/s
C_{geeh}	geehC	13	1
$N_{0,\,eeh}$	N0eeh	3.3e17	cm^{-3}
E_{geeh}	geehE	0.66	1
C_{p0}	cp0	8.5e-32	cm^6/s
C_{gehh}	gehhC	7.5	1
$N_{0,\,ehh}$	N0ehh	7e17	cm^{-3}
E_{gehh}	gehhE	0.63	1
$C_{\Delta n}$	cDn	3e-29	cm^6/s
$\exp_{\Delta n}$	expDn	0.92	1

Constant Carrier Generation

The simplest generation model computes a constant carrier generation G_{const}. It is activated in the `Physics` section as follows:

```
Physics {
   Recombination (
      ConstantCarrierGeneration (value = 1e10)   # [cm^-3 s^-1]
   )
}
```

Alternatively, the value of G_{const} can be specified in the parameter file:

```
ConstantCarrierGeneration {
   value = 1e10                  # [cm^-3 s^-1]
}
```

You can ramp the generation rate by specifying a corresponding `Goal` in a `Quasistationary` command:

```
Goal { Model = "ConstantCarrierGeneration"
       Parameter = "value"
       Value = 1e20}
```

To visualize G_{const}, plot the value of `PMIRecombination`:

```
Plot {
    PMIRecombination
}
```

The model also can be specified regionwise or materialwise.

NOTE   The constant carrier generation model is functionally equivalent to the constant optical generation model presented in Constant Optical Generation on page 543.

Avalanche Generation

Electron–hole pair production due to avalanche generation (impact ionization) requires a certain threshold field strength and the possibility of acceleration, that is, wide space charge regions. If the width of a space charge region is greater than the mean free path between two ionizing impacts, charge multiplication occurs, which can cause electrical breakdown. The reciprocal of the mean free path is called the ionization coefficient α. With these coefficients for electrons and holes, the generation rate can be expressed as:

$$G_{\mathrm{ii}} = \frac{1}{q}(\alpha_n|\vec{J_n}| + \alpha_p|\vec{J_p}|) \tag{437}$$

where $\vec{J_n}$ and $\vec{J_p}$ are the electron and hole current density vectors described in Introduction to Carrier Transport Models on page 181.

Sentaurus Device implements several models for the ionization coefficients: van Overstraeten–de Man, Okuto–Crowell, Lackner, University of Bologna, the new University of Bologna, and Hatakeyama.

Sentaurus Device allows you to select the appropriate driving force for the simulation, that is, the method used to compute the accelerating field. The choices include `GradQuasiFermi`, `Eparallel`, `CarrierTempDrive`, and `ElectricField` (see Driving Force on page 426).

Using Avalanche Generation

Avalanche generation is switched on by using the keyword `Avalanche` in the `Recombination` statement in the `Physics` section. The keywords `eAvalanche` and `hAvalanche` specify separate models or driving forces for the electron and hole ionization coefficients, respectively.

The model is selected by using one of the keywords `vanOverstraeten`, `Okuto`, `Lackner`, `UniBo`, `UniBo2`, or `Hatakeyama`. The default model is `vanOverstraeten`.

The driving force is selected using one of the keywords `GradQuasiFermi`, `Eparallel`, `CarrierTempDrive`, or `ElectricField`. The default driving force is `GradQuasiFermi`.

The following example selects the default van Overstraeten–de Man model for the electron impact ionization process with a driving force derived from electron temperature, and selects the Okuto–Crowell model for holes using the default driving force based on `GradQuasiFermi`:

```
Physics {
   Recombination(eAvalanche(CarrierTempDrive) hAvalanche(Okuto)... )
}
```

To include a dependency on energy bandgap in the avalanche generation models, specify the keyword `BandgapDependence` as an argument to `Avalanche`, `eAvalanche`, or `hAvalanche` (see the model descriptions in the next sections). For example:

```
Physics {
   Recombination(Avalanche(Lackner BandgapDependence))
}
```

To plot the avalanche generation rate, specify `AvalancheGeneration` in the `Plot` section. To plot either of the two terms on the right-hand side of Eq. 437 separately, specify `eAvalanche` or `hAvalanche`. To plot α_n or α_p, specify `eAlphaAvalanche` or `hAlphaAvalanche`, respectively.

By default, the electron and hole current density vectors $\vec{J}_n$ and $\vec{J}_p$ in Eq. 437 are computed in a mesh element using the Scharfetter–Gummel approximation applied to each element edge (see Discretization on page 1011), and this is consistent with the computation of $\nabla \cdot \vec{J}_n$ and $\nabla \cdot \vec{J}_p$ in Eq. 53, p. 181. This approximation is a good one to describe structures where the current density is low along the direction of large electrostatic potential change, such as the channel area of a MOSFET, but such a condition of low current density in the direction of potential change might not be satisfied for power-device applications. As a result, the Scharfetter–Gummel approximation in the avalanche generation term might lead to a requirement to have a very fine mesh or might result in small steps to be taken at a voltage ramp.

To overcome these issues, you can use another approximation for $\vec{J}_n$ and $\vec{J}_p$ in Eq. 437, which is based on the representation of these current density vectors as $\vec{J}_n = -q\mu_n n \nabla \Phi_n$ and $\vec{J}_p = -q\mu_p p \nabla \Phi_p$ (see Eq. 56, p. 183 and Eq. 57, p. 183). This approximation assumes that the carrier densities n and p are constant in elements and also makes the current density vectors constant in an element. Typically, you could see a small change in the breakdown voltage with this approximation, but it provides better convergence and stability properties.

To activate this alternative approximation, specify the following option:

```
Math {
    AvalDensGradQF
}
```

The contribution that avalanche generation makes to the device equations is determined by multiplying the avalanche generation rate by the element-vertex control volumes (areas in two dimensions) computed by the `AverageBoxMethod` algorithm. However, as noted in Truncated Obtuse Elements on page 1016, the total vertex control volume for an obtuse element is not the same as the total geometric volume for the element and can sometimes be several times larger. This can result in an exaggerated number of avalanche-generated carriers from such elements, which can contribute to premature breakdown. This might be the case if you observe that the breakdown voltage is much lower than expected, and the avalanche generation in the structure is confined to one or a few elements. To prevent this, an option is available to use truncated element-vertex volumes for the avalanche calculations, where the total truncated vertex volume for an element is exactly equal to the geometric volume. To activate this option, specify:

```
Math {
    ElementVolumeAvalanche
}
```

Sometimes, mostly for 3D breakdown simulations, nearly flat elements can cause convergence and also premature breakdown problems (due to singular numeric errors). Such nearly flat elements have a very small volume and excluding these elements does not affect breakdown voltage, but it helps to resolve problems with numeric singularity. To exclude such elements from the avalanche generation calculations, use the following option:

```
Math {
    AvalFlatElementExclusion = <float>   #[0 to 90 degree]
}
```

In two dimensions, this option excludes elements from contributing to avalanche generation if all the angles are less than the specified value or larger than the 180°-specified value. In three dimensions, this option excludes elements if the maximum vertex *volume angle* for the element is less than the specified value, where the vertex volume angle is computed as the arcsine of the unit-edge volume (scalar triple product of the unit vectors along the three element edges that meet at the vertex).

> **NOTE** This option excludes only flat elements that have, by definition, poor angles at every vertex (very close to 0° or 180° in two dimensions). In three dimensions, for the case of a 90° angle between three edges of a vertex in an element (this case represents a good element), the vertex unit-edge volume is the maximum (equal to 1), and this makes the vertex volume angle equal to 90° as well. For a nearly flat element, both the unit-edge volume and the volume angle are nearly zero.

The value to be used for `AvalFlatElementExclusion` must not exceed 1–2°. Otherwise, too many elements may be excluded from the avalanche generation, causing a shift in breakdown voltage to higher values.

To control and see the locations of nearly flat elements in a device structure, you can specify an option to plot the minimum and maximum volume angles for each element as follows:

```
Plot {
    AvalFlatElementMin/Element AvalFlatElementMax/Element
}
```

van Overstraeten – de Man Model

This model is based on the Chynoweth law [18]:

$$\alpha(F_{ava}) = \gamma a \exp\left(-\frac{\gamma b}{F_{ava}}\right) \tag{438}$$

with:

$$\gamma = \frac{\tanh\left(\frac{\hbar\omega_{op}}{2kT_0}\right)}{\tanh\left(\frac{\hbar\omega_{op}}{2kT}\right)} \tag{439}$$

The factor γ with the optical phonon energy $\hbar\omega_{op}$ expresses the temperature dependence of the phonon gas against which carriers are accelerated. The coefficients a, b, and $\hbar\omega_{op}$, as measured by van Overstraeten and de Man [19], are applicable over the range of fields 1.75×10^5 Vcm^{-1} to 6×10^5 Vcm^{-1} and are listed in Table 81.

Two sets of coefficients a and b are used for high and low ranges of electric field. The values `a(low),b(low)` are used in the low field range up to E_0 and the values `a(high),b(high)` apply in the high field above E_0. For electrons, the impact ionization coefficients are by default the same in both field ranges.

If `BandgapDependence` is specified as an argument to `Avalanche`, the coefficient b in Eq. 438 is replaced with:

$$b \rightarrow \frac{\beta E_g}{q\lambda} \tag{440}$$

where E_g is the energy bandgap, λ is the optical-phonon mean free path for the carrier, and β is a proportionality constant. Default values for λ and β are listed in Table 81 on page 417.

You can adjust the coefficient values in the Sentaurus Device parameter set `vanOverstraetendeMan`.

Table 81   Coefficients for van Overstraeten–de Man model (Eq. 438) for silicon

Symbol	Parameter name	Electrons	Holes	Valid range of electric field	Unit
a	`a(low)`	7.03×10^5	1.582×10^6	$1.75 \times 10^5\,\mathrm{Vcm}^{-1}$ to E_0	cm^{-1}
	`a(high)`	7.03×10^5	6.71×10^5	E_0 to $6 \times 10^5\,\mathrm{Vcm}^{-1}$	
b	`b(low)`	1.231×10^6	2.036×10^6	$1.75 \times 10^5\,\mathrm{Vcm}^{-1}$ to E_0	V/cm
	`b(high)`	1.231×10^6	1.693×10^6	E_0 to $6 \times 10^5\,\mathrm{Vcm}^{-1}$	
E_0	`E0`	4×10^5	4×10^5		V/cm
$\hbar\omega_{\mathrm{op}}$	`hbarOmega`	0.063	0.063		eV
λ	`lambda`	62×10^{-8}	45×10^{-8}		cm
β	`beta(low)`	0.678925	0.815009	$1.75 \times 10^5\,\mathrm{Vcm}^{-1}$ to E_0	1
	`beta (high)`	0.678925	0.677706	E_0 to $6 \times 10^5\,\mathrm{Vcm}^{-1}$	

Okuto–Crowell Model

Okuto and Crowell [20] suggested the empirical model:

$$\alpha(F_{\mathrm{ava}}) = a \cdot \left(1 + c(T - T_0)\right) F_{\mathrm{ava}}^{\gamma} \exp\left[-\left(\frac{b[1 + d(T - T_0)]}{F_{\mathrm{ava}}}\right)^{\delta}\right] \tag{441}$$

where $T_0 = 300\,\mathrm{K}$ and the user-adjustable coefficients are listed in Table 82 with their default values for silicon. These values apply to the range of electric field from $10^5\,\mathrm{Vcm}^{-1}$ to $10^6\,\mathrm{Vcm}^{-1}$.

If `BandgapDependence` is specified as an argument to `Avalanche`, the coefficient b in Eq. 441 is replaced with:

$$b \to \frac{\beta E_{\mathrm{g}}}{q\lambda} \tag{442}$$

where E_{g} is the energy bandgap, λ is the optical-phonon mean free path for the carrier, and β is a proportionality constant. Default values for λ and β are listed in Table 82 on page 418.

You can adjust the coefficient values in the parameter set `Okuto`.

Table 82   Coefficients for Okuto–Crowell model ([Eq. 441](#)) for silicon

Symbol	Parameter name	Electrons	Holes	Unit
a	a	0.426	0.243	V^{-1}
b	b	4.81×10^5	6.53×10^5	V/cm
c	c	3.05×10^{-4}	5.35×10^{-4}	K^{-1}
d	d	6.86×10^{-4}	5.67×10^{-4}	K^{-1}
γ	gamma	1	1	1
δ	delta	2	2	1
λ	lambda	62×10^{-8}	45×10^{-8}	cm
β	beta	0.265283	0.261395	1

Lackner Model

Lackner [21] derived a pseudo-local ionization rate in the form of a modification to the Chynoweth law, assuming stationary conditions. The temperature-dependent factor γ was introduced to the original model:

$$\alpha_\nu(F_{ava}) = \frac{\gamma a_\nu}{Z} \exp\left(-\frac{\gamma b_\nu}{F_{ava}}\right) \quad \text{where} \quad \nu = n, p \tag{443}$$

with:

$$Z = 1 + \frac{\gamma b_n}{F_{ava}} \exp\left(-\frac{\gamma b_n}{F_{ava}}\right) + \frac{\gamma b_p}{F_{ava}} \exp\left(-\frac{\gamma b_p}{F_{ava}}\right) \tag{444}$$

and:

$$\gamma = \frac{\tanh\left(\dfrac{\hbar\omega_{op}}{2kT_0}\right)}{\tanh\left(\dfrac{\hbar\omega_{op}}{2kT}\right)} \tag{445}$$

The default values of the coefficients a, b, and $\hbar\omega_{op}$ are applicable in silicon for the range of the electric field from $10^5\,\text{Vcm}^{-1}$ to $10^6\,\text{Vcm}^{-1}$.

If `BandgapDependence` is specified as an argument to `Avalanche`, the b coefficients in Eq. 443 and Eq. 444 are replaced with:

$$b \rightarrow \frac{\beta E_{\mathrm{g}}}{q\lambda} \tag{446}$$

where E_{g} is the energy bandgap, λ is the optical-phonon mean free path for the carrier, and β is a proportionality constant.

Table 83 lists the default model parameters. The model parameters are accessible in the parameter set `Lackner`.

Table 83   Coefficients for Lackner model (Eq. 443) for silicon

Symbol	Parameter name	Electrons	Holes	Unit
a	a	1.316×10^6	1.818×10^6	cm^{-1}
b	b	1.474×10^6	2.036×10^6	V/cm
$\hbar\omega_{\mathrm{op}}$	hbarOmega	0.063	0.063	eV
λ	lambda	62×10^{-8}	45×10^{-8}	cm
β	beta	0.812945	0.815009	1

University of Bologna Impact Ionization Model

The University of Bologna impact ionization model was developed for an extended temperature range between 25°C and 400°C (see also New University of Bologna Impact Ionization Model on page 421 for an updated version of this model). It is based on impact ionization data generated by the Boltzmann solver HARM [22]. It covers a wide range of electric fields ($50\,\mathrm{kVcm}^{-1}$ to $600\,\mathrm{kVcm}^{-1}$) and temperatures ($300\,\mathrm{K}$ to $700\,\mathrm{K}$). It is calibrated against impact ionization measurements [23][24] in the whole temperature range.

The model reads:

$$\alpha(F_{\mathrm{ava}}, T) = \frac{F_{\mathrm{ava}}}{a(T) + b(T)\exp\left[\dfrac{d(T)}{F_{\mathrm{ava}} + c(T)}\right]} \tag{447}$$

The temperature dependence of the model parameters, determined by fitting experimental data, reads (for electrons):

$$a(T) = a_0 + a_1 t^{a_2} \qquad b(T) = b_0 \qquad c(T) = c_0 + c_1 t + c_2 t^2 \qquad d(T) = d_0 + d_1 t + d_2 t^2 \tag{448}$$

and for holes:

$$a(T) = a_0 + a_1 t \qquad b(T) = b_0 \exp[b_1 t] \qquad c(T) = c_0 t^{c_1} \qquad d(T) = d_0 + d_1 t + d_2 t^2 \tag{449}$$

where $t = T/1\,\mathrm{K}$.

If `BandgapDependence` is specified as an argument to `Avalanche`, then $d(T)$ is modified as follows:

$$d(T) \to \left(\frac{\beta E_g}{q\lambda} / d_0\right)(d_0 + d_1 t + d_2 t^2) \tag{450}$$

where E_g is the energy bandgap, λ is the optical-phonon mean free path for the carrier, and β is a proportionality constant.

Table 84 lists the default model parameters. The model parameters are accessible in the parameter set `UniBo`.

Table 84   Coefficients for University of Bologna impact ionization model for silicon

Symbol	Parameter name	Electrons	Holes	Unit
a_0	ha0	4.3383	2.376	V
a_1	ha1	-2.42×10^{-12}	1.033×10^{-2}	V
a_2	ha2	4.1233	0	1
b_0	hb0	0.235	0.17714	V
b_1	hb1	0	-2.178×10^{-3}	1
c_0	hc0	1.6831×10^4	9.47×10^{-3}	Vcm^{-1}
c_1	hc1	4.3796	2.4924	Vcm^{-1}, 1
c_2	hc2	0.13005	0	Vcm^{-1}, 1
d_0	hd0	1.2337×10^6	1.4043×10^6	Vcm^{-1}
d_1	hd1	1.2039×10^3	2.9744×10^3	Vcm^{-1}
d_2	hd2	0.56703	1.4829	Vcm^{-1}
λ	lambda	62×10^{-8}	45×10^{-8}	cm
β	beta	0.680414	0.562140	1

NOTE   When the University of Bologna impact ionization model is selected for both carriers, that is, `Recombination(Avalanche(UniBo))`, Sentaurus Device also enables Auger generation (see Auger Recombination on page 408). Specify `Auger(-WithGeneration)` to disable this generation term if necessary.

New University of Bologna Impact Ionization Model

The impact ionization model described in University of Bologna Impact Ionization Model on page 419 was developed further in [25][26][27] to cover an extended temperature range between 25°C and 500°C (773 K). It is based on impact ionization data generated by the Boltzmann solver HARM [22] and is calibrated against specially designed impact ionization measurements [23][24].

It covers a wide range of electric fields. The model reads:

$$\alpha(F_{ava}, T) = \frac{F_{ava}}{a(T) + b(T)\exp\left[\dfrac{d(T)}{F_{ava} + c(T)}\right]} \tag{451}$$

where the coefficients a, b, c, and d are polynomials of T:

$$a(T) = \sum_{k=0}^{3} a_k\left(\frac{T}{1\,\mathrm{K}}\right)^k \tag{452}$$

$$b(T) = \sum_{k=0}^{10} b_k\left(\frac{T}{1\,\mathrm{K}}\right)^k \tag{453}$$

$$c(T) = \sum_{k=0}^{3} c_k\left(\frac{T}{1\,\mathrm{K}}\right)^k \tag{454}$$

$$d(T) = \sum_{k=0}^{3} d_k\left(\frac{T}{1\,\mathrm{K}}\right)^k \tag{455}$$

If `BandgapDependence` is specified as an argument to `Avalanche`, $d(T)$ is modified as follows:

$$d(T) \rightarrow \left(\frac{\beta E_{\mathrm{g}}}{q\lambda} \Big/ d_0\right) \sum_{k=0}^{3} d_k \left(\frac{T}{1\,\mathrm{K}}\right)^k \tag{456}$$

where E_{g} is the energy bandgap, λ is the optical-phonon mean free path for the carrier, and β is a proportionality constant.

Table 85 lists the default model parameters. The model parameters are accessible in the parameter set `UniBo2`.

Table 85   Coefficients for UniBo2 impact ionization model for silicon

Symbol	Electrons		Holes		Unit
	Parameter Name	Value	Parameter Name	Value	
a_0	a0_e	4.65403	a0_h	2.26018	V
a_1	a1_e	-8.76031×10^{-3}	a1_h	0.0134001	V
a_2	a2_e	1.34037×10^{-5}	a2_h	-5.87724×10^{-6}	V
a_3	a3_e	-2.75108×10^{-9}	a3_h	-1.14021×10^{-9}	V
b_0	b0_e	-0.128302	b0_h	0.058547	V
b_1	b1_e	4.45552×10^{-3}	b1_h	-1.95755×10^{-4}	V
b_2	b2_e	-1.0866×10^{-5}	b2_h	2.44357×10^{-7}	V
b_3	b3_e	9.23119×10^{-9}	b3_h	-1.33202×10^{-10}	V
b_4	b4_e	-1.82482×10^{-12}	b4_h	2.68082×10^{-14}	V
b_5	b5_e	-4.82689×10^{-15}	b5_h	0	V
b_6	b6_e	1.09402×10^{-17}	b6_h	0	V
b_7	b7_e	-1.24961×10^{-20}	b7_h	0	V
b_8	b8_e	7.55584×10^{-24}	b8_h	0	V
b_9	b9_e	-2.28615×10^{-27}	b9_h	0	V
b_{10}	b10_e	2.73344×10^{-31}	b10_h	0	V
c_0	c0_e	7.76221×10^3	c0_h	1.95399×10^4	Vcm^{-1}
c_1	c1_e	25.18888	c1_h	-104.441	Vcm^{-1}
c_2	c2_e	-1.37417×10^{-3}	c2_h	0.498768	Vcm^{-1}
c_3	c3_e	1.59525×10^{-4}	c3_h	0	Vcm^{-1}

Table 85   Coefficients for UniBo2 impact ionization model for silicon (Continued)

Symbol	Electrons		Holes		Unit
	Parameter Name	Value	Parameter Name	Value	
d_0	d0_e	7.10481×10^5	d0_h	2.07712×10^6	Vcm^{-1}
d_1	d1_e	3.98594×10^3	d1_h	993.153	Vcm^{-1}
d_2	d2_e	-7.19956	d2_h	7.77769	Vcm^{-1}
d_3	d3_e	6.96431×10^{-3}	d3_h	0	Vcm^{-1}
λ	lambda_e	62×10^{-8}	lambda_h	45×10^{-8}	cm
β	beta_e	0.391847	beta_h	0.831470	1

NOTE   The name of the UniBo2 model is case sensitive. Both in the command
file and the parameter file, the exact spelling of UniBo2 must be used.

Hatakeyama Avalanche Model

The Hatakeyama avalanche model has been proposed [32] to describe the anisotropic behavior
in 4H-SiC power devices. The impact ionization coefficient α is obtained according to the
Chynoweth law [18]:

$$\alpha = \gamma a e^{-\frac{\gamma b}{F}} \tag{457}$$

with:

$$\gamma = \frac{\tanh\left(\frac{\hbar\omega_{op}}{2kT_0}\right)}{\tanh\left(\frac{\hbar\omega_{op}}{2kT}\right)} \tag{458}$$

The coefficients a and b are computed dependent on the direction of the driving force $\vec{F}$. For
this purpose, the driving force $\vec{F}$ is decomposed into a component F_{0001} parallel to the
anisotropic axis 0001 and a remaining component $F_{11\bar{2}0}$ perpendicular to the anisotropic axis.

The norm $F = \left\|\vec{F}\right\|_2$ satisfies the equation:

$$F^2 = F_{0001}^2 + F_{11\bar{2}0}^2 \tag{459}$$

Based on the two projections F_{0001} and $F_{11\bar{2}0}$, the coefficients a and b then are computed as follows:

$$B = \frac{F}{\sqrt{\left(\frac{F_{11\bar{2}0}}{b_{11\bar{2}0}}\right)^2 + \left(\frac{F_{0001}}{b_{0001}}\right)^2}} \tag{460}$$

$$a = a_{11\bar{2}0}^{\left(\frac{BF_{11\bar{2}0}}{b_{11\bar{2}0}F}\right)^2} a_{0001}^{\left(\frac{BF_{0001}}{b_{0001}F}\right)^2} \tag{461}$$

$$A = \log\frac{a_{0001}}{a_{11\bar{2}0}} \tag{462}$$

$$b = B\sqrt{1 - \theta A^2 \left(\frac{BF_{11\bar{2}0}F_{0001}}{Fb_{11\bar{2}0}b_{0001}}\right)^2} \tag{463}$$

With the default $\theta = 1$, the coefficient b may become undefined for large values of the driving force F (the argument of the square root in Eq. 463 becomes negative). This can only happen if:

$$F > \frac{2\min(b_{0001}, b_{11\bar{2}0})}{\left|\log\frac{a_{0001}}{a_{11\bar{2}0}}\right|} \tag{464}$$

By setting $\theta = 0$, you have $b = B$, and the coefficients a and b only depend on the direction of the driving force $\vec{F}$, but not its magnitude.

Table 86   Parameters and default values for 4H-SiC coefficients for the Hatakeyama model

Symbol	Parameter name	Electrons	Holes	Unit
a_{0001}	a_0001	1.76×10^8	3.41×10^8	cm^{-1}
$a_{11\bar{2}0}$	a_1120	2.10×10^7	2.96×10^7	cm^{-1}
b_{0001}	b_0001	3.30×10^7	2.50×10^7	V/cm
$b_{11\bar{2}0}$	b_1120	1.70×10^7	1.60×10^7	V/cm
$\hbar\omega_{op}$	hbarOmega	0.19	0.19	eV
θ	theta	1	1	1

Driving Force

In contrast to other avalanche models in Sentaurus Device (see Driving Force on page 426), which only use the magnitude F of the driving force, the Hatakeyama avalanche model requires a vectorial driving force $\vec{F}$ to compute the coefficients a and b. Depending on the driving force model, the following expressions are used:

- `ElectricField`: The driving force $\vec{F}$ is defined as the straight electric field $\vec{E}$.
- `Eparallel`: The driving force $\vec{F}$ is given by (where $\vec{j}$ is the electron or hole current density):

$$\vec{F} = \frac{\vec{j}}{\|\vec{j}\|}\vec{j}^T\vec{E} \tag{465}$$

- `GradQuasiFermi`: The driving force $\vec{F}$ is given by (where Φ is the electron or hole quasi-Fermi potential):

$$\vec{F} = \nabla\Phi \tag{466}$$

- `CarrierTempDrive`: The driving force $\vec{F}$ is given by (where E^{eff} is the effective field obtained from the electron or hole carrier temperature):

$$\vec{F} = \frac{\vec{j}}{\|\vec{j}\|}E^{\text{eff}} \tag{467}$$

See also Avalanche Generation With Hydrodynamic Transport on page 427.

Anisotropic Coordinate System

In a 2D simulation, Sentaurus Device assumes that the y-axis in the crystal system is the anisotropic axis 0001, and the x-axis in the crystal system is the isotropic axis $11\bar{2}0$. In a 3D simulation, the z-axis in the crystal system is the anisotropic axis, and the x-axis and y-axis span the isotropic plane.

The simulation coordinate system relative to the crystal system is defined by the X and Y vectors in the `LatticeParameters` section of the parameter file (see Crystal and Simulation Coordinate Systems on page 781 and Coordinate Systems on page 887).

Usage

The Hatakeyama avalanche model uses a special-purpose interpolation formula to compute the coefficients a and b based on the direction of the driving force. This formula differs from the standard approach as described in Anisotropic Avalanche Generation on page 791.

NOTE   The Hatakeyama avalanche model must not be used together with an
`Aniso(Avalanche)` specification in the `Physics` section.

Driving Force

In Sentaurus Device, the driving force F_{ava} for impact ionization can be computed as the
component of the electrostatic field in the direction of the current, $F_{\mathrm{ava}} = \vec{F} \cdot \hat{J}_{n,p}$, (keyword
`Eparallel`), or the value of the gradient of the quasi-Fermi level, $F_{\mathrm{ava}} = |\nabla \Phi_{n,p}|$, (keyword
`GradQuasiFermi`). For these two possibilities, F_{ava} is affected by the keyword
`ParallelToInterfaceInBoundaryLayer` (see Field Correction Close to Interfaces on
page 375). For hydrodynamic simulations, F_{ava} can be computed from the carrier temperature
(keyword `CarrierTempDrive`, see Avalanche Generation With Hydrodynamic Transport on
page 427). The default model is `GradQuasiFermi` and, only for hydrodynamic simulations,
it is `CarrierTempDrive`. See Table 235 on page 1437 for a summary of keywords.

The option `ElectricField` is used to perform breakdown simulations using the 'ionization
integral' method (see Approximate Breakdown Analysis on page 428).

Interpolation of Avalanche Driving Forces

As with high-field saturation mobility, Sentaurus Device provides interpolation of avalanche
driving forces to the electric field at low carrier concentrations, which can sometimes improve
convergence behavior.

For the `GradQuasiFermi` driving force, interpolation to the electric field is described in
Interpolation of the GradQuasiFermi Driving Force on page 373. As noted there, you can
specify the following keywords for the interpolation parameters for electrons and holes in the
`Math` section:

■ `RefDens_eGradQuasiFermi_ElectricField`

■ `RefDens_hGradQuasiFermi_ElectricField`

These keywords affect the calculation of the driving forces for *both* high-field saturation
mobility and avalanche generation.

For the `Eparallel` driving force, interpolation to the electric field is given by:

$$F_{\mathrm{ava},n} = \frac{n}{n+n_0}\left(\vec{F}\cdot\frac{\vec{J}_n}{J_n}\right) + \frac{n_0}{n+n_0}|\vec{F}| \tag{468}$$

You can specify the reference densities for electrons and holes in the `Math` section by using the following parameters:

- `RefDens_eEparallel_ElectricField_Aval`
- `RefDens_hEparallel_ElectricField_Aval`

Avalanche Generation With Hydrodynamic Transport

If the hydrodynamic transport model is used, the default driving force F_{ava} equals an effective field E^{eff} obtained from the carrier temperature. The usual conversion of local carrier temperatures to effective fields E^{eff} is described by the algebraic equations:

$$n\mu_n\left(E_n^{eff}\right)^2 = n\frac{3k}{2q}\frac{T_n - T}{\lambda_n\tau_{en}} \tag{469}$$

$$p\mu_p\left(E_p^{eff}\right)^2 = p\frac{3k}{2q}\frac{T_p - T}{\lambda_p\tau_{ep}} \tag{470}$$

which are obtained from the energy conservation equation under time-independent, homogeneous conditions. Eq. 469 and Eq. 470 have been simplified in Sentaurus Device by using the assumption $\mu_n E_n^{eff} = v_{sat,n}$ and $\mu_p E_p^{eff} = v_{sat,p}$. This assumption is true for high values of the electric field. However, for low field, the impact ionization rate is negligibly small.

The parameters λ_n and λ_p are fitting coefficients (default value 1) and their values can be changed in the parameter set `AvalancheFactors`, where they are represented as `n_l_f` and `p_l_f`, respectively.

The conventional conversion formulas Eq. 469 and Eq. 470 can be activated by specifying parameters $\Upsilon_n = 0$, $\Upsilon_p = 0$ in the same `AvalancheFactors` section.

The simplified conversion formulas discussed above predict a linear dependence of effective electric field on temperature for high values of carrier temperature. For silicon, however, Monte Carlo simulations do not confirm this behavior. To obtain a better agreement with Monte Carlo data, additional heat sinks must be taken into account by the inclusion of an additional term in the equations for E^{eff}.

Such heat sinks arise from nonelastic processes, such as the impact ionization itself. Sentaurus Device supports the following model to account for these heat sinks:

$$nv_{sat,n}E_n^{eff} = n\frac{3k}{2q}\frac{T_n - T}{\lambda_n\tau_{en}} + \frac{\Upsilon_n}{q}(E_g + \delta_n k T_n)\alpha_n n v_{sat,n} \tag{471}$$

A similar equation E_p^{eff} is used to determine E_p^{eff}. To activate this model, set the parameters Υ_n and Υ_p to 1. This is the default for silicon, where the generalized conversion formula Eq. 471 gives good agreement with Monte Carlo data for $\delta_n = \delta_p = 3/2$. For all other materials, the default of the parameters Υ_n and Υ_p is 0.

Table 87   Hydrodynamic avalanche model: Default parameters

Symbol	Parameter name	Default value
λ_n	n_l_f	1
λ_p	p_l_f	1
Υ_n	n_gamma	1
Υ_p	p_gamma	1
δ_n	n_delta	1.5
δ_p	p_delta	1.5

NOTE   This procedure ensures that the same results are obtained as with the conventional local field–dependent models in the bulk case. Conversely, the temperature-dependent impact ionization model usually gives much more accurate predictions for the substrate current in short-channel MOS transistors.

Approximate Breakdown Analysis

Junction breakdown due to avalanche generation is simulated by inspecting the ionization integrals:

$$I_n = \int_0^W \alpha_n(x) \; e^{-\int_x^W (\alpha_n(x') - \alpha_p(x')) \; dx'} \; dx \tag{472}$$

$$I_p = \int_0^W \alpha_p(x) \; e^{-\int_0^x (\alpha_p(x') - \alpha_n(x')) \; dx'} \; dx \tag{473}$$

where α_n, α_p are the ionization coefficients for electrons and holes, respectively, and W is the width of the depletion zone. The integrations are performed along field lines through the depletion zone. Avalanche breakdown occurs if an ionization integral equals one. Eq. 472 describes electron injection (electron primary current) and Eq. 473 describes hole injection. Since these breakdown criteria do not depend on current densities, a breakdown analysis can

be performed by computing only the Poisson equation and ionization integrals under the assumption of constant quasi-Fermi levels in the depletion region.

Using Breakdown Analysis

To enable breakdown analysis, Sentaurus Device provides the driving force `ElectricField`, which can be computed even for constant quasi-Fermi levels. This driving force is less physical than the others available in Sentaurus Device. Therefore, Synopsys discourages using it for any purpose other than approximate breakdown analysis.

`ComputeIonizationIntegrals` in the `Math` section switches on the computation of the ionization integrals for ionization paths crossing the local field maxima in the semiconductor. By default, Sentaurus Device reports only the path with the largest I_{mean}. With the addition of the keyword `WriteAll`, information about the ionization integrals for all computed paths is written to the log file.

The `Math` keyword `BreakAtIonIntegral` is used to terminate the quasistationary simulation when the largest ionization integral is greater than one.

The complete syntax of this keyword is `BreakAtIonIntegral(<number> <value>)` where a quasistationary simulation finishes if the `number` ionization integral is greater than `value`, and the ionization integrals are ordered with respect to decreasing value:

```
Math { BreakAtIonIntegral }
```

Three optional keywords in the `Plot` section specify the values of the corresponding ionization integrals that are stored along the breakdown paths:

```
Plot { eIonIntegral | hIonIntegral | MeanIonIntegral }
```

These ionization integrals can be visualized using Sentaurus Visual.

A typical command file of Sentaurus Device is:

```
Electrode {
   { name="anode"  Voltage=0 }
   { name="cathode" Voltage=600 }
}
File {
   grid    = "@grid@"
   doping  = "@doping@"
   current = "@plot@"
   output  = "@log@"
   plot    = "@data@"
}
```

```
Physics {
   Mobility (DopingDependence HighFieldSaturation)
   Recombination(SRH Auger Avalanche(ElectricField))
}
Solve {
   Quasistationary(
   InitialStep=0.02 MaxStep=0.01 MinStep=0.01
   Goal {name=cathode voltage=1000}
   )
   { poisson }
}
Math {
   Iterations=100
   BreakAtIonIntegral
   ComputeIonizationIntegrals(WriteAll)
}
Plot {
   eIonIntegral hIonIntegral MeanIonIntegral
   eDensity hDensity
   ElectricField/Vector
   eAlphaAvalanche hAlphaAvalanche
}
```

Approximate Breakdown Analysis With Carriers

Sentaurus Device allows ionization integrals to be calculated when solving the electron and hole current continuity equations. In this case, however, impact ionization–generated carriers will be included self-consistently in the solution, and the benefits of performing an approximate breakdown analysis (faster simulations with fewer convergence issues) will be lost.

To prevent the self-consistent inclusion of impact ionization–generated carriers in the solution of the device equations, specify the option `AvalPostProcessing` in the `Math` section:

```
Math { AvalPostProcessing }
```

This option allows ionization integrals to be calculated even when solving for carriers, but retains the benefits of an approximate breakdown analysis.

Band-to-Band Tunneling Models

Sentaurus Device provides several band-to-band tunneling models:

- Schenk model (see Schenk Model on page 433).
- Hurkx model (see Hurkx Band-to-Band Model on page 435).
- A family of simple models (see Simple Band-to-Band Models on page 434).
- Nonlocal path model (see Dynamic Nonlocal Path Band-to-Band Tunneling Model on page 436).

The Schenk, Hurkx, and simple models use a common approach to suppress artificial band-to-band tunneling near insulator interfaces and for rapidly varying fields (see Tunneling Near Interfaces and Equilibrium Regions on page 435).

Using Band-to-Band Tunneling

Band-to-band tunneling is controlled by the `Band2Band` option of `Recombination`:

```
Recombination( ...
   Band2Band (
      Model = Schenk | Hurkx | E1 | E1_5 | E2 | NonlocalPath
      DensityCorrection = Local | None
      InterfaceReflection | -InterfaceReflection
      FranzDispersion | -FranzDispersion
      ParameterSetName = (<string>...)
   )
)
```

The following options for `Model` are available:

- `Schenk` selects the Schenk model.
- `Hurkx` selects the Hurkx model.
- `E1`, `E1_5`, and `E2` select one of the simple models.
- `NonlocalPath` selects the nonlocal path model.

The keyword `DensityCorrection` is used by the Schenk, Hurkx, and simple models, and its default value is `None`. A value of `Local` activates a local-density correction (see Schenk Density Correction on page 434).

The option `InterfaceReflection` is used by the nonlocal path model, and this option is switched on by default. This option allows a tunneling path reflected at

semiconductor–insulator interfaces. When it is switched off, band-to-band tunneling is neglected when the tunneling path encounters semiconductor–insulator interfaces.

The option `FranzDispersion` is used by the nonlocal path model, and this option is switched off by default. When it is switched on, the Franz dispersion relation (Eq. 777, p. 730) instead of the Kane dispersion relation (Eq. 482, p. 438) for the imaginary wavevector is used in the direct tunneling process. The indirect tunneling process is not affected by this option.

All models use `ParameterSetName`. It specifies a list of names of `Band2BandTunneling` parameter sets. For each name, band-to-band tunneling is computed using the parameters in the named parameter set, and the results are all added to give the total band-to-band tunneling rate. Without `ParameterSetName`, only the band-to-band tunneling obtained with the unnamed `Band2BandTunneling` parameter set is computed.

The following example will use the nonlocal path model, summing the contributions obtained with the `phonon-assisted` and `direct` parameter sets:

```
Band2Band(
    Model=NonlocalPath
    ParameterSetName=("phonon-assisted" "direct")
)
```

For backward compatibility:

- `Band2Band` alone (without parameters) selects the Schenk model with local-density correction.

- `Band2Band(Hurkx)` selects the Hurkx model without density correction.

- `Band2Band(E1)`, `Band2Band(E1_5)`, and `Band2Band(E2)` select one of the simple models.

The parameters for all band-to-band models are available in the `Band2BandTunneling` parameter set. The parameters specific to individual models are described in the respective sections. The parameter `MinField` (specified in Vcm^{-1}) is used by the Schenk, Hurkx, and simple models for smoothing at small electric fields. A value of zero (the default) disables smoothing.

Named `Band2BandTunneling` parameter sets are specified in the parameter file, for example:

```
Band2BandTunneling "phonon-assisted" { ... }
```

which specifies a parameter set with the name `phonon-assisted`. Note that parameters in named `Band2BandTunneling` parameter sets do not have default values, so you must specify values for all the parameters used by the model you select in the command file.

Schenk Model

Phonon-assisted band-to-band tunneling cannot be neglected in steep p-n junctions (with a doping level of $1 \times 10^{19}\, cm^{-3}$ or more on both sides) or in high normal electric fields of MOS structures. It must be switched on if the field, in some regions of the device, exceeds (approximately) $8 \times 10^5\, V/cm$. In this case, defect-assisted tunneling (see SRH Field Enhancement on page 396) must also be switched on.

Band-to-band tunneling is modeled using the expression [28]:

$$R_{net}^{bb} = AF^{7/2} \frac{\tilde{n}\tilde{p} - n_{i,\,eff}^2}{(\tilde{n} + n_{i,eff})(\tilde{p} + n_{i,eff})} \left[\frac{(F_C^{\mp})^{-3/2} \exp\left(-\frac{F_C^{\mp}}{F}\right)}{\exp\left(\frac{\hbar\omega}{kT}\right) - 1} + \frac{(F_C^{\pm})^{-3/2} \exp\left(-\frac{F_C^{\pm}}{F}\right)}{1 - \exp\left(-\frac{\hbar\omega}{kT}\right)} \right] \tag{474}$$

where $\tilde{n}$ and $\tilde{p}$ equal n and p for `DensityCorrection=None`, and are given by Eq. 476 for `DensityCorrection=Local`.

The critical field strengths read:

$$F_C^{\pm} = B(E_{g,eff} \pm \hbar\omega)^{3/2} \tag{475}$$

The upper sign in Eq. 474 refers to tunneling generation ($np < n_{i,eff}^2$) and the lower sign refers to recombination ($np > n_{i,eff}^2$). The quantity $\hbar\omega$ denotes the energy of the transverse acoustic phonon.

For Fermi statistics and quantization, Eq. 474 is modified in the same way as for SRH recombination (see Eq. 382, p. 392).

The parameters [28] are given in Table 88 and can be accessed in the parameter set `Band2BandTunneling`. The defaults were obtained assuming the field direction to be $\langle 111 \rangle$.

Table 88   Coefficients for band-to-band tunneling (Schenk model)

Symbol	Parameter name	Default value	Unit
A	A	8.977×10^{20}	$cm^{-1}s^{-1}V^{-2}$
B	B	2.14667×10^7	$Vcm^{-1}eV^{-3/2}$
$\hbar\omega$	hbarOmega	18.6	meV

Schenk Density Correction

The modified electron density reads:

$$\tilde{n} \;=\; n\Big(\frac{n_{\mathrm{i,eff}}}{N_{\mathrm{C}}}\Big)^{\frac{\gamma_n |\nabla E_{\mathrm{F},n}|}{F}} \tag{476}$$

and there is a similar relation for $\tilde{p}$. The parameters $\gamma_n \;=\; n/(n + n_{\mathrm{ref}})$ and $\gamma_p \;=\; p/(p + p_{\mathrm{ref}})$ work as discussed in Schenk TAT Density Correction on page 398. The reference densities n_{ref} and p_{ref} are specified (in cm^{-3}) by the DenCorRef parameter pair in the Band2BandTunneling parameter set. An additional parameter MinGradQF (specified in eVcm^{-1}) is available for smoothing at small values of the gradient for the Fermi potential.

Simple Band-to-Band Models

Sentaurus Device provides a family of simple band-to-band models. Compared to advanced models, the most striking weakness of the simple models is that they predict a nonzero generation rate even in equilibrium. A general expression for these models can be written for the generation term [29] as:

$$G^{\mathrm{b2b}} \;=\; A F^{P} \exp\Big(-\frac{B}{F}\Big) \tag{477}$$

Depending on the value of Model, P takes the value 1, 1.5, or 2.

Table 89 lists the coefficients of models and their defaults. The coefficients A and B can be changed in the parameter set Band2BandTunneling.

Table 89   Coefficients for band-to-band tunneling (simple models)

Model	P	A	B
E1	1	$1.1 \times 10^{27}\ \mathrm{cm}^{-2}\mathrm{s}^{-1}\mathrm{V}^{-1}$	$21.3 \times 10^{6}\ \mathrm{Vcm}^{-1}$
E1_5	1.5	$1.9 \times 10^{24}\ \mathrm{cm}^{-1.5}\mathrm{s}^{-1}\mathrm{V}^{-1.5}$	$21.9 \times 10^{6}\ \mathrm{Vcm}^{-1}$
E2	2	$3.4 \times 10^{21}\ \mathrm{cm}^{-1}\mathrm{s}^{-1}\mathrm{V}^{-2}$	$22.6 \times 10^{6}\mathrm{Vcm}^{-1}$

Hurkx Band-to-Band Model

Similar to the other band-to-band tunneling models, in the Hurkx model [30], the tunneling carriers are modeled by an additional generation–recombination process. Its contribution is expressed as:

$$R_{\text{net}}^{\text{bb}} = A \cdot D \cdot \left(\frac{F}{1\,\text{V/cm}}\right)^P \exp\left(-\frac{BE_g(T)^{3/2}}{E_g(300\text{K})^{3/2}F}\right) \tag{478}$$

where:

$$D = \frac{np - n_{\text{i,eff}}^2}{(n + n_{\text{i,eff}})(p + n_{\text{i,eff}})}(1 - |\alpha|) + \alpha \tag{479}$$

Here, specifying $\alpha = 0$ gives the original Hurkx model, whereas $\alpha = -1$ gives only generation ($D = -1$), and $\alpha = 1$ gives only recombination ($D = 1$). Therefore, if $D < 0$, it is a net carrier generation model. If $D > 0$, it is a recombination model. For Fermi statistics and quantization, Eq. 479 is modified in the same way as for SRH recombination (see Eq. 382).

For DensityCorrection=Local, n and p in Eq. 479 are replaced by $\tilde{n}$ and $\tilde{p}$ (see Schenk Density Correction on page 434).

The coefficients A (in $\text{cm}^{-3}\text{s}^{-1}$), B (in V/cm), P, and α can be specified in the Band2BandTunneling parameter set. By default, Sentaurus Device uses $\alpha = 0$ and the parameters from the E2 model (see Table 89 on page 434). Different values for the generation (Agen, Bgen, Pgen) and recombination (Arec, Brec, Prec) of carriers are supported. For example, to change the parameters to those used in [30], use:

```
Band2BandTunneling {
    Agen = 4e14  # [1/(cm³s)]
    Bgen = 1.9e7 # [V/cm]
    Pgen = 2.5   # [1]
    Arec = 4e14  # [1/(cm³s)]
    Brec = 1.9e7 # [V/cm]
    Prec = 2.5   # [1]
    alpha = 0    # [1]
}
```

Tunneling Near Interfaces and Equilibrium Regions

Physically, band-to-band tunneling occurs over a certain tunneling distance. If the material properties or the electric field change significantly over this distance, Eq. 474, Eq. 477, and

Eq. 478 become inaccurate. In particular, near insulator interfaces, band-to-band tunneling vanishes, as no states to tunnel to are available in the insulator.

In some parts of the device (near equilibrium regions), it is possible that the electric field is large but changes rapidly, so that the actual tunneling distance (the distance over which the electrostatic potential change amounts to the band gap) is bigger and, therefore, tunneling is much smaller than expected from the local field alone.

To account for these effects, two additional control parameters are introduced in the `Band2BandTunneling` parameter set:

```
dDist = <value>  # [cm]
dPot = <value>   # [V]
```

By default, both these parameters equal zero. Sentaurus Device disables band-to-band tunneling within a distance `dDist` from insulator interfaces. If `dPot` is nonzero (reasonable values for `dPot` are of the order of the band gap), Sentaurus Device disables band-to-band tunneling at each point where the change of the electrostatic potential in field direction within a distance of `dPot`/F is smaller than `dPot`/2.

Dynamic Nonlocal Path Band-to-Band Tunneling Model

Sufficient band-bending caused by electric fields or heterostructures can make electrons in the valence band valley (Γ-valley in the k-space), at a certain location, reach the conduction band valley (Γ-, X-, or L-valley in the k-space) at different locations using direct or phonon-assisted band-to-band tunneling process.

The present model implements the nonlocal generation of electrons and holes caused by direct and phonon-assisted band-to-band tunneling processes [31]. In direct semiconductors such as GaAs and InAs, the direct tunneling process is usually dominant. On the other hand, the phonon-assisted tunneling process is dominant in indirect semiconductors such as Si and Ge. If the energy differences between the conduction band valleys are small, it is possible that both the direct and the phonon-assisted tunneling processes are important.

The generation rate is obtained from the nonlocal path integration, and electrons and holes are generated nonlocally at the ends of the tunneling path. As a result, the position-dependent electron and hole generation rates are different in the present model. The model can be applied to heterostructure devices with abrupt and graded heterojunctions.

The main difference between the present model and the band-to-band tunneling model based on the nonlocal mesh (see Band-to-Band Contributions to Nonlocal Tunneling Current on page 734) is that the tunneling path is determined dynamically based on the energy band profile rather than predefined by the nonlocal mesh. Therefore, the present model does not require user-specification of the nonlocal mesh.

The model dynamically searches for the tunneling path with the following assumptions:

- The tunneling path starts from the valence band minus the valence band offset in a region where the nonlocal path model is active.

- The tunneling path is a straight line with its direction opposite to the gradient of the valence band at the starting position. The valence band offset does not change the direction of the tunneling path.

- The tunneling energy is equal to the valence band energy minus the valence band offset at the starting position and is equal to the conduction band energy plus the conduction band offset at the ending position.

- When the tunneling path encounters Neumann boundaries or semiconductor–insulator interfaces, it undergoes specular reflection.

- The tunneling path ends at the conduction band plus the conduction band offset.

If the path crosses a region where the nonlocal path model is not active, by default, the tunneling from this path is discarded. If the `-eB2BGenWithinSelectedRegions` flag is specified in the global `Math` section, tunneling for all paths entirely within semiconductor regions are accounted for.

> **NOTE** By default, nonlocal derivative terms in the Jacobian matrix are not taken into account. To use AC or noise analysis with the present model, computation of nonlocal derivatives must be switched on (see Using Nonlocal Path Band-to-Band Model on page 440). The lack of derivative terms can degrade convergence when the high-field saturation mobility model is switched on or the series resistance is defined at electrodes.

Band-to-Band Generation Rate

For a given tunneling path of length l that starts at $x = 0$ and ends at $x = l$, holes are generated at $x = 0$ and electrons are generated at $x = l$. The net hole recombination rate at $x = 0$ due to the direct band-to-band tunneling process R_{net}^d can be written as:

$$R_{net}^d = |\nabla E_V(0)| C_d \exp\left(-2\int_0^l \kappa dx\right)\left[\left(\exp\left[\frac{\varepsilon - E_{F,n}(l)}{kT(l)}\right] + 1\right)^{-1} - \left(\exp\left[\frac{\varepsilon - E_{F,p}(0)}{kT(0)}\right] + 1\right)^{-1}\right] \tag{480}$$

$$C_d = \frac{g\pi}{36h}\left(\int_0^l \frac{dx}{\kappa}\right)^{-1}\left[1 - \exp\left(-k_m^2 \int_0^l \frac{dx}{\kappa}\right)\right] \tag{481}$$

where:

- h is Planck's constant.

- g is the degeneracy factor.

- $\varepsilon = E_V(0) - \Delta_V(0) = E_C(l) + \Delta_C(l)$ is the tunneling energy.

- Δ_C is the conduction band offset. Δ_C can be positive if the considered tunneling process involves the conduction band valley whose energy minimum is greater than the conduction band energy E_C. $\Delta_C > 0$ increases the effective band gap.

- Δ_V is the valence band offset, and $\Delta_V > 0$ increases the effective band gap.

- κ is the magnitude of the imaginary wavevector obtained from the Kane two-band dispersion relation [31]:

$$\kappa = \frac{1}{\hbar}\sqrt{m_r E_{g,\mathrm{tun}}(1 - \alpha^2)} \tag{482}$$

$$\alpha = -\frac{m_0}{2m_r} + 2\sqrt{\frac{m_0}{2m_r}\left(\frac{\varepsilon - E_V + \Delta_V}{E_{g,\mathrm{tun}}} - \frac{1}{2}\right) + \frac{m_0^2}{16m_r^2} + \frac{1}{4}} \tag{483}$$

$$\frac{1}{m_r} = \frac{1}{m_V} + \frac{1}{m_C} \tag{484}$$

$E_{g,\mathrm{tun}} = E_{g,\mathrm{eff}} + \Delta_C + \Delta_V$ is the effective band gap including the band offsets, and k_m is the maximum transverse momentum determined by the maximum valence-band energy $\varepsilon_{\max}$ and the minimum conduction-band energy $\varepsilon_{\min}$:

$$k_m^2 = \min(k_{vm}^2, k_{cm}^2) \tag{485}$$

$$k_{vm}^2 = \frac{2m_V(\varepsilon_{\max} - \varepsilon)}{\hbar^2} \tag{486}$$

$$k_{cm}^2 = \frac{2m_C(\varepsilon - \varepsilon_{\min})}{\hbar^2} \tag{487}$$

In the Kane two-band dispersion relation, the effective mass in the conduction band m_C and the valence band m_V are related [31]:

$$\frac{1}{m_C} = \frac{1}{2m_r} + \frac{1}{m_0} \tag{488}$$

$$\frac{1}{m_V} = \frac{1}{2m_r} - \frac{1}{m_0} \tag{489}$$

The net hole recombination rate due to the phonon-assisted band-to-band tunneling process R_{net}^p can be written as:

$$R_{net}^p = |\nabla E_V(0)| C_p \exp\left(-2\int_0^{x_0} \kappa_V dx - 2\int_{x_0}^l \kappa_C dx\right)\left[\left(\exp\left[\frac{\varepsilon - E_{F,n}(l)}{kT(l)}\right] + 1\right)^{-1} - \left(\exp\left[\frac{\varepsilon - E_{F,p}(0)}{kT(0)}\right] + 1\right)^{-1}\right] \quad (490)$$

$$C_p = \int_0^l \frac{g(1 + 2N_{op})D_{op}^2}{2^6\pi^2\rho\varepsilon_{op}E_{g,tun}}\sqrt{\frac{m_V m_C}{hl\sqrt{2m_r E_{g,tun}}}}dx\left(\int_0^{x_0}\frac{dx}{\kappa_V}\right)^{-1}\left(\int_{x_0}^l\frac{dx}{\kappa_C}\right)^{-1}\left[1 - \exp\left(-k_{vm}^2\int_0^{x_0}\frac{dx}{\kappa_V}\right)\right]\left[1 - \exp\left(-k_{cm}^2\int_0^l\frac{dx}{\kappa_C}\right)\right] \quad (491)$$

where D_{op}, ε_{op}, and $N_{op} = [\exp(\varepsilon_{op}/kT) - 1]^{-1}$ are the deformation potential, energy, and number of optical phonons, respectively, ρ is the mass density, and κ_V and κ_C are the magnitude of the imaginary wavevectors from the Keldysh dispersion relation:

$$\kappa_V = \frac{1}{\hbar}\sqrt{2m_V|\varepsilon - E_V + \Delta_V|}\,\Theta(\varepsilon - E_V + \Delta_V) \quad (492)$$

$$\kappa_C = \frac{1}{\hbar}\sqrt{2m_C|E_C + \Delta_C - \varepsilon|}\,\Theta(E_C + \Delta_C - \varepsilon) \quad (493)$$

and x_0 is the location where $\kappa_V = \kappa_C$.

As Eq. 480, p. 437 and Eq. 490 are the extension of the results in [31] to arbitrary band profiles, these expressions are reduced to the well-known Kane and Keldysh models in the uniform electric-field limit [31]:

$$R_{net} = A\left(\frac{F}{F_0}\right)^P \exp\left(-\frac{B}{F}\right) \quad (494)$$

where $F_0 = 1\,\text{V/cm}$, $P = 2$ for the direct tunneling process, and $P = 2.5$ for the phonon-assisted tunneling process.

At $T = 300\,\text{K}$ without the bandgap narrowing effect, the prefactor A and the exponential factor B for the direct tunneling process can be expressed by [31]:

$$A = \frac{g\pi m_r^{1/2}(qF_0)^2}{9h^2[E_g(300\text{K}) + \Delta_C + \Delta_V]^{1/2}} \quad (495)$$

$$B = \frac{\pi^2 m_r^{1/2}[E_g(300\text{K}) + \Delta_C + \Delta_V]^{3/2}}{qh} \quad (496)$$

For the phonon-assisted tunneling process, A and B can be expressed by [31]:

$$A = \frac{g(m_V m_C)^{3/2}(1 + 2N_{op})D_{op}^2(qF_0)^{5/2}}{2^{21/4}h^{5/2}m_r^{5/4}\rho\varepsilon_{op}[E_g(300K) + \Delta_C + \Delta_V]^{7/4}} \tag{497}$$

$$B = \frac{2^{7/2}\pi m_r^{1/2}[E_g(300K) + \Delta_C + \Delta_V]^{3/2}}{3qh} \tag{498}$$

Using Nonlocal Path Band-to-Band Model

The nonlocal path band-to-band model is activated by setting `Model=NonlocalPath` in the `Band2Band` option of the command file. Multiple processes with different parameters are supported by using the `ParameterSetName` option and multiple named `Band2BandTunneling` parameter sets (see Using Band-to-Band Tunneling on page 431).

> **NOTE** Each tunneling path (characterized by a particular parameter set name) must have a consistent tunneling process (either direct or phonon-assisted tunneling process) in different regions. For example, specifying `Ppath=0` (direct tunneling) in silicon regions and specifying `Ppath` greater than zero (phonon-assisted tunneling) in polysilicon regions will induce an error message.

`MaxTunnelLength` in the parameter file specifies the maximum length of the tunneling path. If the length reaches `MaxTunnelLength` before a valid tunneling path is found, the band-to-band tunneling is neglected.

You can choose between two input parameter sets in the `Band2BandTunneling` section:

- The first parameter set consists of (m_C, m_V, g, Δ_C, Δ_V) in the case of direct tunneling or (m_C, m_V, gD_{op}^2/ρ, ε_{op}, Δ_C, Δ_V) in the case of phonon-assisted tunneling.
- The second parameter set consists of (A, B, m_V/m_C, Δ_C, Δ_V) in the case of direct tunneling or (A, B, m_V/m_C, ε_{op}, Δ_C, Δ_V) in the case of phonon-assisted tunneling.

> **NOTE** The temperature-specific band gap $E_g(300K) + \Delta_C + \Delta_V$ in Eq. 495 to Eq. 498 is used solely for the definitions of the A and B parameters to be consistent with the Kane and Keldysh models in the uniform electric-field limit. Internally, the second parameter set is transformed into the first parameter set. The band gap that is used for the WKB integrals features all dependencies (for example, mole fraction, temperature, and stress) as specified in the `Physics` section.

Specifying $\varepsilon_{op} = 0$ selects the direct tunneling process. When $\varepsilon_{op} = 0$ and the option `FranzDispersion` is switched on in the `Band2Band` option of the command file, the

magnitude of the imaginary wavevector is obtained from the Franz two-band dispersion relation (Eq. 777, p. 730) instead of the Kane two-band dispersion relation (Eq. 482, p. 438).

Specifying $\varepsilon_{op} > 0$ selects the phonon-assisted tunneling process. When $m_V / m_C = 0$, m_V and m_C are determined from Eq. 488, p. 438 and Eq. 489, p. 438.

In the parameter file, the parameter pairs `QuantumPotentialFactor` and `QuantumPotentialPosFac` in the `Band2BandTunneling` parameter set specify the prefactors for the electron and hole quantum potentials obtained from the density gradient model (see Density Gradient Quantization Model on page 294) that can be added to the effective band gap for tunneling. By default, they are zero, such that the quantum potentials are neglected in the computation of the generation rate. When they are nonzero, the quantum potentials multiplied by the corresponding prefactors are added to the conduction and valence band edges when the transmission coefficient is computed. For `QuantumPotentialFactor`, an addition is performed irrespective of the sign of the quantum potential. For `QuantumPotentialPosFac`, an addition is performed only when the quantum potential is positive, that is, only where quantization causes an effective widening of the band gap. For example, the following section causes the electron and hole quantum potentials to be added to the band gap wherever they cause an effective widening of the band gap:

```
Band2BandTunneling {
    ...
    QuantumPotentialPosFac = 1 1
}
```

Table 90 lists the coefficients of models and their defaults. These parameters can be mole fraction dependent. The default parameters A and B are obtained from [30].

Table 90   Default parameters for nonlocal path band-to-band tunneling model

Symbol	Parameter name	Default value	Unit
A	`Apath`	4×10^{14}	$cm^{-3}s^{-1}$
B	`Bpath`	1.9×10^{7}	Vcm^{-1}
gD_{op}^2/ρ	`Cpath`	0	J^2cmkg^{-1}
g	`degeneracy`	0	1
Δ_C	`Dcpath`	0	eV
Δ_V	`Dvpath`	0	eV
m_C	`m_c`	0	m_0
m_V	`m_v`	0	m_0
ε_{op}	`Ppath`	0.037	eV
m_V/m_C	`Rpath`	0	1

Handling of Derivatives

Due to the dynamic search for tunnel paths, the structure of the system Jacobian depends on solution variables. Therefore, the nonzero entries of the Jacobian are not known *a priori*. The possible entries are estimated before entering the Newton loop.

The computation of nonlocal derivative terms is controlled in the global `Math` section, in the `Quasistationary` statement (see Quasistationary Ramps on page 74) and in the `Transient` statement (see Transient Ramps on page 91) using the `NonlocalPath` section.

Using the `Derivative` option in the `NonlocalPath` section, the computation of nonlocal derivatives can be switched on (`Derivative=1`) and switched off (`Derivative=0`). By default, the computation of nonlocal derivatives is switched off.

If nonlocal derivatives are computed, different strategies are available, using the `Strategy` option, to fill the system Jacobian:

■ If `Strategy=1`, all previously collected Jacobian entries are registered as possible nonzero entries for the next Newton loop. The collection bin of possible Jacobian entries is emptied at the beginning of the `Quasistationary` and `Transient` ramps.

■ If `Strategy=2`, Jacobian entries that occur only during the last `N` Newton iterations are registered as possible nonzero entries for the next Newton loop.

■ If `Strategy=3`, it automatically activates and deactivates the computation of nonlocal derivatives during the `Quasistationary` and `Transient` ramps, depending on the step size. If the step size is smaller than `MinStep`, nonlocal derivatives are computed. If the step size is greater than `MaxStep`, nonlocal derivatives are not computed. Jacobian entries that occur during the last `N` Newton iterations are registered as possible nonzero entries for the next Newton loop.

For example:

```
NonlocalPath (
   Derivative=1
   Strategy=3
   N=5
   MinStep=1.0e-5
   MaxStep=1.0e-2
)
```

NOTE The inclusion of nonlocal derivatives is computationally heavy and reduces the sparsity of the system Jacobian. Simulation times will increase.

Postprocessing Mode

To estimate the nonlocal tunneling generation rate without convergence difficulties and without computationally heavy nonlocal derivatives, Sentaurus Device provides the postprocessing mode of the dynamic nonlocal path band-to-band tunneling model.

The postprocessing mode can be switched on (`Postprocessing`) and switched off (`-Postprocessing`) in the `NonlocalPath` section. By default, the postprocessing mode is switched off. Specifying the `NonlocalPath` section in the `Quasistationary` or `Transient` statement overwrites the specifications of the `NonlocalPath` section in the global `Math` section.

In the postprocessing mode, generation rates due to the dynamic nonlocal path band-to-band tunneling model are excluded from the continuity equations. Based on this solution without nonlocal tunneling, Sentaurus Device calculates the nonlocal tunneling generation rates in a postprocessing step.

> **NOTE** In the postprocessing mode, nonlocal tunneling is not computed self-consistently. There is no feedback of the nonlocal tunneling generation rates on the solution that has been used to calculate the nonlocal tunneling generation rates.

The tunneling generation currents are computed according to $J^{n/p} = q \int R_{net}^{n/p}(r) d^3 r$ where the integration volume expands over all semiconductor regions. If postprocessing is activated, the electron and hole tunneling generation currents `eBand2BandGenerationCurrent` and `hBand2BandGenerationCurrent` are written in units of C/s into the plot file.

Frozen Tunneling Direction

In some cases, the estimation of the tunneling direction pointing along the negative gradient of the valence band energy can be a tunneling direction of minor importance. Furthermore, freezing the tunneling direction can support numeric stability to achieve convergence. You can specify the tunneling direction by setting `direction=<vector>` in the `NonlocalPath` section.

Visualizing Nonlocal Band-to-Band Generation Rate

To plot the electron and hole generation rates, specify `eBand2BandGeneration` and `hBand2BandGeneration` in the `Plot` section, respectively.

> **NOTE** `Band2BandGeneration` is equal to `hBand2BandGeneration`.

Bimolecular Recombination

The bimolecular recombination model describes the interaction of electron–hole pairs and singlet excitons (see Singlet Exciton Equation on page 235).

Physical Model

The rate of electron–hole pair and singlet exciton recombination follows the Langevin form, that is, it is proportional to the carrier mobility. The bimolecular recombination rate is given by:

$$R_{\text{bimolec}} = \gamma \cdot \frac{q}{\varepsilon_0 \varepsilon_r} \cdot (\mu_n + \mu_p) \left(np - n_{i,\text{eff}}^2 \frac{n_{\text{se}}}{n_{\text{se}}^{\text{eq}}} \right) \tag{499}$$

where:

- γ is a prefactor for the singlet exciton.
- q is the elementary charge.
- ε_0 and ε_r denote the free space and relative permittivities, respectively.
- Electron and hole mobilities are given by μ_n and μ_p, accordingly.
- n, p, and $n_{i,\text{eff}}$ describe the electron, hole, and effective intrinsic density, respectively.
- n_{se} is the singlet exciton density.
- $n_{\text{se}}^{\text{eq}}$ denotes the singlet-exciton equilibrium density.

Using Bimolecular Recombination

The bimolecular recombination model is activated by using the keyword `Bimolecular` as an argument of the `Recombination` statement in the `SingletExciton` section (see Table 254 on page 1449). It is switched off by default and can be activated regionwise (see Singlet Exciton Equation on page 235). An example is:

```
Physics (Region="EML-ETL") {
   SingletExciton (
      Recombination ( Bimolecular )
   )
}
```

Table 91 lists the parameter of the bimolecular recombination model, which is accessible in the `SingletExciton` section of the parameter file.

Table 91   Default parameter for bimolecular recombination

Symbol	Parameter name	Default value	Unit
γ	gamma	0.25	1

Exciton Dissociation Model

The exciton dissociation model describes the dissociation of singlet excitons into electron–hole pairs at semiconductor–semiconductor and semiconductor–insulator interfaces.

Physical Model

The rate of singlet exciton interface dissociation is modeled as:

$$R_{se,diss}^{surf} = v_{se,0}\sigma_{se-N_{diss}}N_{se,diss}^{surf}(n_{se} - n_{se}^{eq})$$ (500)

where:

$$v_{diss}^{surf} = v_{se,0}\sigma_{se-N_{diss}}N_{se,diss}^{surf}$$ (501)

is the singlet exciton recombination velocity in cm/s , $\sigma_{se-N_{diss}}$ is the capture cross-section of exciton dissociation centers with the surface density $N_{se,diss}^{surf}$, $v_{se,0}$ is the singlet exciton thermal velocity, and n_{se} and n_{se}^{eq} are the exciton and equilibrium exciton densities, respectively.

In the dissociation process, a singlet exciton generates an electron–hole pair. The rate in Eq. 500 is a recombination rate for the singlet exciton equation and a generation rate for the electron and hole continuity equations.

Using Exciton Dissociation

The exciton dissociation model is activated using the keyword `Dissociation` as an argument of the `Recombination` statement in the `SingletExciton` section (see Table 254 on page 1449). It is switched off by default and can be activated regionwise (see Singlet Exciton Equation on page 235).

The following example activates exciton dissociation at the `EML/ETL` region interface:

```
Physics (RegionInterface="EML/ETL") {
   SingletExciton (Recombination ( Dissociation ))
}
```

Table 92 lists the parameters of the exciton dissociation model, which is accessible in the `SingletExciton` section of the parameter file.

Table 92   Default parameters for exciton dissociation model

Symbol	Parameter name	Default value	Unit
$\sigma_{se-N_{diss}}$	`ex_dXsection`	1×10^{-8}	cm^2
$N_{se,diss}^{surf}$	`N_diss`	1×10^{10}	cm^{-2}

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CHAPTER 17 Traps and Fixed Charges

This chapter presents information on how traps are handled by Sentaurus Device.

Traps are important in device physics. For example, they provide doping, enhance recombination, and increase leakage through insulators. Several models (for example, Shockley–Read–Hall recombination, described in Shockley–Read–Hall Recombination on page 391) depend on traps implicitly, but do not actually model them. This chapter describes models that take the occupation and the space charge stored on traps explicitly into account. It also describes the specification of fixed charges.

Sentaurus Device provides several trap types (electron and hole traps, fixed charges), five types of energetic distribution (level, uniform, exponential, Gaussian, and table), and various models for capture and emission rates, including the V-model (optionally, with field-dependent cross sections), the J-model, and nonlocal tunneling. Traps are available for both bulk and interfaces.

A simple model restricted to insulator fixed charges is described in Insulator Fixed Charges on page 471.

Basic Syntax for Traps

The specification of trap distributions and trapping models appears in the `Physics` section. In contrast to other models, most model parameters are specified here as well. Parameter specifications in the parameter file serve as defaults for those in the command file.

Traps can be specified for interfaces or bulk regions. Specifications take the form:

```
Physics (Region="gobbledygook"){
   Traps(
      ( <trap specification> )
      ( <trap specification> )
      ...
   )
}
```

and likewise for `Material`, `RegionInterface`, and `MaterialInterface`. Above, each `<trap specification>` describes one particular trap distribution, and the models and parameters applied to it. When only a single trap specification is present, the inner pair of

parentheses can be omitted. Table 325 on page 1488 summarizes the options that can appear in the trap specification.

> **NOTE** Wherever a contact exists at a specified region interface, Sentaurus Device does not recognize the interface traps within the bounds of the contact because the contact itself constitutes a region and effectively overwrites the interface between the two 'material' regions. This is true even if the contact is not declared in the `Electrode` statement.

Trap Types

The keywords `FixedCharge`, `Acceptor`, `Donor`, `eNeutral`, and `hNeutral` select the type of trap distribution:

- `FixedCharge` traps are always completely occupied.

- `Acceptor` and `eNeutral` traps are uncharged when unoccupied and they carry the charge of one electron when fully occupied.

- `Donor` and `hNeutral` traps are uncharged when unoccupied and they carry the charge of one hole when fully occupied.

Energetic and Spatial Distribution of Traps

The keywords `Level`, `Uniform`, `Exponential`, `Gaussian`, and `Table` determine the energetic distribution of traps. They select a single-energy level, a uniform distribution, an exponential distribution, a Gaussian distribution, and a user-defined table distribution, respectively:

$$
\begin{cases}
N_0 & \text{for } E = E_0 & \text{for } \texttt{Level} \\
N_0 & \text{for } E_0 - 0.5E_S < E < E_0 + 0.5E_S & \text{for } \texttt{Uniform} \\
N_0 \exp\left(-\left|\dfrac{E - E_0}{E_S}\right|\right) & & \text{for } \texttt{Exponential} \\
N_0 \exp\left(-\dfrac{(E - E_0)^2}{2E_S^2}\right) & & \text{for } \texttt{Gaussian} \\
\begin{cases} N_1 & \text{for } E = E_1 \\ \dots & \dots \\ N_m & \text{for } E = E_m \end{cases} & & \text{for } \texttt{Table}
\end{cases}
\tag{502}
$$

N_0 is set with the `Conc` keyword. For a `Level` distribution, `Conc` is given in cm^{-3} (for regionwise or materialwise specifications) or cm^{-2} (for interface-wise specifications). For the

other energetic distributions, `Conc` is given in $\text{eV}^{-1}\text{cm}^{-3}$ or $\text{eV}^{-1}\text{cm}^{-2}$. For `FixedCharge`, the sign of `Conc` denotes the sign of the fixed charges. For the other trap types, `Conc` must not be negative.

For a `Table` distribution, individual levels are given as a pair of energies (in eV) and the corresponding concentrations (in $\text{eV}^{-1}\text{cm}^{-3}$ or $\text{eV}^{-1}\text{cm}^{-2}$). Depending on the presence of the keywords `fromCondBand`, `fromMidBandGap`, or `fromValBand`, the energy levels in the table are relative to the conduction band, intrinsic energy, or valence band, respectively. To obtain the absolute concentration (in cm^{-3} or cm^{-2}) for each level, the energy range between the smallest and the largest energy in the table is split into intervals. The boundaries of the intervals are the energies that are in the middle between adjacent energies in the table. The absolute concentration of a level is the product of the size of the energy interval that contains it and the concentration specified in the table. If the table contains only one level, an interval size of 1 eV is assumed. For example:

```
Traps ((Table=(-0.1 1e15 0 1e16 0.1 1e15) fromMidBandGap))
```

creates a trap level at the midgap with a concentration of $0.1\,\text{eV} \times 10^{16}\,\text{cm}^{-3}\,\text{eV}^{-1} = 10^{15}\,\text{cm}^{-3}$, and a level at both 0.1 eV above and below the midgap, with a concentration of $0.05\,\text{eV} \times 10^{15}\,\text{cm}^{-3}\,\text{eV}^{-1} = 5\times10^{13}\,\text{cm}^{-3}$.

E_0 and E_S are given in eV by `EnergyMid` and `EnergySig`. The energy of the center of the trap distribution, E_trap^0, is obtained from E_0 depending on the presence of one of the keywords `fromCondBand`, `fromMidBandGap`, or `fromValBand`:

$$E_\text{trap}^0 = \begin{cases} E_\text{C} - E_0 - E_\text{shift} & \texttt{fromCondBand} \\ [E_\text{C} + E_\text{V} + kT\ln(N_\text{V}/N_\text{C})]/2 + E_0 + E_\text{shift} & \texttt{fromMidBandGap} \\ E_\text{V} + E_0 + E_\text{shift} & \texttt{fromValBand} \end{cases} \tag{503}$$

Internally, Sentaurus Device approximates trap-energy distributions by discrete energy levels. The number of levels defaults to 13 and is set by `TrapDLN` in the `Math` section.

In Eq. 503, E_shift is zero (the default) or is computed by a PMI specified with `EnergyShift=<model name>` or `EnergyShift=(<model name>, <int>)`. The PMI depends on the electric field and the lattice temperature. By default, these quantities are taken at the location of the trap; alternatively, with `ReferencePoint=<vector>`, you can specify a coordinate in the device from where these quantities are to be taken. For more details, see Trap Energy Shift on page 1205.

For traps located at interfaces, `Region` or `Material` allows you to specify the region or material on one side of the interface; the energy specification then refers to the band structure on that side. For heterointerfaces, the charge and recombination rate due to the traps will be fully accounted for on that side. Without this side specification, the energy parameters refer to the bands that you see when you plot the band edges, which usually originate from the lower

bandgap material. The charge and recombination rates due to traps are evenly distributed on both sides.

Note that if the trap energies are not referred to the side of the material with lower bandgap, the correction of trap energies is performed at 300 K. This implies that if you perform a temperature-dependent simulation with traps at an interface between materials that have different temperature dependency, you should use both heterointerfaces and `Region` or `Material` for the side specification, to make the correct specification of trap energies easier.

By default, the trap energies refer to effective band edges, that is, band edges that include bandgap narrowing. By specifying `Reference=BandGap`, trap energies refer to band edges that do not include bandgap narrowing.

By default, the energy range of traps for `Uniform`, `Gaussian`, and `Exponential` trap distributions are truncated to the effective bandgap at 300 K. Truncation is controlled by the `Cutoff` keyword. A value of `None` disables truncation, a value of `Simple` activates a truncation approach used by previous versions of Sentaurus Device (ignoring mole fraction dependency of the band gap), and a value of `BandGap` truncates to the band gap at 300 K without bandgap narrowing. Note that the truncation approach does not affect the band edges to which trap energies refer during simulation: These are always the solution-dependent band edges, including temperature dependency. The `Level` and `Table` traps are never truncated to the band gap.

By default, trap concentrations are uniform over the domain for which they are specified. With `SFactor= "<dataset_name>"`, the given dataset determines the spatial distribution. If `Conc` is zero or is omitted, the dataset determines the density directly. For `Uniform`, `Gaussian`, and `Exponential` trap distributions, this is the total density (in cm^{-3} or cm^{-2}) of the integrated energy distribution. If `Conc` is nonzero, the `SFactor` is scaled by the maximum of its absolute value and multiplied by N_0. Datasets available for `SFactor` are `DeepLevels`, `xMoleFraction`, and `yMoleFraction` (read from the doping file), and `eTrappedCharge` and `hTrappedCharge` (read from the file specified by `DevFields` in the `File` section), as well as the PMI user fields (read from the file specified by `PMIUserFields` in the `File` section).

Alternatively, with `SFactor = "<pmi_model_name>"`, the spatial distribution is computed using the PMI. See Space Factor on page 1190 for more details. During a transient simulation, this PMI gives the possibility to have a time-dependent trap concentration. In this case, spatial distribution can be computed based on the solution from the previous time step available through the PMI.

`SpatialShape` selects a multiplicative modifier function for the trap concentration. If `SpatialShape` is `Uniform` (the default), the multiplier for point (x, y, z) is:

$$\Theta(\sigma_x - |x - x_0|)\Theta(\sigma_y - |y - y_0|)\Theta(\sigma_z - |z - z_0|) \tag{504}$$

If `SpatialShape` is `Gaussian`, the multiplier is:

$$\exp\left(-\frac{(x-x_0)^2}{2\sigma_x^2} - \frac{(y-y_0)^2}{2\sigma_y^2} - \frac{(z-z_0)^2}{2\sigma_z^2}\right) \tag{505}$$

In Eq. 504 and Eq. 505, (x_0, y_0, z_0) and $(\sigma_x, \sigma_y, \sigma_z)$ are given (in μm) by the `SpaceMid` and `SpaceSig` options, respectively. By default, the components of `SpaceSig` are huge, so that the multiplier becomes one.

Specifying Single Traps

The keyword `SingleTrap` has been provided to simplify the specification of parameters to mimic the behavior of a single carrier trap or single fixed-charge trap. Including `SingleTrap` in the trap specification results in the following behavior:

- The coordinates specified with `SpaceMid=`(x_0, y_0, z_0) snap to the nearest node in the material, region, or interface that is specified as part of the `Physics` command. If a global `Physics` specification is used, the coordinates snap to the nearest node in the device.

- `SpatialShape=Uniform` is used automatically for the trap. You do not need to specify this parameter.

- `SpaceSig=(1e-6, 1e-6, 1e-6)` is used automatically for the trap. This is intended to confine the trap to a single node. You do not need to specify this parameter.

- The trap concentration is computed automatically such that a filled trap corresponds to one electronic charge. If `Conc` is specified by users, it is ignored.

- `SingleTrap` is only allowed with a `Level` energetic distribution for carrier traps (`eNeutral`, `hNeutral`, `Acceptor`, or `Donor`) or with `FixedCharge` traps.

- When `SingleTrap` is specified with `FixedCharge`, the sign of `Conc` (if specified) is used for the sign of the fixed charge. If `Conc` is not specified or if `Conc=0` is specified, the fixed charge is positive. To obtain a negative fixed charge with `SingleTrap`, specify any negative value for `Conc`.

- For 2D simulations, `AreaFactor` specified in the `Physics` section is used for the z-direction width when calculating the `SingleTrap` concentration.

For example, the following command file fragment places two single-electron traps at the silicon–oxide interface:

```
Physics (MaterialInterface="Silicon/Oxide") {
  Traps (
    (SingleTrap eNeutral Level EnergyMid=0 fromMidBandGap
    SpaceMid=(0.0,0.0,0.1))
```

```
        (SingleTrap eNeutral Level EnergyMid=0 fromMidBandGap
        SpaceMid=(0.2,0.0,0.3))
    )
}
```

Trap Randomization

The spatial distribution of traps can be randomized by including the keyword `Randomize` in the trap specification. Specifying `Randomize` results in the following behavior:

- If `SingleTrap` is specified, the location of the single trap is randomized in the material, region, or interface that is specified as part of the `Physics` command. If a global `Physics` specification is used, the location of the single trap is randomized in the whole device. If `SpaceMid` is specified, it is ignored.

- If `SingleTrap` is not specified, the concentration of traps at each node is randomized. This is accomplished by first determining the average number of traps at a node based on the spatial distribution created from the trap specification. This is used as the expectation value for a Poisson-distribution random number generator to obtain a new random number of traps at the node. Finally, this is converted back to a trap concentration.

- `Randomize` is only allowed with a `Level` energetic distribution for carrier traps (`eNeutral`, `hNeutral`, `Acceptor`, or `Donor`) or with `FixedCharge` traps.

- If `Randomize` is specified, the randomization is different every time the command file is executed. However, this behavior can be altered by specifying `Randomize` with an integer argument:

  - `Randomize < 0`: No randomization occurs.

  - `Randomize = 0`: Same as `Randomize` without an argument. The randomization is different for every execution of the command file.

  - `Randomize > 0`: The specified number is used as the seed for the random number generator. This allows a particular randomization to be repeated for repeated executions of the same command file on the same platform.

Examples

Randomize location of a single electron trap at the silicon–oxide interface:

```
Physics (MaterialInterface="Silicon/Oxide") {
  Traps (
    (SingleTrap Randomize eNeutral Level EnergyMid=0 fromMidBandGap)
  )
}
```

Randomize a Gaussian spatial distribution of traps in silicon:

```
Physics (Material="Silicon") {
   Traps (
      (eNeutral Conc=1e16 Level EnergyMid=0 fromMidBandGap
      Randomize SpatialShape=Gaussian
      SpaceMid=(0.0,0.0,0.05) SpaceSig=(0.05,0.05,0.05))
   )
}
```

Trap Models and Parameters

Trap Occupation Dynamics

The electron occupation f^n of a trap is a number between 0 and 1, and changes due to the capture and emission of electrons:

$$\frac{\partial f^n}{\partial t} = \sum_i r_i^n \tag{506}$$

$$r_i^n = (1 - f^n)c_i^n - f^n e_i^n \tag{507}$$

c_i^n denotes an electron capture rate for an empty trap and e_i^n denotes an electron emission rate for a full trap, respectively. The sum in Eq. 506 is over all capture and emission processes. For example, the capture of an electron from the conduction band is a process distinct from the capture of an electron from the valence band.

For the stationary state, the time derivative in Eq. 506 vanishes. The occupation becomes:

$$f^n = \frac{\sum c_i^n}{\sum (c_i^n + e_i^n)} \tag{508}$$

and the net electron capture rate due to process k becomes:

$$r_k^n = \frac{c_k^n \sum e_i^n - e_k^n \sum c_i^n}{\sum (c_i^n + e_i^n)} \tag{509}$$

The previous equations are given in the electron picture, which is the most natural one for `eNeutral` or `Acceptor` traps. For `hNeutral` and `Donor` traps, you might prefer to use the

equivalent hole picture. Use the relations $c_i^p = e_i^n$, $e_i^p = c_i^n$, $f^p = 1 - f^n$, and $r_i^p = -r_i^n$ to translate the electron picture into the hole picture.

Figure 20 illustrates the two equivalent pictures.
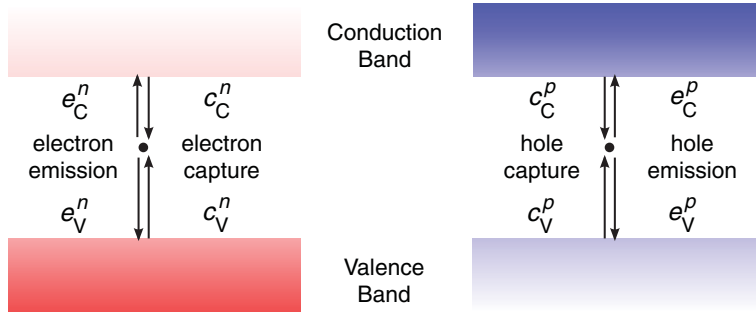
Figure 20   Trap occupation dynamics: (*left*) electron picture and (*right*) hole picture

In particular, in the stationary state, for traps with concentration N_0, the V-model (see Local Trap Capture and Emission on page 457) and Eq. 509 lead to the Shockley–Read–Hall recombination rate:

$$R_{\text{net}} = \frac{N_0 v_{\text{th}}^n v_{\text{th}}^p \sigma_n \sigma_p (np - n_{\text{i,eff}}^2)}{v_{\text{th}}^n \sigma_n (n + n_1 / g_n) + v_{\text{th}}^p \sigma_p (p + p_1 / g_p)}$$ (510)

Each capture and emission process couples the trap to a reservoir of carriers. If only a single process would be effective, in the stationary state, the trap would be in equilibrium with the reservoir for this process. This consideration (the 'principle of detailed balance') relates capture and emission rates:

$$e_i = \frac{c_i}{g} \exp\left(\frac{E_{\text{trap}} - E_{\text{F}}^i}{kT_i}\right)$$ (511)

Here, E_{trap} is the energy of the trap, E_{F}^i is the Fermi energy of the reservoir, T_i is the temperature of the reservoir, and g is the degeneracy factor. Sentaurus Device supports distinct degeneracy factors g_n and g_p for coupling to the conduction and valence bands. They default to 1 and are set with eGfactor and hGfactor in the command file, and with the G parameter pair in the Traps parameter set.

Capture and emission rates are either local (see Local Trap Capture and Emission on page 457) or nonlocal (see Tunneling and Traps on page 463). Sentaurus Device does not solve the current continuity equations in insulators and, therefore, supports local rates only for traps in semiconductors or at semiconductor interfaces. Therefore, traps in insulators that are not connected to a semiconductor region by a nonlocal model do not have any capture and emission processes, and their occupation is undefined (except for FixedCharge 'traps'). Sentaurus Device ignores them.

Local Trap Capture and Emission

The electron capture rate from the conduction band at the same location as the trap is:

$$c_C^n = \sigma_n \left[(1 - g_n^J) v_{th}^n n + g_n^J \frac{J_n}{q} \right] \tag{512}$$

and similarly, the hole capture rate from the valence band is $c_V^p = \sigma_p [(1 - g_p^J) v_{th}^p p + g_p^J J_p / q]$.

g_n^J and g_p^J are set with `eJfactor` and `hJfactor` in the command file, and with the `Jcoef` parameter pair in the `Traps` parameter set. g_n^J and g_p^J can take any value between 0 and 1. When zero (the default), the V-model is obtained, and when 1, the J-model (popular for modeling radiation problems) is obtained.

The electron emission rate to the conduction band is $e_C^n = v_{th}^n \sigma_n \gamma_n n_1 / g_n + e_{const}^n$ and the hole emission to the valence band is $e_V^p = v_{th}^p \sigma_p \gamma_p p_1 / g_p + e_{const}^p$. For $g_n^J = e_{const}^n = 0$ and $g_p^J = e_{const}^p = 0$, these rates obey the principle of detailed balance.

Above, $n_1 = N_C \exp[(E_{trap} - E_C)/kT]$ and $p_1 = N_V \exp[(E_V - E_{trap})/kT]$. For Fermi statistics or with quantization (see Chapter 14 on page 283), γ_n and γ_p are given by Eq. 47 and Eq. 48, p. 177 (see Fermi Statistics on page 176), whereas otherwise, $\gamma_n = \gamma_p = 1$.

v_{th}^n and v_{th}^p are the thermal velocities. Sentaurus Device offers two options, selected by the `VthFormula` parameter pair in the `Traps` parameter set (default is 1):

$$v_{th}^{n,p} = \begin{cases} v_o^{n,p} \sqrt{\dfrac{T}{300K}} & \text{VthFormula=1} \\[2ex] \sqrt{\dfrac{3kT}{m_{n,p}(300\,K)}} & \text{VthFormula=2} \end{cases} \tag{513}$$

$v_0^{n,p}$ are given by the `Vth` parameter pair in the `Traps` section of the parameter file.

Sentaurus Device offers several options for the cross sections σ_n and σ_p. In any case, trap cross sections are derived from the constant cross sections σ_n^0 and σ_p^0, which are set by the `eXsection` and `hXsection` keywords in the command file, and by the `Xsec` parameter pair in the `Traps` parameter set.

By default, the cross sections are constant: $\sigma_n = \sigma_n^0$ and $\sigma_p = \sigma_p^0$.

e_{const}^n and e_{const}^p represent the constant emission rate terms for carrier emission from the trap level to the conduction and valence band. They can be set by the `eConstEmissionRate` and `hConstEmissionRate` keywords in the command file, and by the `ConstEmissionRate` parameter pair in the `Traps` parameter set (default $e_{\text{const}}^n = 0 \text{ s}^{-1}$, $e_{\text{const}}^p = 0 \text{ s}^{-1}$).

The option `SimpleCapt` restricts the field enhancement to the cross sections used by the emission rates. That is, for the computation of e_C^n and e_V^n, σ_n and σ_p are used and, for the computation of c_C^n and c_V^n, σ_n^0 and σ_n^0 are used. Using different cross sections for capture and emission violates the principle of detailed balance. By default, the same cross sections are used for capture and emission rates.

J-Model Cross Sections

This model is activated by the `ElectricField` keyword in the command file. It is intended for use with the J-model and reads:

$$\sigma_{n,p} = \sigma_{n,p}^0 \left(1 + a_1 \left| \frac{F}{1\,\text{Vm}^{-1}} \right|^{p_1} + a_2 \left| \frac{F}{1\,\text{Vm}^{-1}} \right|^{p_2} \right)^{p_0} \tag{514}$$

where a_1, a_2, p_0, p_1, and p_2 are adjustable parameters available as parameter pairs `a1`, `a2`, `p0`, `p1`, and `p2` in the `Traps` parameter set. Using the `SimpleCapt` option restricts the field enhancement of cross sections to the emission rates only.

Hurkx Model for Cross Sections

The Hurkx model is selected by the `Tunneling(Hurkx)` keyword in the command file. The cross sections are obtained from σ_n^0 and σ_p^0 using Eq. 399, p. 399. Using the `SimpleCapt` option restricts the field enhancement of cross sections to the emission rates only.

Poole–Frenkel Model for Cross Sections

The Poole–Frenkel model [1] is frequently used for the interpretation of transport effects in dielectrics and amorphous films. The model predicts an enhanced emission probability Γ_{pf} for charged trap centers where the potential barrier is reduced because of the high external electric field.

The model is selected by the `PooleFrenkel` keyword in the `Traps` specification (in the `Physics` section) of the command file. In the Poole–Frenkel model:

$$
\sigma_{n,p}^{\text{enh}} = \sigma_{n,p}^{0}(1 + \Gamma_{\text{pf}})
$$
$$
\Gamma_{\text{pf}} = \frac{1}{\alpha^2}[1 + (\alpha - 1)\exp(\alpha)] - \frac{1}{2} \tag{515}
$$
$$
\alpha = \frac{1}{kT}\sqrt{\frac{q^3 F}{\pi \varepsilon_{\text{pf}}}}
$$

If `PooleFrenkel` is used without options, for `Donor` and `hNeutral` traps, $\sigma_n = \sigma_n^{\text{enh}}$ and $\sigma_p = \sigma_p^{0}$ and, for `Acceptor` and `eNeutral` traps, $\sigma_p = \sigma_p^{\text{enh}}$ and $\sigma_n = \sigma_n^{0}$. If `PooleFrenkel` with the option `Electron` is used, $\sigma_n = \sigma_n^{\text{enh}}$ irrespective of trap type. If `PooleFrenkel` is used with the option `Hole`, $\sigma_p = \sigma_p^{\text{enh}}$ irrespective of trap type. The specifications `PooleFrenkel(Electron)` and `PooleFrenkel(Hole)` can be used together to activate the model for exchange with conduction and valence bands simultaneously. ε_{pf} is an adjustable parameter and is set by the `epsPF` parameter pair in the `PooleFrenkel` parameter set.

Using the `SimpleCapt` option restricts the field enhancement of cross sections to the emission rates only.

Local Capture and Emission Rates Based on Makram-Ebeid–Lannoo Phonon-Assisted Tunnel Ionization Model

The Makram-Ebeid–Lannoo model [2] is a phonon-assisted tunnel emission model for carriers trapped on deep semiconductor levels, with its main application in two-band charge transport in silicon nitride [3].

In this model, the deep trap acts as an oscillator or core embedded in the nitride lattice, attracting electrons (electron trap) or holes (hole trap). The deep trap is defined by the phonon energy W_{ph}, the thermal energy W_T and the optical energy W_{opt}. The trap ionization rate is given by:

$$
P = \sum_{n=-\infty}^{\infty} \exp\left[\frac{n W_{\text{ph}}}{2kT} - S\coth\frac{W_{\text{ph}}}{2kT}\right] I_n\left(\frac{S}{\sinh(W_{\text{ph}}/(2kT))}\right) P_i(W_T + n W_{\text{ph}}) \tag{516}
$$

$$
P_i(W) = \frac{eF}{2\sqrt{2mW}}\exp\left(-\frac{4\sqrt{2m}}{3\hbar eF}W^{3/2}\right) \tag{517}
$$

where I_n is the modified Bessel function of the order n, $S = (W_{\text{opt}} - W_T)/W_{\text{ph}}$, and $P_i(W)$ is the tunnel escape rate through the triangle barrier of height W.

Sentaurus Device implements the Makram-Ebeid–Lannoo model for `Level` traps, `eNeutral` and `hNeutral`. The electron emission rate to the conduction band e_C^n and the hole emission to the valence band e_V^p are the trap ionization rates described by Eq. 516 with the corresponding W_{ph}, W_T and W_{opt} defining the associated deep trap.

The electron capture rate from the conduction band c_C^n and the hole capture rate from the valence band c_V^p are computed based on user selection. They can be obtained from the emission rates by the principle of detailed balance or using the constant capture cross-sections:
$c_C^n = \sigma_n^0 \left[(1 - g_n^J) v_{th}^n n + g_n^J \frac{J_n}{q} \right]$, $c_V^p = \sigma_p^0 [(1 - g_p^J) v_{th}^p p + g_p^J J_p / q]$.

The model is selected by the keyword `Makram-Ebeid` in the command file of the trap parameter set. When the `Makram-Ebeid` keyword with no options is used, the trap couples to both the conduction and valence bands through Makram-Ebeid–Lannoo trap emission rates. When `Makram-Ebeid` is used with the option `electron` in parentheses, an `eNeutral` trap couples to the conduction band through the Makram-Ebeid –Lannoo emission rate and to the valence band using the default emission rate. Similarly, `Makram-Ebeid` with `hole` in parentheses couples an `hNeutral` trap to the valence band through the Makram-Ebeid–Lannoo emission rate and to the conduction band using the default emission rate.

For example, to couple `eNeutral Level` traps described by the Makram–Ebeid–Lannoo model to both the conduction and valence bands, you must specify the following in the command file:

```
Traps(
    ...
    (eNeutral Level ... Makram-Ebeid)
)
```

To couple the `eNeutral Level` trap through the Makram–Ebeid–Lannoo emission rate only to the conduction band, while keeping the default emission rate to the valence band, you must specify:

```
Traps(
    ...
    (eNeutral Level ... Makram-Ebeid(electron))
)
```

The electron capture rate from the conduction band to an `eNeutral` trap (e_C^n) and the hole capture rate from the valence band to an `hNeutral` trap (c_V^p) are, by default, computed from the corresponding emission rates using the detailed balance principle. By using the keyword `simpleCapt` in parentheses as an option for `Makram-Ebeid`, capture rates are computed as $c_C^n = \sigma_n \left[(1 - g_n^J) v_{th}^n n + g_n^J \frac{J_n}{q} \right]$ for exchange with the conduction band and $c_V^p = \sigma_p [(1 - g_p^J) v_{th}^p p + g_p^J J_p / q]$ for exchange with the valence band, where g_n^J and g_p^J are set with `eJfactor` and `hJfactor` in the command file and with the `Jcoef` parameter pair in the `Traps` parameter set. g_n^J and g_p^J can take any value between 0 and 1. When zero or not

specified (the default), the V-model is obtained with the simplified rates $c_C^n = \sigma_n^0 v_{th}^n n$ and $c_V^p = \sigma_p^0 v_{th}^p p$, respectively. When 1, the J-model is obtained.

The deep trap parameters W_{ph}, W_T, and W_{opt} can be adjusted in the `Makram-Ebeid` section of the parameter file. Their default values are $W_{ph} = 0.06\,\mathrm{eV}$, $W_T = 1.4\,\mathrm{eV}$, and $W_{opt} = 2.8\,\mathrm{eV}$. In addition, the Makram-Ebeid–Lannoo tunneling masses m can be adjusted in the parameter file. The default value is 0.5 for both electrons and holes.

For example, to change the W_{ph}, W_T, and W_{opt} parameters in AlN, you must specify:

```
Material = "AlN") {
   Makram-Ebeid(
      mt    = 0.3 ,0.5    #[1]
      Wph   = 0.065       #[eV]
      Wt    = 1.43        #[eV]
      Wopt  = 2.7         #[eV]
   )
}
```

Local Capture and Emission Rates From PMI

As an alternative to models described above, the local capture and emission rates c_C^n, c_V^p, e_C^n, and e_V^p can be computed directly using a physical model interface (PMI). Using this PMI only makes sense for `Level` traps. For more details, see Trap Capture and Emission Rates on page 1200.

Trap-to-Trap Tunneling

Trap-to-trap tunneling between single-level discrete traps is supported. Discrete traps of the same type, located in the same region, can be coupled through tunneling. Only `eNeutral` and `hNeutral` types are supported with only one type at a time.

Trap-to-trap tunneling is activated by specifying a `SingleTrap` entry in the `Traps` section of the `Physics` section. The `SingleTrap` entry must contain the keyword `Location` where the positions of the discrete traps involved in the trap-to-trap tunneling process are defined (at least two discrete traps must be specified). In addition, the `SingleTrap` entry must contain the keywords `Coupled=Tunneling`, indicating that the traps are coupled through tunneling. In the `Solve` section, the explicit trap equation must be activated to solve for the trap occupation probability.

For example, to activate trap-to-trap tunneling between a system of three discrete traps of type eNeutral located in a Si_3N_4 region, the following syntax is used:

```
Physics(Region="reg1") {
   Traps(
      ...
      (SingleTrap eNeutral Level EnergyMid=0 fromMidBandGap
      Coupled=Tunneling
      Location=( (0, 0, 0.1) (0, 0.1, 0.1) (0 0.2 0.2) )
      )
      ...
   )
}

Quasistationary(
   InitialStep=1e-4 MaxStep=1e-2 MinStep=1e-8
   Goal { name="gate" Voltage=55 }
){ Coupled{ poisson electron hole traps } }
```

The traps involved in the tunneling process are snapped to the closest vertex with, at most, one trap allowed per vertex. Because the traps are discrete, having a good mesh in the regions where trap-to-trap tunneling occurs is important to obtain meaningful results.

The local trapped carrier density is such that, in the control volume adjusted for dimension around the vertex where the trap is located, there is one trapped charge if the trapped is occupied, or zero otherwise.

The traps involved in the trap-to-trap tunneling processes are regarded as single-mode oscillators embedded in the dielectric matrix [6] with a capture rate described by:

$$c_i = \sum_{j \neq i} C_f \frac{\hbar W_T \sqrt{\pi}}{m_t m_0 r_{j,i}^2 Q_0 \sqrt{kT}} \exp\left(-\frac{W_{opt} - W_T}{2kT}\right) \exp\left(-\frac{2r_{j,i}\sqrt{2m_t m_0 W_T}}{\hbar}\right) \exp\left(-\frac{E_{trap}^i - E_{trap}^j + \left|E_{trap}^i - E_{trap}^j\right|}{2kT}\right) f_j \quad (518)$$

where:

- Transitions occur between localized state i with energy E_{trap}^i and neighbouring localized states j with energies E_{trap}^j.
- W_{opt} is the trap optical ionization energy.
- W_T is the trap thermal ionization energy.
- $Q_0 = \sqrt{2(W_{opt} - W_T)}$.
- $r_{i,j}$ is the spatial distance between traps i and j involved in the transition.
- f_j is the localized trap j occupation probability.
- C_f is a multiplication factor, which is 1 by default.
- m_t is the trap-to-trap tunneling mass.

Tunneling between two traps is activated only if the spatial distance between them is smaller than the user-defined parameter R_{cutoff}, which limits the interaction distance for tunneling. By default, the parameter is infinite, so potentially all traps in the region are considered. You should adjust R_{cutoff} to reduce the size of the Jacobian and numeric issues. Ideally, R_{cutoff} should be of the order of the spatial distance between traps to allow only first-order neighbor interactions.

The transition rate parameters W_{opt}, W_{T}, R_{cutoff}, m_t, and C_f are available through the parameter file in the region trap section.

Table 93   Parameters and their default values for trap-to-trap tunneling

Symbol	Parameter name	Default value	Unit
W_{opt}	T2T_Wopt	3	eV
W_{T}	T2T_WT	1.5	eV
R_{cutoff}	T2T_Rcutoff	1×10^{30}	cm
C_f	T2T_factor	1	1
m_t	T2T_m	0.5	1

Tunneling and Traps

Traps can be coupled to nearby interfaces and contacts by tunneling. Sentaurus Device models nonlocal tunneling to traps as the sum of an inelastic, phonon-assisted process and an elastic process [4][5]. To use the nonlocal tunneling model for tunneling to traps:

■ For each interface or contact that you want to couple to traps by tunneling, generate a nonlocal mesh (see Nonlocal Meshes on page 146). A nonlocal mesh describes the tunneling paths between the vertices where the traps are located, and the interface or contact for which the nonlocal mesh is constructed.

■ Specify eBarrierTunneling (for coupling to the conduction band) and hBarrierTunneling (for coupling to the valence band) in the trap specification in the command file. Provide the names of the nonlocal meshes the trap must be coupled to using the NonLocal option of eBarrierTunneling and hBarrierTunneling.

■ Adjust TrapVolume, HuangRhys, and PhononEnergy (see below), as well as the tunneling masses and the interface-specific prefactors (see Nonlocal Tunneling Parameters on page 726).

For example:

```
Traps((
   hNeutral Conc=1e15 fromMidBandGap EnergyMid=0 Level TrapVolume=1e-7
   eBarrierTunneling(Nonlocal="NLM1" Nonlocal="NLM2")
))
```

NOTE   To model trap-assisted tunneling through a barrier that contains traps, at least two separate nonlocal meshes are needed, one for each side of the barrier.

The electron capture rate for the phonon-assisted transition from the conduction band is:

$$c_{C,phonon}^{n} = \frac{\sqrt{m_t m_0^3 k^3 T_n^3} g_C}{\hbar^3 \sqrt{\chi}} V_T S \omega \left[\frac{\alpha(S-l)^2}{S} + 1 - \alpha \right] \exp\left[-S(2f_B + 1) + \frac{\Delta E}{2kT} + \chi \right] \tag{519}$$

$$\times \left(\frac{z}{l+\chi} \right)^l F_{1/2}\left(\frac{E_{F,n} - E_C(0)}{kT_n} \right) \frac{|\Psi(z_o)|^2}{|\Psi(0)|^2}$$

where:

- V_T is the interaction volume of the trap.

- S is the Huang–Rhys factor.

- $\hbar\omega$ is the energy of the phonons involved in the transition.

- α is a dimensionless parameter.

These parameters are set by `TrapVolume` (in μm^3), `HuangRhys` (dimensionless), `PhononEnergy` (in eV), and `alpha` (dimensionless) in the command file, and by parameters of the same name in the `Traps` parameter set. V_T, S, and $\hbar\omega$ default to 0, and α defaults to 1. `TrapVolume` must be positive when tunneling is activated.

In Eq. 519, l is the number of the phonons emitted in the transition, $f_B = [\exp(\hbar\omega/kT) - 1]^{-1}$ is the Bose–Einstein occupation of the phonon state, $z = 2S\sqrt{f_B(f_B + 1)}$ and $\chi = \sqrt{l^2 + z^2}$. The dissipated energy is $\Delta E = E_C + 3kT_n/2 - E_{trap}$. The Fermi energy and the electron temperature are obtained at the interface or contact, while the lattice temperature is obtained at the site z_0 of the trap. m_t is the relative (dimensionless) tunneling mass, and g_C is the prefactor for the Richardson constant at the interface or contact. See Nonlocal Tunneling Parameters on page 726 for more details regarding these parameters.

The electron capture rate for the elastic transition from the conduction band is:

$$c_{C,elastic}^{n} = \frac{\sqrt{8m_t} m_0^{3/2} g_C}{\hbar^4 \pi} V_T [E_C(z_o) - E_{trap}]^2 \Theta[E_{trap} - E_C(0)] \sqrt{E_{trap} - E_C(0)} f\left(\frac{E_{F,n} - E_{trap}}{kT_n} \right) \frac{|\Psi(z_o)|^2}{|\Psi(0)|^2} \tag{520}$$

where $f(x) = 1/(1 + \exp(-x))$. The emission rates are obtained from the capture rates by the principle of detailed balance (see Eq. 511). The hole terms are analogous to the electrons terms.

However, `hBarrierTunneling` for contacts and metals is nonphysical and, therefore, ignored.

The ratio of wavefunction is obtained from Γ_{CC} described in WKB Tunneling Probability on page 729 as:

$$\frac{|\Psi(z_o)|^2}{|\Psi(0)|^2} = \frac{v(0)}{v(z_0)}\Gamma_{CC} \tag{521}$$

where v denotes the (possibly imaginary) velocities. To avoid singularities, for the inelastic transition with the WKB tunneling model, the velocity $v(z_o)$ at the trap site is replaced by the thermal velocity. For the inelastic process, Γ_{CC} is computed at the tunneling energy $E_C + kT_n/2$ and, for elastic process, at energy E_{trap}. For the tunneling probability, the default one-band model and the `TwoBand` option are available, as described in WKB Tunneling Probability on page 729.

Trap Numeric Parameters

When used with Fermi statistics, the trap model sometimes leads to convergence problems, especially at the beginning of a simulation when Sentaurus Device tries to find an initial solution. This problem can often be solved by changing the numeric damping of the trap charge in the nonlinear Poisson equation.

To this end, set the `Damping` option to the `Traps` keyword in the global `Math` section to a nonnegative number, for example:

```
Math {
    Traps(Damping=100)
}
```

Larger values of `Damping` increase damping of the trap charge; a value of `0` disables damping. The default value is `10`. Depending on the particular example, increasing damping can improve or degrade the convergence behavior. There are no guidelines regarding the optimal value of this parameter.

At nonheterointerface vertices, bulk traps are considered only from the region with the lowest band gap. In cases where the bulk traps from other regions are important, use `RegionWiseAssembly` in `Traps` of the global `Math` section, which properly considers bulk traps from all adjacent regions.

Visualizing Traps

To plot the concentration of electrons trapped in `eNeutral` and `Acceptor` traps and of negative fixed charges, specify `eTrappedCharge` in the `Plot` section. Similarly, for the concentration of holes trapped in `hNeutral` or `Donor` traps and positive fixed charges, specify `hTrappedCharge`. These datasets include the contribution of interface charges as well. To that end, Sentaurus Device converts the interface densities to volume densities and, therefore, their contribution depends on the mesh spacing. To plot the interface charges separately as interface densities, use `eInterfaceTrappedCharge` and `hInterfaceTrappedCharge`.

Specify `TotalTrapConcentration` to plot the absolute value of the net bulk trap concentration. Similarly, specify `TotalInterfaceTrapConcentration` to plot the absolute value of the net interface trap concentration. These quantities do not account for occupancy.

For backward compatibility, for traps specified in insulators, at vertices on interfaces to semiconductors, the charge density in the insulator parts associated with the vertices will be reassigned to the semiconductor parts. This involves the rescaling of the densities with the ratio of the volumes of the two parts and, typically, this leads to a distortion of the data for visualization. However, the distortion has no effect on the actual solution.

To plot the recombination rates for the conduction band and valence band due to trapping and de-trapping, specify `eGapStatesRecombination` and `hGapStatesRecombination`, respectively.

In addition, Sentaurus Device allows you to plot trapped carrier density and occupancy probability versus energy at positions specified in the command file.

The plot file is a `.plt` file and its name must be defined in the `File` section by the `TrappedCarPlotFile` keyword:

```
File {
   ...
   TrappedCarPlotFile = "itraps_trappedcar"
}
```

The plotting is activated by including the `TrappedCarDistrPlot` section (similar to the `CurrentPlot` section) in the command file:

```
TrappedCarDistrPlot {
   MaterialInterface="Silicon/Oxide" {(0.5 0)}
   ...
}
```

The positions defining where the trapped carrier density, occupancy probability, and trap density versus energies are to be plotted are specified materialwise or regionwise in the `TrappedCarDistrPlot` section, grouped on regions, materials, region interfaces, and material interfaces.

A set of coordinates of positions in parentheses follows the region or region interface:

```
TrappedCarDistrPlot {
   MaterialInterface="Silicon/Oxide" {(0.5 0)}
   RegionInterface="Region_2/Region_3" {(0.1 0.001)}
   Region="Region_1" {(0.3 0) (0 0) (-0.1 0.2)}
   Material="Silicon" {(0.27 0) (0 0.01)}
   ...
}
```

For each position defined by its coordinates, Sentaurus Device searches for the closest vertex inside the corresponding region or on the corresponding region interface. This is the actual position where the plotting is performed.

The difference between user coordinates and actual coordinates is displayed in the log file for each valid position in the `TrappedCarDistrPlot` section in the following format:

```
[Position(User)     ClosestVertex    PositionClosestVertex]
[(2.4000,-0.1000)      718              (2.3130,-0.0500)]
[(2.5000,-0.1000)      743              (2.3500,-0.0500)]
```

In addition, a simplified syntax for a global position inside the device is available:

```
TrappedCarDistrPlot {
   (0.5 0)
   ...
}
```

In this case, the closest vertex is used in distribution plotting.

Based on trap types and positions, a unique entry is created in the generated graph. The naming is `TrapTypeCounter(position)`, where `Counter` is used when multiple traps of the same type are used. For each of these entries, the `Energy`, `TrappedChargeDistribution`, `DistributionFunction`, and `TrapDensity` fields are available for plotting. In addition, for each entry, `eQuasiFermi` and `hQuasiFermi` are available for plotting. This allows you to monitor the evolution of `DistributionFunction` relative to quasi-Fermi levels.

Explicit Trap Occupation

For the investigation of, for example, time-delay effects, it may be advantageous to start a transient simulation from an initial state with either totally empty or totally filled trap states. However, depending on the position of the equilibrium Fermi level, it may be impossible to reach such an initial state from steady-state or quasistationary simulations (for example, it may be a metastable state with a very long lifetime).

For this purpose, two different mechanisms are available to initialize trap occupancies in the `Solve` section.

The first mechanism is invoked by `TrapFilling` in the `Set` and `Unset` statements of the `Solve` section. Table 203 on page 1398 summarizes the syntax of these statements, and Trap Examples on page 470 presents an example. This mechanism is deprecated with the exception of the `-degradation` option.

The second mechanism, invoked by `Traps` in a `Set` statement within a `Solve` section, allows you to set trap occupancies for individual named traps to spatial- and solution-independent values, and to freeze and unfreeze the trap occupancies of all traps. To set a trap you need to define an identifying `Name` in its definition in `Traps`, which enables you to reference this trap in the `Set` command. The `Frozen` option allows you to freeze the trap occupancies for subsequent `Solve` statements and to unfreeze them again. Freezing traps implies that the traps are decoupled from both the conduction band and valence band, that is, their recombination terms are set to zero. Observe that `Frozen` applies to all defined traps. Traps not explicitly initialized in the `Set` are frozen at their actual values. The options of `Traps` in `Set` are summarized in Table 203.

```
Device "MOS" {
   Physics { ...
      Traps ( ( Name="t1" eNeutral ... ) ( Name="t2" hNeutral ... ) ... )
   }
}

System { ...
   MOS "mos1" ( ... ) { ... }
}

Solve { ...
   Set ( Traps ( "mos1"."t1" = 1. Frozen ) )
   ...
   Set ( Traps ( -Frozen ) )
   ...
}
```

Here in the example, some traps are named. In the first `Set`, the trap `"t1"` of device `"mos1"` is explicitly set to one. Due to the `Frozen` option, trap `"t1"` is frozen at the specified value and trap `"t2"` is frozen at its actual value. The second `Set` releases all traps again.

To set all the trap occupancies to a certain value between 0 and 1, you must specify the `Value` keyword as an option for `Traps`. In this case, the occupancy of all the traps (with or without names) is set to the value specified by the `Value` keyword.

In the following examples, the trap occupancies are set to 1, the equivalent of `TrapFilling=Full`, and then they are released later in the simulation using the `-Frozen` option:

```
Solve { ...
   Set ( Traps ( "mos1".value = 1. Frozen ) )
   ...
   Set ( Traps ( -Frozen ) )
   ...
}
```

or:

```
Solve { ...
   Set ( Traps ( value = 1. Frozen ) )
   ...
   Set ( Traps ( -Frozen ) )
   ...
}
```

NOTE   Freezing and unfreezing of traps using the `Solve-Set-Traps` command implies freezing and unfreezing of multistate configurations, respectively (see Manipulating MSCs During Solve on page 486). If the incomplete ionization model is used, dopant ionization is affected as well (see Chapter 13 on page 277).

Options to Include Traps in Doping

The effect of traps on some physical models can be treated in an approximate manner by treating trap concentration as additional doping. Two options are available for this purpose:

```
Traps (
   <trap-specifications>
   [Add2TotalDoping | Add2TotalDoping(ChargeTraps)]
)
```

If `Add2TotalDoping` is specified, the trap concentration is added to both the acceptor or donor doping concentration (depending on the sign of the trap) and the total doping concentration. This affects models that depend on acceptor, donor, and total doping concentrations such as mobility and lifetime. However, this option has no effect on *mobility calculations* if a `MobilityDoping` file is used (see Mobility Doping File on page 384) or if incomplete ionization–dependent mobility is used (see Incomplete Ionization–Dependent Mobility Models on page 382).

If `Add2TotalDoping(ChargedTraps)` is specified, the *charged* trap concentration is added to the acceptor or donor doping concentration *for mobility calculations only*. However, this option has no effect if a `MobilityDoping` file is used (see Mobility Doping File on page 384) or if incomplete ionization–dependent mobility is used (see Incomplete Ionization–Dependent Mobility Models on page 382).

Trap Examples

The following example of a trap statement illustrates one donor trap level at the intrinsic energy with a concentration of $1{\times}10^{15}\,\mathrm{cm}^{-3}$ and capture cross sections of $1{\times}10^{-14}\,\mathrm{cm}^2$:

```
Traps(Donor Level EnergyMid=0 fromMidBandGap
   Conc=1e15 eXsection=1e-14 hXsection=1e-14)
```

This example shows trap specifications appropriate for a polysilicon TFT, with four exponential distributions:

```
Traps( (eNeutral Exponential fromCondBand Conc=1e21 EnergyMid=0
   EnergySig=0.035 eXsection=1e-10 hXsection=1e-12)
   (eNeutral Exponential fromCondBand Conc=5e18 EnergyMid=0
   EnergySig=0.1 eXsection=1e-10 hXsection=1e-12)
   (hNeutral Exponential fromValBand Conc=1e21 EnergyMid=0
   EnergySig=0.035 eXsection=1e-12 hXsection=1e-10)
   (hNeutral Exponential fromValBand Conc=5e18 EnergyMid=0
   EnergySig=0.2 eXsection=1e-12 hXsection=1e-10) )
```

The following `Solve` statement fills traps consistent with a high electron and a low hole concentration; performs a `Quasistationary`, keeping that trap filling; and, finally, simulates the transient evolution of the trap occupation:

```
Solve{
   Set(TrapFilling=n)
   Quasistationary{...}
   Unset(TrapFilling)
   Transient{...}
}
```

Insulator Fixed Charges

Sentaurus Device supports special syntax for fixed charges in insulators and at insulator interfaces. Insulator fixed charges are defined as options to `Charge` in the `Physics` section:

```
Physics (Material="Oxide"){
   Charge (
      (<charge specification>)
      (<charge specification>)
   )
}
```

and likewise for `Region`, `RegionInterface`, and `MaterialInterface`. When only a single specification is present, the inner pair of parentheses can be omitted. For bulk insulator charges, the only relevant parameter is `Conc`, the concentration, specified in $q\text{cm}^{-3}$.

Fixed charges at interfaces can be specified with either Gaussian or uniform distributions:

```
Charge([Uniform | Gaussian]
   Conc = <float>       # [cm-2]
   SpaceMid = <vector>  # [um]
   SpaceSig = <vector>  # [um]
```

The parameter `Conc` specifies the maximum surface charge concentration σ_0 in $q\text{cm}^{-2}$. `SpaceMid` and `SpaceSig` have the same meaning as for traps (see Energetic and Spatial Distribution of Traps on page 450). They are optional for `Uniform` distributions but mandatory for `Gaussian` distributions. Table 282 on page 1466 summarizes the options that can appear in the `Charge` specification.

References

[1]   L. Colalongo *et al.*, "Numerical Analysis of Poly-TFTs Under Off Conditions," *Solid-State Electronics*, vol. 41, no. 4, pp. 627–633, 1997.

[2]   S. Makram-Ebeid and M. Lannoo, "Quantum model for phonon-assisted tunnel ionization of deep levels in a semiconductor," *Physical Review B*, vol. 25, no. 10, pp. 6406–6424, 1982.

[3]   K. A. Nasyrov *et al.*, "Two-bands charge transport in silicon nitride due to phonon-assisted trap ionization," *Journal of Applied Physics*, vol. 96, no. 8, pp. 4293–4296, 2004.

[4]   A. Palma *et al.*, "Quantum two-dimensional calculation of time constants of random telegraph signals in metal-oxide–semiconductor structures," *Physical Review B*, vol. 56, no. 15, pp. 9565–9574, 1997.

[5]   F. Jiménez-Molinos et al., "Direct and trap-assisted elastic tunneling through ultrathin gate oxides," *Journal of Applied Physics*, vol. 91, no. 8, pp. 5116–5124, 2002.

[6]   K. A. Nasyrov and V. A. Gritsenko, "Charge transport in dielectrics via tunneling between traps," *Journal of Applied Physics*, vol. 109, no. 9, p. 093705, 2011.

CHAPTER 18 Phase and State Transitions

This chapter presents a framework for the simulation of local phase or state transitions.

State transitions appear in device physics in various forms. Typical examples are the charge traps as described in Chapter 17 on page 449. In phase-change memory (PCM) devices, different phases (for example, crystalline and amorphous) of chalcogenides are used to store information and can be modeled with the framework described here. Furthermore, in the hydrogen transport degradation model (see MSC–Hydrogen Transport Degradation Model on page 500), diffusing mobile hydrogen species may be trapped in localized states.

In this chapter, a general modeling framework called *multistate configuration* (MSC) is presented to describe transitions between phases or states. The framework allows the specification of an arbitrary number of states that interact locally by an arbitrary number of transitions. The states can be charged and carry hydrogen atoms. Transitions between two states may interact with the conduction and valence band, or with hydrogen diffusion equations to preserve charge and the number of hydrogen atoms. The structure of transitions is limited to a linear local dependency between the state occupation rates. However, arbitrary nonlinear local dependency on the solution variables of the transport equations are allowed using PMI models. The state occupation rates are solved self-consistently with the transport model both for stationary and dynamic characteristics.

Multistate Configurations and Their Dynamic

A multistate configuration (MSC) is defined by the number of states N and the state occupation probabilities s_1, …, s_N satisfying the condition:

$$\sum_i s_i = 1 \tag{522}$$

For two states i and j, an arbitrary number of transitions (described by capture and emission rates) is allowed. The dynamic equation is then given by:

$$\dot{s}_i = \sum_{j \neq i} \sum_{t \in T_{ij}} c_{ij} s_j - e_{ij} s_i \tag{523}$$

where T_{ij} is the set of transitions between i and j. For such a transition $t \in T_{ij}$ with capture and emission rates c and e, respectively, you have $c = c_{ij} = e_{ji}$ and $e = e_{ij} = c_{ji}$ if i and j denote the reference state and interacting state, respectively. The problem can be written in the compact form:

$$\dot{s} = Ts \tag{524}$$

where T is the total transition matrix, composed of the individual transition matrices.

Each state can carry a number K^Q of (positive) charges and a number K^H of hydrogen atoms (both numbers can be positive or negative, and are zero by default). Transitions between two states must satisfy conservation laws for both quantities. Required particles can be taken from several reservoirs. Reservoir particles are characterized by the corresponding numbers K_r^Q and K_r^H, and transitions specify the number P_r of involved reservoir particles. The conservation laws then read:

$$K_i - K_j = \sum_r P_r K_r \tag{525}$$

where K_i and K_j are the characteristic numbers for the reference and interacting states of the transition, respectively. The sum is taken over all reservoirs involved in the transition.

Table 94 lists the available particle reservoirs and their characteristics. The reservoirs of hydrogen atoms, molecules, and ions represent the corresponding mobile species in the hydrogen transport degradation model. Their use is illustrated in Reactions With Multistate Configurations on page 504.

Table 94   MSC particle reservoirs and their characteristics

Description	Identifying string	Particle	Charge K^Q	Hydrogen K^H	Equation
Conduction band	CB	electron	−1	0	Electron
Valence band	VB	hole	1	0	Hole
Hydrogen atoms	HydrogenAtom	H	0	1	HydrogenAtom
Hydrogen molecules	HydrogenMolecule	H_2	0	2	HydrogenMolecule
Hydrogen ions	HydrogenIon	H^+	1	1	HydrogenIon

The resulting space charge and recombination terms with the corresponding equations are taken into account automatically.

Specifying Multistate Configurations

A multistate configuration is specified by an `MSConfig` section placed into an `MSConfigs` section of a (region or material or global or interface) `Physics` section. It is described by its states (at least two) and transitions (each state must be involved in at least one transition) using the keywords `State` and `Transition`. An arbitrary number of `MSConfig` sections is allowed.

```
Physics ( Region = "si" ) {
   MSConfigs (
      MSConfig ( Name = "ca"
         State ( Name = "c" ) State ( Name = "a" )
         Transition ( Name = "t1"
            To="c" From="a" CEModel("pmi_ce_msc" 0))
      )
      ...
   )
}
```

This example specifies a multistate configuration with two states and one transition between them. See Table 311 on page 1480 for the parameters supported by `MSConfig`.

`State` requires a `Name` as an identifier. The state can carry both a number of positive charges by specifying `Charge`, and a number of hydrogen atoms by using `Hydrogen`.

`Transition` requires several parameters. The keyword `CEModel` specifies a transition model including its optional model index (see Transition Models on page 477). The reference and interacting states of the transition are selected by the keywords `To` and `From`, respectively. A `Name` specification is mandatory as well.

A transition between differently charge states (correspondingly for hydrogen atoms) requires additional charged particles to preserve the total charge. With `Reservoirs`, you can specify a list of reservoirs (`CB` and `VB` for the conduction band and valence band, respectively), which provides the necessary number of particles specified by `Particles` as an argument to the reservoir. The conduction band serves as an electron reservoir, and the valence band is a hole reservoir.

Multistate Configurations on Interfaces

You can also define MSCs on interfaces. Therefore, an MSC might look like the following example:

```
Physics (MaterialInterface="Oxide/Silicon") {
   MSConfigs (
      MSConfig (
```

```
                  Name="msc0"
                  State(Name="s0" Charge=0 Hydrogen=1)
                  State(Name="s1" Charge=1 Hydrogen=0)
                  Transition (
                     Name="Depassivation" CEModel("CEModel_PMI",1)
                     To="s1" From="s0"
                     Reservoirs("VB"(Particles=+1) "HydrogenAtom"(Particles=-1))
                     FieldFromInsulator
                  )
            )
        )
    }
```

Observe that, for interface MSCs, the reservoirs refer to bulk reservoirs. At interfaces between the insulator and semiconductor, you can explicitly require that the field from the insulator is selected by using `FieldFromInsulator` in the MSC specification.

Additional Remarks

An `eNeutral` level trap of the form:

```
(Name="eN" eNeutral Conc=1.e+13 CBRate=("pmi_ce0" 0) VBRate=("pmi_ce0" 1))
```

can be specified equivalently as an MSC in the following way:

```
MSConfig ( Name="eN" Conc=1.e+13
    State ( Name="s0" Charge=0 ) State ( Name="s1" Charge=-1 )
    Transition ( Name="tCB" CEModel("pmi_ce0" 0)
       To="s1" From="s0" Reservoirs("CB"(Particles=+1)))
    Transition ( Name="tVB" CEModel("pmi_ce0" 1)
       To="s0" From="s1" Reservoirs("VB"(Particles=+1)))
)
```

For all multistate configurations, the dynamic is always solved implicitly, that is, no extra equation needs to be specified as an argument to the `Coupled` or `Transient` solve statements.

NOTE   Only quasistationary and transient simulations support multistate configurations. Small-signal analysis (see Small-Signal AC Analysis on page 96), harmonic balance analysis (see Harmonic Balance on page 101), and noise analysis (see Chapter 23 on page 675) do not support multistate configurations.

NOTE   The computation of state occupation is influenced by the `TrapFilling` option of the `Set` and `Unset` commands in the `Solve` section (see Table 186 on page 1384). It is frozen if the trap-filling option `Frozen` is set; otherwise, the occupation rates are treated as free. The frozen status is released again by the `Unset(TrapFilling)` command.

The transition dynamic may become numerically unstable, that is, it cannot be solved with sufficient accuracy if, for example, the forward and backward rates of all transitions at one operation point differ by several orders of magnitude. Using `-Elimination` in `MSConfig` applies a different solving algorithm, often improving the numeric robustness in such cases.

The state occupation probabilities can be plotted in groups or individually by specifying `MSConfig` (see Table 332 on page 1496) in the `Plot` section.

Transition Models

The MSC framework allows an arbitrary number of transitions between two states of an MSC. Each transition model can be either the model `pmi_ce_msc`, or a trap capture and emission PMI (see Trap Capture and Emission Rates on page 1200).

The pmi_ce_msc Model

The `pmi_ce_msc` transition model supports the following features:

- Arbitrary number of states and transitions
- Charge states
- Several transition rate models (nucleation, growth, electron and hole exchange)
- Equilibrium computation (necessary for detailed balance processes)
- Energy and particle exchange

States

The states are described by a base energy E_i, a degeneracy factor g_i, the number of negative elementary charges K_i^- (an arbitrary integer), and the energy E_i^- of one electron in the state. The inner energy of the state is then:

$$H_i = E_i + K_i^- E_i^- \tag{526}$$

The electron energy is the sum of the valence band energy and the user-specified value $E_{i,\,\text{user}}^-$.

Equilibrium

The equilibrium occupation probabilities $s*$ are needed to guarantee the detailed balance principle for all transitions. The equilibrium is determined by the state parameters, the temperature, and the Fermi levels of the involved particle reservoirs. You have:

$$Z_i = g_i \exp(-\beta(H_i - K_i^{'} E_F)) \tag{527}$$

$$Z = \sum_i Z_i \tag{528}$$

$$s_i^* = Z_i/Z \tag{529}$$

Here, E_F is the quasi-Fermi energy and β is the thermodynamic beta. The quasi-Fermi energy is approximated inside the PMI. Let the (approximated) intrinsic density n_I and the intrinsic Fermi energy E_I be:

$$n_I = \sqrt{N_C N_V \exp(-\beta E_g)} \tag{530}$$

$$E_I = \frac{1}{2}\left[(E_C + E_V) + kT\ln\left(\frac{N_V}{N_C}\right) \right] \tag{531}$$

Then, the carrier quasi-Fermi energies are approximated from the carrier densities by:

$$E_{F,n} = E_I + kT\ln\left(\frac{n}{n_I}\right) \tag{532}$$

$$E_{F,p} = E_I - kT\ln\left(\frac{p}{n_I}\right) \tag{533}$$

and equilibrium Fermi energy then as:

$$E_F = \frac{1}{2}(E_{F,n} + E_{F,p}) \tag{534}$$

Transitions

Several transition models, listed in Table 95, are available and selected by the `Formula` parameter in the parameter file.

Table 95   The pmi_ce_msc transition models

Description	Formula
Arrhenius law	0
Nucleation according to Peng	1
Growth according to Peng	2
Single trap	7
MSC trap	8

In this section, i denotes the 'to' state, while j specifies the 'from' state of the transition. For most of the models, only the forward reaction rate (capture) is given, while the backward reaction rate (emission) is computed by:

$$\frac{e}{c} = \frac{s_j^*}{s_i^*} \tag{535}$$

if not stated otherwise.

Arrhenius Law (Formula=0)

The forward reaction rate (capture) is given by:

$$c = r_0 \exp(-\beta E_{\text{act}}) \tag{536}$$

where r_0 is the maximal transition frequency and E_{act} is the activation energy.

Nucleation According to Peng (Formula=1)

A nucleation model, in analogy to the model in [1], [2], and [3], is given by:

$$c_{\text{N}} = r_0 \exp(-\beta(E_{\text{act}} + \Delta G^*(T))) \tag{537}$$

where:

$$\Delta G^*(T) = \frac{16\pi}{3} \frac{\gamma_{\text{SL}}^3}{\Delta G(T)^2} \tag{538}$$

$$\Delta G(T) = \begin{cases} \Delta H_2\left[1 - \dfrac{T}{T_g}\left(1 - \dfrac{\Delta H_1}{\Delta H_2}\dfrac{T_m - T_g}{T_m}\right)\right] & \text{if} \quad T < T_g \\[2ex] \Delta H_1 \dfrac{T_m - T}{T_m} & \text{if} \quad T_g < T < T_m \\[2ex] 0 & \text{if} \quad T_m < T \end{cases} \tag{539}$$

Growth According to Peng (Formula=2)

Growing crystalline phases is often described by a growth velocity, for example, in [1]. Some of the growing model has been adopted in the following local model, which reads as:

$$c_G = r_0[1 - \exp(-\beta \Delta G(T) v_{MM})]\exp(-\beta E_{act}) \tag{540}$$

if $T < T_m$; otherwise, it is zero.

Single-Trap Transition (Formula=7)

This model depends on the carrier density d_c. It resembles some standard trap models and is intended to be used in two-state MSCs only. If the number of electrons in the reference state is greater than in the interacting state, that is, $K_i > K_j$, then the capture process depends on the electron density and uses $d_c = n$. If $K_i < K_j$, then $d_c = p$; otherwise, you use $d_c = 0$. The capture rate is then given by:

$$c = \sigma v_{th} d_c \tag{541}$$

where σ is the cross section and v_{th} is the thermal velocity. The emission rate for electron capturing is computed as:

$$e = c\exp(\beta(E_T - E_{F,n})) \tag{542}$$

where E_T is the trap energy. For hole-capturing, the emission rate reads as:

$$e = c\exp(\beta(E_{F,p} - E_T)) \tag{543}$$

MSC Trap With Emulated Detailed Balance (Formula=8)

The actual model generalizes the single-trapping model (Formula=7) to general MSC states and transitions. The capture rate is computed as in the single trapping case above. The emission rate, however, is computed as follows. Let N_n and N_p be the number of electrons and holes, respectively, which are destroyed during the process. Then, you have:

$$N_n - N_p = K_i^- - K_j^- \tag{544}$$

and you require:

$$\frac{e}{c} = g_{ji}\exp(-N_n\beta_n(E_{\text{F},n} - \overline{E_\text{C}}) + N_p\beta_p(E_{\text{F},p} - \overline{E_\text{V}}) + \beta_l(-N_n\overline{E_\text{C}} + N_p\overline{E_\text{V}} - H_{ji})) \tag{545}$$

where you used $g_{ji} = g_j/g_i$ and $H_{ji} = H_j - H_i$. The average conduction band and valence band energies are:

$$\overline{E_\text{C}} = E_\text{C} + \frac{3}{2}kT_n \quad \text{and} \quad \overline{E_\text{V}} = E_\text{V} - \frac{3}{2}kT_p \tag{546}$$

In thermal equilibrium, the detailed balance principle is satisfied.

Model Parameters

The model requires parameters for all states and transitions to allow a consistent computation of the thermal equilibrium of the MSC as a whole. Therefore, the parameters are grouped into global, state, and transition parameters.

The parameters `nb_states` and `nb_transitions` determine the number of states and transitions, respectively, and must be both consistent with the command file specification. The parameter `sindex<int>` specifies for the `<int>`-th state a parameter index, which determines a prefix for the state parameters. For example, given `sindex0=5`, the parameters prefixed with `s5_` are read for the 0-th state. A similar parameter index selection is available for transitions using the parameters `tindex<int>` (for example, `tindex2=7` reads the parameters prefixed by `t7_`).

For transitions, the specified parameter index must coincide with the model index of the transition in the command file.

Table 96   Global parameters

Name	Symbol	Default	Unit	Range	Description
plot	–	0	–	{0,1}	Plots some properties to screen
nb_states	–	0	–	>=0, integer	Number of states
nb_transitions	–	0	–	>=0, integer	Number of transitions
sindex<int>	–	–	–	>=0, integer	Parameter index of `<int>`-th state
tindex<int>	–	–	–		Parameter index of `<int>`-th transition

Table 97   Global material and default transition parameters of pmi_ce_msc

Name	Symbol	Default	Unit	Range	Description
E_g	E_g	0.5	eV	>0.	Band gap
N_C	N_C	1×10^{19}	cm^{-3}	>0.	Electron density-of-states
N_V	N_V	1×10^{19}	cm^{-3}	>0.	Hole density-of-states
Tm	T_m	1×10^{100}	K	>0.	Melting temperature
Tg	T_g	1×10^{100}	K	>0.	Glass temperature
DeltaH1	ΔH_1	0.	J/cm^3	>0.	Heat of solid-to-liquid
DeltaH2	ΔH_2	0.	J/cm^3	>0.	Heat of amorphous-to-crystalline
GammaSL	γ_{SL}	0.	J/cm^2	>0.	Interfacial free-energy density
MM_volume	v_{MM}	0.	cm^3	>0.	Monomer volume
Reference_E_T	–	0	–	{0,1,2}	Reference energy for E_T

Table 98   Reference_E_T interpretation

Value	Symbol	Description
0	$E_T = (E_C + E_V)/2 + E_{T,\,user}$	Midgap
1	$E_T = E_C - E_{T,\,user}$	Conduction band
2	$E_T = E_V + E_{T,\,user}$	Valence band

Table 99   State parameters

Name	Symbol	Default	Unit	Range	Description
E	E_i	0.	eV	real	Constant base energy
g	g_i	1.	1	>0.	Degeneracy
charge	$-K_i^-$	0	1	integer	Number of positive elementary charges
E_charge	$E_{i,\,user}^-$	0.	eV	real	Particle energy with respect to valence band
E_nb_Tpairs	–	0	–	>=0	Number of interpolation points for base energy
E_Tp<int>_X	–	–	K		Temperature of <int>-th interpolation point
E_Tp<int>_Y	–	–	eV		Energy of <int>-th interpolation point

Alternatively, the base energy can be described as a piecewise linear (pwl) function of the temperature: With `E_nb_Tpairs`, you specify the number of interpolation points. For the `<int>`-th interpolation point ($0 \leq$ `<int>` $<$ E_nb_Tpairs), you must specify with `E_Tp<int>_X` the temperature and with `E_Tp<int>_Y`, the corresponding energy. The pwl specification is used if `E_nb_Tpairs` is greater than zero.

Some transition parameters are inherited from the global specification (see Table 97 on page 482). They can be overwritten for specific transitions by using the appropriate parameter prefix. Table 100 lists additional transition parameters.

Table 100 Transition parameters of pmi_ce_msc

Name	Symbol	Default	Unit	Range	Description
CB_nb_particles	N_n	0	1	integer	Particle number of reservoir CB
E_T	$E_{T, user}$	0.	eV	real	Trap energy
Eact	E_{act}	0.	eV	real	Activation energy
formula	–	–	–	Table 95 on page 479	Model selection
r0	r_0	1.	Hz	>0.	Maximal frequency
s0	–	–	–		Parameter index of 'to' state
s1	–	–	–		Parameter index of 'from' state
sigma	σ	1×10^{-15}	cm^2	>0	Cross section
VB_nb_particles	N_p	0	1	integer	Particle number of reservoir VB
vth	v_{th}	1×10^7	cm/s	>0	Thermal velocity

Interaction of Multistate Configurations With Transport

Multistate configurations (MSCs) have a direct impact on the transport through their charge density and their recombination rates with selected reservoirs. Furthermore, several physical models can be made explicitly dependent on the occupation probabilities of a specific MSC by using the PMI.

Apparent Band-Edge Shift

The keywords `eBandEdgeShift`, `hBandEdgeShift`, or `BandEdgeShift` in an `MSConfig` section switch on band-edge shift models for the conduction band, the valence band, or both, respectively. The model itself is either the MSC-dependent `pmi_msc_abes` model (see The

pmi_msc_abes Model on page 484) or a user-defined `PMI_MSC_ApparentBandEdgeShift`
model as described in Multistate Configuration–Dependent Apparent Band-Edge Shift on
page 1147.

The apparent band-edge shifts become visible only if the density gradient transport model is
used. To avoid the implicit use of the density gradient quantum correction model, the (electron
and hole) `gamma` parameters in the `QuantumPotentialParameters` parameter set must be
set to zero in the parameter file.

A typical simulation is:

```
Physics {
   MSConfigs (
      MSConfig ( ...
         eBandEdgeShift ( "pmi_abes" 0 )
         hBandEdgeShift ( "pmi_abes" 1 )
      )
   )
   eQuantumPotential
   hQuantumPotential
}
Solve {
   Coupled { Poisson Electron Hole Temperature eQuantumPotential
      hQuantumPotential }
   Transient ( ... ) {
      Coupled { Poisson Electron Hole Temperature eQuantumPotential
      hQuantumPotential }
   }
}
```

Here, the user PMI model `pmi_abes` has been used for both the conduction and valence bands.

The pmi_msc_abes Model

The `pmi_msc_abes` model depends on the lattice temperature T and, if an MSC is specified,
on the state occupation probabilities s_i, and it reads as:

$$\Lambda = \sum_i \Lambda_i(T) s_i \qquad (547)$$

where the sum is taken over all MSC states, and $\Lambda_i(T)$ is the apparent band-edge shift (ABES)
of state i.

The model is activated by using (here, for electrons, a MSC named `"m0"`, and a model index `5`)
as described above:

```
eBandEdgeShift ( "pmi_msc_abes" 5 )
```

The model uses a two-level or three-level hierarchy (depending on `use_mi_pars`) to determine the state parameters, namely, the global, the model index, and the state parameters. Table 101 lists the global parameters.

Table 101   Global, model-string, and state parameters of pmi_msc_abes

Name	Symbol	Default	Unit	Range	Description
`plot`	–	`0`	–	`{0,1}`	Plot parameter to screen
`use_mi_pars`	–	`0`	–	`{0,1}`	Use model index for parameter set
`lambda`	Λ	`0.`	eV	`real`	Constant value
`lambda_nb_Tpairs`	–	`0`	–	`>=0`	Number of interpolation points
`lambda_Tp<int>_X`	–	–	K	`>0.`	Temperature at `<int>`-th interpolation point
`lambda_Tp<int>_Y`	–	–	eV	`real`	Value at `<int>`-th interpolation point

The names of model index parameters are prefixed with:

```
mi<model_index>_
```

The state parameters have one of the prefixes depending on the value of `use_mi_pars`:

```
mi<model_index>_<state_name>_
<state_name>_
```

The `lambda_` parameters enable either a constant or pwl apparent band-edge shift for each state, which is fully analogous to the specification described in The pmi_msc_heatcapacity Model on page 900.

Thermal Conductivity, Heat Capacity, and Mobility

The following models allow the dependency on MSC occupation probabilities:

- The pmi_msc_thermalconductivity Model on page 912
- The pmi_msc_heatcapacity Model on page 900
- The pmi_msc_mobility Model on page 324

Descriptions of PMIs for MSC-dependent thermal conductivity, heat capacity, and mobility can be found in Multistate Configuration–Dependent Thermal Conductivity on page 1173, Multistate Configuration–Dependent Heat Capacity on page 1180, and Multistate Configuration–Dependent Bulk Mobility on page 1113, respectively.

Manipulating MSCs During Solve

The MSC dynamic is, in general, solved implicitly. However, sometimes it may be useful to manipulate the computations. For example, you may want to initialize MSCs with nonsteady-state solutions or to freeze the dynamic of MSCs because time constants are very large compared to electronic and thermal effects. Furthermore, it may be of interest to disable specific MSC transitions for certain applications (for example, in phase-change memory applications to freeze phases but to allow electronic transitions). The available mechanisms are described here.

Explicit State Occupations

You can set explicitly the state occupations of MSCs to a spatial-independent and solution-independent value, and freeze and unfreeze the dynamic of the MSCs during `Solve` by using `MSConfigs` in a `Set` command (see Table 195 on page 1393 for a summary of options).

To set the state occupations of an MSC, you use the `MSConfig` command within `MSConfigs`, identify the MSC by using its name (and, for mixed-mode simulations, the device name using `Device`), and specify the occupancies for the involved states using `State`.

The state occupations are then set collectively and normalized implicitly, while unspecified states default to zero occupation. The `Frozen` option of `MSConfigs` applies to all existing MSCs and freezes the state occupations at the set or actual values. To unfreeze the dynamics of the MSCs again, the `-Frozen` option is used.

The following example illustrates the syntax for single-device simulations:

```
Physics {
  MSConfigs ( ...
    MSConfig ( Name="msc1" State ( Name="s0" ) State ( Name="s1" ) ... )
  )
}
Solve { ...
  Set (
    MSConfigs (
      MSConfig ( Name="msc1"
        State (Name="s0" Value=0.1) State (Name="s1" Value=0.4) )
      Frozen                             # freeze the MSC dynamic
    )
  )
  ...
  Set ( MSConfigs ( -Frozen ) )          # unfreeze the MSC dynamic
}
```

Here, the occupancies of states `s0` and `s1` of the MSC `msc1` are set to 0.2 and 0.8, respectively, due to the implicit normalization; all other states are unoccupied.

> **NOTE** Freezing and unfreezing MSCs implies freezing and unfreezing traps, respectively (see the `Solve-Set-Traps` command in Explicit Trap Occupation on page 468).

Manipulating Transition Dynamics

You can manipulate the transition dynamic by accessing prefactors for individual transition forward (capture) and backward (emission) reaction rates. This means that the modified rate $\tilde{c} = \kappa c$ (κ is the prefactor, and c is the true reaction rate) is used in the dynamic equation. By setting selected transition prefactors to zero, you can decouple states into independent groups. Especially, if you decouple a certain state from all others, the state is frozen, that is, it retains its occupation in the subsequent analysis. With:

```
Set( (Device="d1" MSConfig="m7" Transition="t3" CPreFactor=0. EPreFactor=0.) )
```

both reaction rates of the specified transition are set to zero (`PreFactor` can be used for common settings of both reaction rates). Omitting one of the specifying string keywords `Device`, `MSConfig`, and `Transition` applies the setting to all corresponding objects in the `Device-MSConfig-Transition` hierarchy.

> **NOTE** The prefactors affect only subsequent computations, but they do not change the physical parameters of the MSC.

Example: Two-State Phase-Change Memory Model

Phase-change memory (PCM) devices store a bit as the phase (crystalline or amorphous) of a (chalcogenide) material. Reading information takes advantage of the different conductances of the phases. Storing information requires switching the phases. To switch to the amorphous phase, a high current is passed through the material, heating up the device above the melting point. When switching off the current, the molten material cools so rapidly that it cannot crystallize, but remains in a metastable amorphous phase. To switch to the crystalline phase, the material is reheated more gently. The material remains solid, but the temperature is sufficient that the phase can relax to the equilibrium crystalline phase.

The PCM device is modeled by a two-state model representing the crystalline and amorphous phase using an MSC with two uncharged states. The transition is modeled by the Arrhenius law formula (`Formula=0`) of the `pmi_ce_msc` transition model. The model has four parameters:

- The base energies and the degeneracy factors of the states determine the equilibrium.

- The activation energy E_{act} and r_0 of the transition determine the velocity of the transition.

A short interpretation is given:

Let $s = s_{\text{c}}$ denote the degree of crystallization of the material and $s_{\text{a}} = 1 - s$, the amorphization rate. Assuming an energy difference $\delta E > 0$ between the amorphous and crystalline phases, and that the amorphous phase has $g > 1$ times more microscopic realizations than the crystalline state, in equilibrium $s = 1/[g \exp(-\delta E/kT) + 1]$, that is, the amorphous state is preferred at higher temperatures. The critical temperature where the equilibrium occupation rates s_{c} and s_{a} are equal is $T_{\text{crit}} = \delta E/k \ln(g)$.

The dynamic is given by crystallization and amorphization rates $r_{\text{c}} = r_0 \exp(-E_{\text{act}}/kT)$ and $r_{\text{a}} = r_0 g \exp(-(E_{\text{act}} + \delta E)/kT)$, respectively, assuming a simple Arrhenius law for the crystallization rate. Here, r_0 is the maximal crystallization rate, and E_{act} is the activation energy.

References

[1] C. Peng, L. Cheng, and M. Mansuripur, "Experimental and theoretical investigations of laser-induced crystallization and amorphization in phase-change optical recording media," *Journal of Applied Physics*, vol. 82, no. 9, pp. 4183–4191, 1997.

[2] S. Senkader and C. D. Wright, "Models for phase-change of $Ge_2Sb_2Te_5$ in optical and electrical memory devices," *Journal of Applied Physics*, vol. 95, no. 2, pp. 504–511, 2004.

[3] D.-H. Kim *et al.*, "Three-dimensional simulation model of switching dynamics in phase change random access memory cells," *Journal of Applied Physics*, vol. 101, p. 064512, March 2007.

CHAPTER 19 Degradation Models

This chapter discusses the degradation models used in Sentaurus Device.

Overview

A necessary part of predicting CMOS reliability is the simulation of the time dependence of interface trap generation. To cover as wide a range as possible, this simulation should accurately reflect the physics of the interface trap formation process. Although the mechanisms of interface trap generation are not completely understood, it is generally accepted that they involve silicon-hydrogen (Si-H) bond breakage and subsequent hydrogen transport, and various physical models have been proposed in the literature.

Sentaurus Device provides several degradation models that account for time-dependent trap generation:

- Trap degradation model (see Trap Degradation Model on page 490)

  This simple model captures the reaction-diffusion theory with hydrogen atom transport in the gate oxide.

- Multistate configuration (MSC)–hydrogen transport degradation model (see MSC–Hydrogen Transport Degradation Model on page 500)

  This model accounts for 3D transport of hydrogen atoms, ions, and molecules in all regions. Complex reaction dynamics related to Si-H bond breakage at the silicon–oxide interface are described with the MSC framework.

- Two-stage negative bias temperature instability (NBTI) degradation model (see Two-Stage NBTI Degradation Model on page 509)

  This model proposed by Grasser *et al.* [1] and Goes *et al.* [2] is related to the creation of E' centers and P_b centers (oxide and interface dangling bonds).

- Extended nonradiative multiphonon (eNMP) model [3] (see Extended Nonradiative Multiphonon Model on page 513)

  This four-state model includes metastable states and accounts for the behavior of oxide defects related to NBTI.

- Hot-carrier stress (HCS) degradation model (see Hot-Carrier Stress Degradation Model on page 519)

This is a general degradation model suitable for MOS-based devices. It includes mechanisms for hot-carrier stress degradation and field-enhanced thermal degradation.

Trap Degradation Model

Disorder-induced variations among the Si-H activation energies at the passivated Si–SiO$_2$ interface have been shown [4] to be a plausible source of the sublinear time dependence of this trap generation process. Diffusion of hydrogen from the passivated interface was used to explain some time dependencies [5]. In addition, this could be due to a Si-H density–dependent activation energy [6], which may be due to the effects of Si-H breaking on the electrical and chemical potential of hydrogens at the interface. Furthermore, the field dependence of the activation energy due to the Poole–Frenkel effect can be considered, so that all these factors lead to enhanced trap formation kinetics.

Trap Formation Kinetics

The main assumption about trap formation is that initially dangling silicon bonds at the Si–SiO$_2$ interface were passivated by hydrogen (H) or deuterium (D) [7], and degradation is a depassivation process where hot carrier interactions with Si-H/D bonds or other mechanisms are responsible for this. The equations of the model are solved self-consistently with all transport equations.

Power Law and Kinetic Equation

The experimental data for the kinetics of interface trap formation [8] shows that the time dependence of trap generation can be described by a simple power law: $N_{it} - N_{it}^0 = N_{hb}^0 / (1 + (\nu t)^{-\alpha})$, where N_{it} is the concentration of interface traps, and N_{hb}^0 and N_{it}^0 are the initial concentrations of Si-H bonds (or the concentration of hydrogen on Si bonds) and interface traps, respectively.

Assuming $N = N_{hb}^0 + N_{it}^0$ total Si bonds at the interface, the remaining number of Si-H bonds at the interface after stress is $N_{hb} = N - N_{it}$ and follows the power law:

$$N_{hb} = \frac{N_{hb}^0}{1 + (\nu t)^{\alpha}} \tag{548}$$

Based on experimental observations, the power α is stress dependent and varies between 0 and 1.

From first-order kinetics [4], it is expected that the Si-H concentration during stress obeys:

$$\frac{dN_{hb}}{dt} = -\nu N_{hb}$$

(549)

where ν is a reaction constant that can be described by $\nu \propto \nu_A \exp(-\varepsilon_A / kT)$ in the Arrhenius approximation, ε_A is the Si-H activation energy, and T is the Si-H temperature. The exponential kinetics given by this equation ($N_{hb} = N_{hb}^0 \exp(-\nu t)$) do not fully describe the experimental data because a constant activation energy will behave like the power law in Eq. 548, but with power $\alpha \approx 1$.

Si-H Density–Dependent Activation Energy

This section describes an activation energy parameterization to capture the sublinear power law for the time dependence of interface trap generation. There is evidence that the hydrogen atoms, when removed from the silicon, remain negatively charged [9]. If this correct, the hydrogen can be expected to remain in the vicinity of the interface and will affect the breaking of additional silicon-hydrogen bonds by changing the electrical potential.

The concentration of released hydrogen is equal to $N - N_{hb}$, so the activation energy dependence (assuming the activation energy changes logarithmically with the breaking of Si-H) can be expressed as:

$$\varepsilon_A = \varepsilon_A^0 + (1 + \beta)kT\ln\left(\frac{N - N_{hb}}{N - N_{hb}^0}\right)$$

(550)

where the last term represents the Si-H density–dependent change with a prefactor $1 + \beta$. Note that $(N - N_{hb})/(N - N_{hb}^0)$ is the fraction of traps generated to the total initial traps, and this gives the form of the chemical potential of Si-H bonds with the prefactor $1 + \beta$.

The numeric solution of the kinetic equation with the varying activation energy above clearly shows that such a Si-H density–dependent activation energy gives a power law, and the power α is a function of the prefactor $1 + \beta$. From the available experimental data of interface trap generation, it was noted that for negative gate biases $\alpha > 0.5$, but for positive ones $\alpha < 0.5$. It is interesting that the solution of the above kinetic equation gives $\alpha \approx 0.5$ in the equilibrium case where a unity prefactor is used. In nonequilibrium, a polarity-dependent modification of the prefactor (field stretched and pressed Si-H bonds) is possible.

Diffusion of Hydrogen in Oxide

Another model that can interpret negative bias temperature instability (NBTI) phenomena and different experimental slopes in degradation kinetics is the R-D model [10]. This model

considers hydrogen in oxide, which diffuses from the silicon–oxide interface, but the part of the hydrogen that remains at the interface controls the degradation kinetics.

The diffusion of hydrogen in oxide can be expressed as follows:

$$D\frac{dN_{\mathrm{H}}}{dx} = \frac{dN_{\mathrm{hb}}}{dt} \qquad\qquad x = 0$$

$$\frac{dN_{\mathrm{H}}}{dt} = D\frac{d^2N_{\mathrm{H}}}{dx^2} \qquad\qquad 0 < x < x_{\mathrm{P}} \qquad\qquad (551)$$

$$D\frac{dN_{\mathrm{H}}}{dx} = -k_{\mathrm{P}}(N_{\mathrm{H}} - N_{\mathrm{H}}^0) \qquad\qquad x = x_{\mathrm{P}}$$

where N_{H} is a concentration of hydrogen in oxide, $D = D_0\exp(-\varepsilon_{\mathrm{H}}/kT)$ is its diffusion coefficient, $x = 0$ is a coordinate of the silicon–oxide interface, $x = x_{\mathrm{P}}$ is the coordinate of the oxide–polysilicon gate interface (which is equal to the oxide thickness), k_{P} is the surface recombination velocity at the oxide–polysilicon gate interface, and N_{H}^0 is an equilibrium (initial) concentration of hydrogen in the oxide.

Model Equations and Syntax

To use the trap degradation model, specify the `Degradation` keyword as part of a `Traps` specification in the command file. This invokes the general kinetic equation (left column of Eq. 552) with an added passivation term. To use the power law form of the model (right column of Eq. 552), specify `Degradation(PowerLaw)`:

<u>Kinetic</u>

$$\frac{dN_{\mathrm{hb}}}{dt} = -\nu N_{\mathrm{hb}} + \gamma(N - N_{\mathrm{hb}})$$

$$\gamma = \gamma_0[N_{\mathrm{H}}/N_{\mathrm{H}}^0 + \Omega(N_{\mathrm{hb}}^0 - N_{\mathrm{hb}})]$$

$$\gamma_0 = \frac{N_{\mathrm{hb}}^0}{N - N_{\mathrm{hb}}^0}\nu_0$$

<u>Power Law</u>

$$N_{\mathrm{hb}} = \frac{N_{\mathrm{hb}}^0}{1 + (\nu t)^\alpha}$$

$$\alpha = 0.5 + \beta \qquad\qquad (552)$$

In Eq. 552, γ_0 is the passivation constant, which is computed automatically by default to provide the equilibrium, but it can also be specified directly in the command file. Ω is the passivation volume (by default, it is equal to zero) and represents a simple model for the retrapping of depassivated hydrogen by dangling silicon bonds. Depassivated hydrogen increases the average hydrogen concentration N_{H} near traps, which is computed from the R-D model (see Diffusion of Hydrogen in Oxide on page 491). If the R-D model is not activated, then $N_{\mathrm{H}}/N_{\mathrm{H}}^0 = 1$.

The parameterized system of equations for the reaction constant ν, based on the trap formation model (see Trap Formation Kinetics on page 490 and [6]), can be expressed as:

$$\nu = \nu_0 \exp\left(\frac{\varepsilon_A^0}{kT_0} - \frac{\varepsilon_A^0 + \Delta\varepsilon_A}{\varepsilon_T} \right) k_{HC} k_{Tun} k_{SHE}$$

$$\varepsilon_T = kT + \delta_{/\!/} |F_{/\!/}|^{\rho_{/\!/}}$$

$$\Delta\varepsilon_A = -\delta_\perp |F_\perp|^{\rho_\perp} + 1 + \beta\varepsilon_T \ln\frac{N - N_{hb}}{N - N_{hb}^0}$$

$$\beta = \beta_0 + \beta_\perp F_\perp + \beta_{/\!/} F_{/\!/}$$

(553)

where:

- ν_0 (given in the command file) is the reaction (depassivation) constant at the passivation equilibrium (for the passivation temperature T_0 and for no changes in the activation energy $\Delta\varepsilon_A = 0$).

- $F_\perp$, $F_{/\!/}$ are the perpendicular and parallel components of the electric field F to the interface where traps are located. The perpendicular electric field $F_\perp$ has a positive sign if the space charge at the interface is positive.

- ε_T is the energy of hydrogen on Si-H bonds and is equal to kT plus some possible gain from hot carriers represented as the additional term that is dependent on the parallel component of the electric field $\delta_{/\!/} |F_{/\!/}|^{\rho_{/\!/}}$.

- $\Delta\varepsilon_A$ is a change of the activation energy because of stretched Si-H bonds [11] by the electric field (first term) and due to a change of the chemical potential (second term) [6]. Effectively, the influence of the chemical potential also can be different in the presence of the electric field, and the coefficient β represents this.

- The coefficients $\delta_\perp, \rho_\perp, \delta_{/\!/}, \rho_{/\!/}$ and $\beta_0, \beta_\perp, \beta_{/\!/}$ are field enhancement parameters for the model.

Reaction Enhancement Factors

In Eq. 553, k_{HC} and k_{Tun} are reaction enhancement factors due to hot-carrier and tunneling current, respectively. They are given by:

$$k_{HC} = 1 + \delta_{HC} \left| \frac{I_{HC}}{I_0} \right|^{\rho_{HC}}$$

(554)

$$k_{Tun} = 1 + \delta_{Tun} \left(\delta_{FN} \left| \frac{I_{FN}}{I_0} \right|^{\rho_{FN}} + \delta_{DTe} \left| \frac{I_{DTe}}{I_0} \right|^{\rho_{DTe}} + \delta_{DTh} \left| \frac{I_{DTh}}{I_0} \right|^{\rho_{DTh}} + \delta_{BTe} \left| \frac{I_{BTe}}{I_0} \right|^{\rho_{BTe}} + \delta_{BTh} \left| \frac{I_{BTh}}{I_0} \right|^{\rho_{BTh}} \right)^{\rho_{Tun}}$$

(555)

where I_{HC} is the local hot-carrier current density (see Hot-Carrier Injection Models on page 737), and I_{FN}, I_{DTe}, I_{DTh}, I_{BTe}, and I_{BTh} are the tunneling current densities from

Fowler–Nordheim tunneling, electron and hole direct tunneling, and electron and hole nonlocal barrier tunneling, respectively (see Tunneling on page 715). In these equations, $I_0 = 1$ A/cm^2.

When the electron energy distribution is available by specifying the keyword `eSHEDistribution` in the `Physics` section (see Using Spherical Harmonics Expansion Method on page 750), you can include the following additional spherical harmonics expansion (SHE) distribution enhancement factor:

$$k_{SHE} = 1 + \delta_{SHE}\left(\frac{qg_v}{2}\int_{\varepsilon_{th}}^{\infty}\left(\min\left[\exp\left(\frac{\varepsilon - \varepsilon_a + \delta_\perp|F_\perp/F_0|^{\rho_\perp}}{kT}\right), 1\right]g(\varepsilon)f(\varepsilon)v(\varepsilon)\right)d\varepsilon\right)^{\rho_{SHE}} \quad (556)$$

where:

- δ_{SHE} is a prefactor.
- ε_{th} is a threshold energy.
- ε_a is an activation energy.
- $\delta_\perp$ is a normal field–induced activation energy–lowering factor.
- $\rho_\perp$ is a normal field–induced activation energy–lowering exponent.
- $F_0 = 1\,\mathrm{V/cm}$.
- g_v is the valley degeneracy.
- g is the density-of-states.
- f is the electron energy distribution.
- v is the magnitude of the electron velocity.
- ρ_{SHE} is an exponent for the SHE current.

The SHE distribution enhancement factor can be specified by the `eSHEDistribution` keyword in the `Traps` statement. Similarly, the `hSHEDistribution` keyword specifies the enhancement factor of the hole energy distribution.

The following example specifies the SHE distribution enhancement factor with $\delta_{SHE} = 100\,\mathrm{cm}^2/\mathrm{A}$, $\varepsilon_{th} = 2$ eV, $\varepsilon_a = 2.1$ eV, $\delta_\perp = 10^{-7}$ eV, $\rho_\perp = 1$, and $\rho_{SHE} = 1$:

```
Physics(MaterialInterface="Silicon/Oxide") {
  Traps(...
    Degradation
    # (delta_SHE  E_th  E_a  delta_p  rho_p  rho_SHE)
    eSHEDistribution=(1.0e2  2  2.1  1.0e-7  1  1)
    ...
  )
}
```

Using the Trap Degradation Model

The `Degradation` model can be activated for any trap level or distribution (see Traps and Fixed Charges on page 449). The keywords related to the `Degradation` model are described in Table 325 on page 1488, along with all other trap-related options, and their syntax is shown here:

```
Physics ( [ RegionInterface | MaterialInterface = "<name1>/<name2>" ] |
          [ Material | Region = "<name>" ] ) {
    Traps (
        <trap_specifications>
        Degradation [(PowerLaw)]
        Conc=<N_it^0>
        BondConc=<N> [BondConcSFactor=["<dataset_name>" | "<pmi_model_name>"]]
        ActEnergy=<ε_A^0>
        DePasCoef=<ν_0>
        [CritConc=<N_crit>]
        [FieldEnhan=(<δ_//> <ρ_//> <δ_⊥> <ρ_⊥>)]
        [PowerEnhan=(<β_0> <β_//> <β_⊥>)]
        [CurrentEnhan=(<δ_Tun> <ρ_Tun> <δ_HC> <ρ_HC>)]
        [FowlerNordheimEnhan=(<δ_FN> <ρ_FN>)]
        [DirectTunnelingEnhan=(<δ_DTe> <ρ_DTe> <δ_DTh> <ρ_DTh>)]
        [BarrierTunnelingEnhan=(<δ_BTe> <ρ_BTe> <δ_BTh> <ρ_BTh>)]
        [eSHEDistribution=(<δ_SHE> <ε_th> <ε_a> <δ_⊥> <ρ_⊥> <ρ_SHE>)]
        [hSHEDistribution=(<δ_SHE> <ε_th> <ε_a> <δ_⊥> <ρ_⊥> <ρ_SHE>)]
        [DiffusionEnhan=(<x_p> <D_0> <ε_H> <k_p> <N_H^0> <N_ox>)]
        [PasCoef=<γ_0>]
        [PasTemp=<T_0>]
        [PasVolume=<Ω>]
    )
    ...
}
```

The total silicon-bond concentration, which represents the maximum concentration of traps that can be generated as the result of degradation, is specified with `BondConc`. It is possible to have a spatially dependent bond concentration by using the parameter `BondConcSFactor` to specify a dataset or a PMI space factor model (see Space Factor on page 1190) that describes the spatial dependency. If `BondConcSFactor` is specified without `BondConc`, the values obtained from the dataset or PMI are used directly. If both `BondConcSFactor` and `BondConc` are specified, the `BondConcSFactor` values are normalized by the largest `BondConcSFactor` value and are then multiplied by `BondConc`.

Device Lifetime and Simulation

The following example illustrates the use of the `Degradation` model:

```
Physics(MaterialInterface="Silicon/Oxide"){
   Traps(Conc=1e8 EnergyMid=0 Acceptor #FixedCharge
      Degradation #(PowerLaw)
         ActEnergy=2 BondConc=1e12
      DePasCoeff=8e-10
      FieldEnhan=(0 1 1.95e-3 0.33)
      CurrentEnhan=(0 1 6e+5 1)
      PowerEnhan=(0 0 -1e-7)
   )
   GateCurrent(GateName="gate" Lucky(CarrierTemperatureDrive) Fowler)
}
```

For this input, the initially specified trap concentration is $10^8 \, \mathrm{cm}^{-2}$ and, in the process of degradation, it can be increased up to $10^{12} \, \mathrm{cm}^{-2}$. The activation energy of hydrogen on Si-H bonds is 2 eV and the depassivation constant at the equilibrium is equal to $8 \times 10^{-10} \, \mathrm{s}^{-1}$. The degradation simulation can be separated into two parts:

- Simulation of extremely stressed devices with existing experimental data and fitting to the data by modification of the field and current-dependent parameters.

- Simulation of normal-operating devices to predict device reliability (lifetime).

For the first part of the degradation simulation, the typical `Solve` section can be:

```
Solve {
   NewCurrentPrefix="tmp"
   coupled (iterations=100) { Poisson }
   coupled { poisson electron hole }
   Quasistationary( InitialStep=0.1 MaxStep=0.2 MinStep=0.0001
            increment=1.5 Goal{name="gate" voltage=-10} )
            { coupled { poisson electron hole } }
   NewCurrentPrefix=""
   coupled { poisson electron hole }
   transient( InitialTime=0 Finaltime = 100000
            increment=2 InitialStep=0.1 MaxStep=100000 ){
         coupled{ poisson electron hole }
   }
}
```

The first `Quasistationary` ramps the device to stress conditions (in this particular case, to high negative gate voltage), the second `transient` simulates the degradation kinetics (up to $10^5 \, \mathrm{s}$, which is a typical time for stress experimental data).

NOTE   The hot carrier currents are postprocessed values and, therefore, `InitialStep` should not be large.

To monitor the trap formation kinetics in transient, you can use `Plot` and `CurrentPlot` statements to output `TotalInterfaceTrapConcentration`, `TotalTrapConcentration`, and `OneOverDegradationTime`, for example:

```
CurrentPlot{
    eDensity(359) Potential(359)
    eInterfaceTrappedCharge(359) hInterfaceTrappedCharge(359)
    OneOverDegradationTime(359) TotalInterfaceTrapConcentration(359)
}
```

where a vertex number is specified to have a plot of the fields at some location on the interface. As a result, the behavior of these values versus time can be seen in the plot file of Sentaurus Device.

The prediction of the device lifetime can be performed in two different ways:

■ Direct simulation of a normal-operating device in transient for a long time (for example, 30 years).

■ Extrapolation of the degradation of a stressed device by computation of the ratio between depassivation constants for stressed and unstressed conditions.

The important value here is the critical trap concentration N_{crit}, which defines an edge between a properly working and improperly working device. Using N_{crit}, the device lifetime τ_{D} is defined as follows (according to different prediction ways):

1. In `transient`, direct computation of time $t = \tau_{\mathrm{D}}$ gives the trap concentration equal to N_{crit}.

2. In `Quasistationary`, if the previously finished `transient` statement computes the device lifetime $\tau_{\mathrm{D}}^{\mathrm{stress}}$ and the depassivation constant ν^{stress} at stress conditions, then $\tau_{\mathrm{D}} = (\nu^{\mathrm{stress}}/\nu)\tau_{\mathrm{D}}^{\mathrm{stress}}$.

So, the plotted value of `OneOverDegradationTime` is equal to $1/\tau_{\mathrm{D}}$ for one trap level and the sum $\sum 1/\tau_{\mathrm{D}}^{i}$ if several trap levels are defined for the degradation. It is computed for each vertex where the degradation model is applied and can be considered as the lifetime of local device area.

For the second approach to device lifetime computation, the following `Solve` statement can be used:

```
Solve {
    NewCurrentPrefix="tmp"
    coupled (iterations=100) { Poisson }
    coupled { poisson electron hole }
```

```
Quasistationary( InitialStep=0.1 MaxStep=0.2 Minstep=0.0001
          increment=1.5 Goal{name="gate" voltage=-10} )
          { coupled { poisson electron hole } }

NewCurrentPrefix=""
coupled { poisson electron hole }
transient( InitialTime=0 Finaltime = 100000
          increment=2 InitialStep=0.1 MaxStep=100000 ){
          coupled{ poisson electron hole }
}

set(Trapfilling=-Degradation)

coupled { poisson electron hole }
Quasistationary( InitialStep=0.1 MaxStep=0.2 Minstep=0.0001 increment=1.5
          Goal{name="gate" voltage=1.5} )
          { coupled { poisson electron hole } }
Quasistationary( InitialStep=0.1 MaxStep=0.2 Minstep=0.0001 increment=1.5
          Goal{name="drain" voltage=3} )
          { coupled { poisson electron hole } }
}
```

The statement `set(Trapfilling=-Degradation)` returns the trap concentrations to their unstressed values (it is not necessary to include, but it may be interesting to check the influence). The first `Quasistationary` statement after the `set` command returns the normal-operating voltage on the gate and, in the second, you can plot the dependence of $1/\tau_\mathrm{D}$ on applied drain voltage. The last dependence could be useful to predict an upper limit of operating voltages where the device will work for a specified time.

Degradation in Insulators

Although the `Degradation` model was designed for trap generation that occurs at semiconductor–insulator interfaces, the model can be used to generate traps at insulator–insulator interfaces or in bulk-insulator regions.

For insulator degradation, Sentaurus Device will set $F_\perp = F$ and $F_\parallel = 0$, and the enhancement factors k_HC, k_Tun, and k_SHE are taken from values computed at the semiconductor–insulator interface.

> **NOTE** To allow traps that are created in insulator regions to be filled with carriers, it is necessary to construct a nonlocal mesh to connect the semiconductor–insulator interface to the regions where traps are generated and to invoke nonlocal tunneling models (see Tunneling and Traps on page 463).

To use this feature:

1. Create a nonlocal mesh that connects the semiconductor interface with the regions where traps are generated. For example:

```
Math {
    NonLocal "NLM_silicon_oxide" (
    MaterialInterface = "Silicon/Oxide"
    Length = 4.1e-7               # Use a length that will reach the traps
}
```

2. Specify nonlocal tunneling and `Traps(Degradation ...)` in the `Physics` section associated with the insulator–insulator interface or the bulk-insulator region where degradation will be used. Degradation parameters must be specified and adjusted as necessary. For example:

```
Physics (RegionInterface="oxide1/oxide2") {
    Traps ((
        eBarrierTunneling(Nonlocal="NLM_silicon_oxide")
        hBarrierTunneling(Nonlocal="NLM_silicon_oxide")
        TrapVolume=1e-6
        HuangRhys=70
        PhononEnergy=0.02
    #
        Degradation
        Conc=1e4 EnergyMid=0 Donor
        ActEnergy=2
        BondConc=1e14
        DePasCoeff=1e-11
        PasTemp=300
        FieldEnhan=(0 1 3.9e-3 0.33)
        CurrentEnhan=(0 1 1 1)
        PowerEnhan=(0 0 -1e-7)
        DiffusionEnhan=(2e-7 1e-13 0.05 1.0 5e10 15)
        PasVolume=5e-10
    ))
}
```

3. In the parameter file, specify a nonzero tunneling mass for all regions or materials where tunneling can occur. For example:

```
Material = "Silicon" {
    BarrierTunneling "NLM_silicon_oxide" { mt = 1, 1 }
}

Material = "Oxide" {
    BarrierTunneling "NLM_silicon_oxide" { mt = 1, 1 }
}
```

MSC–Hydrogen Transport Degradation Model

Bias and temperature stresses generate interface fixed charges and trapped charges near the oxide interface. These immobile charges affect the threshold voltage (see Chapter 7 on page 173) and the carrier mobility (see Mobility Degradation Components due to Coulomb Scattering on page 347). To explain these degradation phenomena, various physical models have been proposed [12][13][14][1]. Although the details of these models are different, they commonly involve charge-trapping, silicon-hydrogen bond depassivation, and hydrogen transport.

To model charge-trapping, interactions between localized trapping centers and mobile carriers must be considered. Contrary to the standard traps in Chapter 17 on page 449, the trapping centers used in the degradation model usually involve hydrogens. Therefore, interactions between the localized trapping centers and mobile hydrogens should be considered. In addition, the trapping centers may have more than two internal states depending on the structural relaxation and the presence of charges and hydrogens [1].

The multistate configurations (MSCs) introduced in Chapter 18 on page 473 can be used to represent these complex trapping centers because the MSCs can handle an arbitrary number of states and their transitions involving the capture and emission of charges and hydrogens.

Finally, hydrogen transport must be considered if the degradation model involves mobile hydrogens. Hydrogen atoms, hydrogen molecules, and hydrogen ions can contribute to the hydrogen transport, and there can be chemical reactions between them [12][13][14].

Sentaurus Device provides the following capabilities to model oxide degradation:

- Transport equations for hydrogen atoms, hydrogen molecules, and hydrogen ions.
- An arbitrary number of interface and bulk reactions among mobile elements (hydrogen atoms, hydrogen molecules, hydrogen ions, electrons, and holes).
- An arbitrary number of interface and bulk reactions among mobile elements and localized states by using the multistate configurations (see Chapter 18 on page 473).

Hydrogen Transport

Transport equations for hydrogen atoms (X_1), hydrogen molecules (X_2), and hydrogen ions (X_3) can be written as:

$$\frac{\partial}{\partial t}[X_i] + \nabla \cdot \left[D_i \exp\left(-\frac{E_{\mathrm{d}i}}{kT}\right)\left(\frac{qK_i^Q}{kT}\vec{F}[X_i] - \nabla[X_i] - \alpha_{\mathrm{td}}[X_i]\nabla \ln T\right)\right] + R_{\mathrm{net}} + r_i([X_i] - [X_i]_0) = 0 \qquad (557)$$

where:

- D_i is the diffusion coefficient.
- E_{di} is the diffusion activation energy.
- α_{td} is the prefactor of the thermal diffusion term.
- K_i^Q is the number of charges for element X_i.
- R_{net} is the net recombination rate due to chemical reactions.
- r_i is the explicit recombination rate.
- $[X_i]_0$ is the initial density.

By default, the initial densities of hydrogen atoms, molecules, and ions are all zero. You can load the initial density of each hydrogen element from the `PMIUserField` by using the `Set` command in the `Solve` section, for example:

```
Solve {
    ...
    Set ( HydrogenAtom = "PMIUserField0" )
    Set ( HydrogenMolecule = "PMIUserField1" )
    Set ( HydrogenIon = "PMIUserField3" )
    ...
}
```

Sentaurus Device uses default values for $D_i \exp(-E_{di}/(kT))$ and α_{td}. You can customize the computation of $D_i \exp(-E_{di}/(kT))$ and α_{td} by using PMI models (for details, see Diffusivity on page 1279). The corresponding command file can be written as:

```
Physics ( Material = "Oxide" ) {
   HydrogenDiffusion(
      HydrogenAtom (
         Diffusivity = pmi_HydrogenDiffusivity
         Alpha = pmi_HydrogenAlpha
      )
      HydrogenMolecule (
         Diffusivity = pmi_HydrogenDiffusivity
         Alpha = pmi_HydrogenAlpha
      )
      HydrogenIon (
         Diffusivity = pmi_HydrogenDiffusivity
         Alpha = pmi_HydrogenAlpha
      )
      ...
   )
}
```

Boundary Conditions

At electrodes, $[X_i] = [X_i]_0$ is assumed as the default boundary condition. You can specify more flexible conditions at each contact. The corresponding command file can be written as:

```
HydrogenBoundary {
   { Name = "cSiTop"
     HydrogenAtom = 1e7                    # [cm-3]
     HydrogenMolecule = reflective
   }
   { Name = "cSiBot"
     HydrogenAtom = reflective
   }
   ...
}
```

Reactions Between Mobile Elements

In the model, you can specify an arbitrary number of bulk and interface chemical reactions between hydrogen atoms (X_1), hydrogen molecules (X_2), hydrogen ions (X_3), electrons (X_4), and holes (X_5). Each reaction is defined by the following reaction equation:

$$\sum_{i=1}^{5} \alpha_i X_i \leftrightarrow \sum_{i=1}^{5} \beta_i X_i \tag{558}$$

where the nonnegative integers α_i and β_i are the particle numbers of element X_i to be removed and created by the forward reaction.

These coefficients must satisfy the charge and hydrogen conservation laws:

$$\sum_{i=1}^{5} (\alpha_i - \beta_i) K_i^Q = 0 \tag{559}$$

$$\sum_{i=1}^{5} (\alpha_i - \beta_i) K_i^H = 0 \tag{560}$$

where K_i^Q and K_i^H are the number of charges and the number of hydrogen atoms for element X_i (for K_i^Q and K_i^H of each mobile element, see Table 94 on page 474).

The forward and reverse reaction rates R_f and R_r are modeled as:

$$R_f = k_f \exp\left(\delta_f F - \frac{E_f}{kT}\right) \prod_{i=1}^{5} \left(\frac{[X_i]}{1 \ /\text{cm}^3}\right)^{\alpha_i} \qquad (561)$$

$$R_r = k_r \exp\left(\delta_r F - \frac{E_r}{kT}\right) \prod_{i=1}^{5} \left(\frac{[X_i]}{1 \ /\text{cm}^3}\right)^{\beta_i} \qquad (562)$$

where:

- F is the magnitude of the electric field $[\text{V/cm}]$.
- k_f and k_r are the forward and reverse reaction coefficients, respectively ($[\text{cm}^{-3}\text{s}^{-1}]$ for bulk reactions and $[\text{cm}^{-2}\text{s}^{-1}]$ for interface reactions).
- δ_f and δ_r are the forward and reverse reaction field coefficients, respectively $[\text{cm V}^{-1}]$.
- E_f and E_r are the forward and reverse reaction activation energies, respectively $[\text{eV}]$.

> **NOTE** For a reaction specified at a semiconductor–insulator interface, the insulator electric field is used instead of the semiconductor electric field.

A reaction can be specified in the `Physics` section as an argument `HydrogenReaction` to the `HydrogenDiffusion` keyword. For example, consider the dimerization of two hydrogen atoms into a hydrogen molecule $2\text{H} \leftrightarrow \text{H}_2$ in the oxide region with $k_f = 10^{-3} \text{ cm}^{-3}\text{s}^{-1}$ and $k_r = 10^2 \text{ cm}^{-3}\text{s}^{-1}$.

The corresponding command file can be written as:

```
Physics ( Material = "Oxide" ) {
   HydrogenDiffusion(
      HydrogenReaction( # 2H <-> H_2
         LHSCoef ( # alpha_i
            HydrogenAtom = 2
            HydrogenMolecule = 0
            HydrogenIon = 0
            Electron = 0
            Hole = 0
         )
         RHSCoef ( # beta_i
            HydrogenAtom = 0
            HydrogenMolecule = 1
            HydrogenIon = 0
            Electron = 0
            Hole = 0
         )
         ForwardReactionCoef = 1.0e-3 # k_f
```

```
            ReverseReactionCoef = 1.0e2 # k_r
            ForwardReactionEnergy = 0 # E_f
            ReverseReactionEnergy = 0 # E_r
            ForwardReactionFieldCoef = 0 # delta_f
            ReverseReactionFieldCoef = 0 # delta_r
         )
         ...
      )
   }
```

The default values of all the coefficients are zero. Table 305 on page 1475 lists the options available for the reaction specification.

For heterointerfaces, the keyword `Region` or `Material` allows you to specify the region or material where the reaction process enters as a generation–recombination rate. In addition, the keyword `FieldFromRegion` or `FieldFromMaterial` allows you to specify the region or material where the electric field is obtained. For example:

```
   Physics ( Material = "Silicon/OxideAsSemiconductor" ) {
      HydrogenDiffusion(
         HydrogenReaction(...
            Material = "Silicon"
            FieldFromMaterial = "OxideAsSemiconductor"
         )
      )
   }
```

Reactions With Multistate Configurations

A multistate configuration (MSC) can be used to model reactions between the mobile hydrogen elements and localized hydrogen states such as silicon-hydrogen bonds at the silicon–oxide interface.

For example, consider a hydrogen depassivation model based on the hole capture process:

$$\text{Si-H} + p \leftrightarrow \text{Si}^+ + \text{H} \tag{563}$$

where Si-H, p, Si$^+$, and H represent the silicon-hydrogen bond, hole, silicon dangling bond, and hydrogen atom, respectively. This reaction can be specified by a two-state MSC defined at the silicon–oxide interface:

```
   Physics ( MaterialInterface = "Silicon/Oxide" ) {
      MSConfigs (
         MSConfig ( Name = "SiHBond" Conc=5.0e12
            State ( Name = "s1" Hydrogen=1 Charge=0 ) # Si-H bond
            State ( Name = "s2" Hydrogen=0 Charge=1 ) # Si^+ dangling bond
```

```
            Transition ( Name = "t21" # Si-H + p <-> H + Si^+
                To="s2" From="s1" CEModel("CEModel_Depassivation" 1)
                Reservoirs("VB"(Particles=+1) "HydrogenAtom"(Particles=-1) )
                FieldFromInsulator
            )
        )
        ...
    )
}
```

The capture and emission rates are obtained from:

$$c_{21} = c_{PMI}(n, p, T, T_n, T_p, F) \prod_{i=1}^{3} \left(\frac{[X_i]}{1 \text{ /cm}^3} \right)^{\alpha_i} \tag{564}$$

$$e_{21} = e_{PMI}(n, p, T, T_n, T_p, F) \prod_{i=1}^{3} \left(\frac{[X_i]}{1 \text{ /cm}^3} \right)^{\beta_i} \tag{565}$$

where c_{PMI} and e_{PMI} are the capture and emission rates specified by the trap capture and emission PMI model, respectively. For more information about multistate configurations, see Chapter 18 on page 473.

> **NOTE**   Contrary to the conventional trap capture and emission PMI model, the insulator electric field can be used in the PMI model at the semiconductor–insulator interface instead of the semiconductor electric field when the keyword `FieldFromInsulator` is set in the transition.

The CEModel_Depassivation Model

The built-in capture and emission model `CEModel_Depassivation` models the hydrogen depassivation process. In the model, the hydrogen depassivation (electron capture) rate induced by hot-electron distribution is written as:

$$c_{PMI} = 2g_v \sigma \int_{\varepsilon_{min}}^{\varepsilon_{max}} v(\varepsilon)g(\varepsilon)f(\varepsilon) \exp\left[\gamma \left(\frac{F}{1 \text{ V/cm}} \right)^\rho - \frac{\Theta(W_f - q\alpha F - \chi\varepsilon)(W_f - q\alpha F - \chi\varepsilon)}{kT} \right] \tag{566}$$

where:

- ε_{min} and ε_{max} are the minimum and maximum kinetic energies of the integration.
- σ is the capture cross-section.
- g_v is the valley degeneracy.

- $v(\varepsilon)$ is the magnitude of the group velocity.
- $g(\varepsilon)$ is the density-of-states.
- $f(\varepsilon)$ is the distribution function.
- γ is the field enhancement prefactor.
- ρ is the field enhancement exponent.
- W_f is the activation energy for the depassivation process.
- α is the field-induced barrier-lowering factor.
- χ is the kinetic energy–induced barrier-lowering factor.

Similarly, the hydrogen depassivation rate induced by cold electrons can be written as:

$$c_{PMI} = \sigma v_{th} n \exp\left[\gamma\left(\frac{F}{1\ V/cm}\right)^\rho - \frac{\Theta(W_f - q\alpha F)(W_f - q\alpha F)}{kT} \right] \tag{567}$$

where v_{th} is the thermal velocity.

As the hydrogen passivation (electron emission) rate is not related to hot carriers, it is modeled simply as:

$$e = e_{PMI} \times \left(\frac{[H]}{1/cm^3} \right) \tag{568}$$

$$e_{PMI} = e_0 \exp\left(-\frac{W_r}{kT} \right) \tag{569}$$

where e_0 is the passivation rate prefactor, and W_r is the activation energy for the passivation process.

The capture-emission model `CEModel_Depassivation` implements Eq. 566 and Eq. 567 for electrons and holes. The additional index in the `CEModel_Depassivation` model selects the equation and the carrier type as follows:

```
MSConfig( ...
   Transition( ... CEModel("CEModel_Depassivation" 0)) # Eq. 567 for electrons
   Transition( ... CEModel("CEModel_Depassivation" 1)) # Eq. 567 for holes
   Transition( ... CEModel("CEModel_Depassivation" 2)) # Eq. 566 for electrons
   Transition( ... CEModel("CEModel_Depassivation" 3)) # Eq. 566 for holes
)
```

To use the `CEModel_Depassivation` model with the index 2 or 3 (hot electron–induced or hot hole–induced degradation), you must specify `eSHEDistribution` or `hSHEDistribution` in the `Physics` section to compute the electron or hole distribution function (see Using Spherical Harmonics Expansion Method on page 750).

The model coefficients and their defaults are given in Table 102. The model coefficients can be changed in the `CEModel_Depassivation` section of the parameter file.

Table 102   Default coefficients for CEModel_Depassivation

Symbol	Parameter name (Electrons)	Default value (Electrons)	Parameter name (Holes)	Default value (Holes)	Unit
σ	Xsec_e	1.0×10^{-24}	Xsec_h	1.0×10^{-24}	cm^2
v_{th}	Vth_e	2.0×10^{7}	Vth_h	2.0×10^{7}	cm/s
γ	gamma_e	2.7×10^{-7}	gamma_h	2.7×10^{-7}	1
ρ	rho_e	1.0	rho_h	1.0	1
α	alpha_e	9.0×10^{-9}	alpha_h	9.0×10^{-9}	cm
χ	chi_e	1.0	chi_h	1.0	1
W_f	Wf_e	0.5	Wf_h	0.5	eV
e_0	e0_e	3.0×10^{-9}	e0_h	3.0×10^{-9}	1/s
W_r	Wr_e	0	Wr_h	0	eV
$d\varepsilon$	dE_e	0.01	dE_h	0.01	eV
ε_{min}	Emin_e	0	Emin_h	0	eV
ε_{max}	Emax_e	5	Emax_h	5	eV

Using MSC–Hydrogen Transport Degradation Model

You can select the regions and interfaces where the hydrogen transport equations are to be solved by specifying the keyword `HydrogenDiffusion` in the corresponding `Physics` section of the command file. For example:

```
Physics ( Material = "Oxide" ) {
   HydrogenDiffusion
}
```

The keyword `HydrogenDiffusion` can be specified with the `HydrogenReaction` arguments (see Reactions Between Mobile Elements on page 502).

Specifying `HydrogenDiffusion` in the interface-specific `Physics` section gives a surface recombination term determined by r_i and $[X_i]_0$ at the corresponding interface.

To activate the transport of hydrogen atoms, hydrogen molecules, and hydrogen ions, the keywords `HydrogenAtom`, `HydrogenMolecule`, and `HydrogenIon` must be specified inside the `Coupled` command of the `Solve` section.

For example, transient drift-diffusion simulation with transport of hydrogen atoms and hydrogen molecules can be specified by:

```
Solve {
   Transient(...) {
      Coupled { Poisson Electron Hole HydrogenAtom HydrogenMolecule }
   }
}
```

The parameters D_i, $E_{\mathrm{d}i}$, $[X_i]_0$, and r_i can be specified in the region-specific and interface-specific `HydrogenDiffusion` parameter set in the parameter file. For example:

```
Material = "Oxide" {
   HydrogenDiffusion {
      HydrogenAtom {
         d0 = 1.0e-13  # [cm^2*s^-1]
         Ed = 0        # [eV]
         atd = 1       # [1]
         n0 = 0        # [cm^-3]
         krec = 0      # [cm^-3*s^-1]
      }
      HydrogenMolecule {
         d0 = 1.0e-14  # [cm^2*s^-1]
         Ed = 0        # [eV]
         atd = 1       # [1]
         n0 = 0        # [cm^-3]
         krec = 0      # [cm^-3*s^-1]
      }
      HydrogenIon {
         ...
      }
   }
}

MaterialInterface = "Oxide/PolySi" {
   HydrogenDiffusion {
      HydrogenAtom {
         n0 = 1        # [cm^-3]
         krec = 1      # [cm^-2*s^-1]
      }
   }
}
```

Here `d0`, `Ed`, `atd`, `n0`, and `krec` correspond to D_i, E_{di}, α_{td}, $[X_i]_0$, and r_i. The default values of D_i, E_{di}, $[X_i]_0$, and r_i are zero; while $\alpha_{td} = 1$ by default.

The keywords for plotting the densities of hydrogen atoms, hydrogen molecules, and hydrogen ions are:

```
Plot { ...
   HydrogenAtom HydrogenMolecule HydrogenIon
}
```

Two-Stage NBTI Degradation Model

Negative bias temperature instability (NBTI) refers to the generation of positive oxide charges and interface traps in MOS structures under negative gate bias at elevated temperature, which affects the threshold voltage and on-currents of PMOSFETs [12].

Sentaurus Device provides a two-stage NBTI degradation model [1][2], which assumes that the NBTI degradation proceeds using a two-stage process:

- The first stage includes the creation of E' centers (dangling bonds in amorphous oxides) from their neutral oxygen vacancy precursors, the charging and discharging of E' centers, and the total annealing of E' centers to neutral oxygen vacancy precursors.
- The second stage considers the creation of poorly recoverable P_b centers (dangling bonds at silicon–oxide interfaces).

In the two-stage NBTI degradation model, the involved energy levels and activation energies are distributed widely and are treated as random variables. A random sampling technique is used to obtain the average change of the interface charge.

> **NOTE** As the two-stage NBTI model is based on the semiclassical carrier density at the semiconductor–insulator interface, it is not recommended to use the model with quantum-correction models.

Formulation

The two-stage NBTI degradation model considers a special trap having four internal states:

- s_1: Oxygen vacancy as a precursor state.
- s_2: Positive E' center.
- s_3: Neutral E' center.
- s_4: Fixed positive charge with a P_b center.

Each NBTI trap is characterized by seven independent random variables:

- E_1: Trap level of the precursor [eV] (by default, $-1.14 \le E_1 < -0.31$).

- E_2: Trap level of the E' center [eV] (by default, $0.01 \le E_2 < 0.3$).

- E_4: Trap level of the P_b center [eV] (by default, $0.01 \le E_4 < 0.5$).

- E_A: Barrier energy of a transition from s_3 to s_1 [eV] (by default, $0.01 \le E_A < 1.15$).

- E_B: Barrier energy of a transition from s_1 to s_2 [eV] (by default, $0.01 \le E_B < 1.15$).

- E_D: Barrier energy of a transition between s_2 to s_4 [eV] (by default, $\langle E_D \rangle = 1.46, (\langle E_D^2 \rangle - \langle E_D \rangle^2)^{1/2} = 0.44$).

- r: Uniform number between 0 and 1. When $r < C$, a transition between s_2 to s_4 is allowed (by default, $C = 0.12$).

E_1, E_2, E_4, E_A, and E_B follow the uniform distribution between their minimum and maximum values. E_D follows the Fermi-derivative distribution characterized by its average and standard deviation. The trap levels E_1, E_2, and E_4 are defined relative to the valence band energy.

The state occupation probability s_i satisfies the normalization condition:

$$\sum_{i=1}^{4} s_i = 1 \tag{570}$$

and the following rate equations:

$$\dot{s}_1 = -s_1 k_{12} + s_3 k_{31} \tag{571}$$

$$\dot{s}_2 = s_1 k_{12} - s_2(k_{23} + k_{24}) + s_3 k_{32} + s_4 k_{42} \tag{572}$$

$$\dot{s}_3 = s_2 k_{23} - s_3(k_{32} + k_{31}) \tag{573}$$

$$\dot{s}_4 = s_2 k_{24} - s_4 k_{42} \tag{574}$$

with the transition rates:

$$k_{12} = e_C^{n,1} + c_V^{p,1} \tag{575}$$

$$k_{23} = c_C^{n,2} + e_V^{p,2} \tag{576}$$

$$k_{32} = e_C^{n,2} + c_V^{p,2} \tag{577}$$

$$k_{31} = \nu_1 \exp(-E_A/kT) \tag{578}$$

$$k_{24} = \nu_2 \exp[-(E_D - \gamma F)/kT]\Theta(C - r) \tag{579}$$

$$k_{42} = \nu_2 \exp[-(E_D + \Delta E_D + \gamma F)/kT]\Theta(C - r) \tag{580}$$

where:

- ν_1 and ν_2 are the attempt frequencies (by default, $\nu_1 = 1.0 \times 10^{13}\,\mathrm{s}^{-1}$ and $\nu_2 = 5.11 \times 10^{15}\,\mathrm{s}^{-1}$).

- γ is the prefactor for the field-dependent barrier energy (by default, $\gamma = 7.4 \times 10^{-8}\,\mathrm{cm} \cdot \mathrm{eV/V}$).

- ΔE_D is the additional barrier energy for k_{42} (by default, $\Delta E_D = 0\,\mathrm{eV}$).

In addition, it is assumed that the hole occupation probability f_{it}^p of the P_b center in the state 4 is determined by:

$$f_{\mathrm{it}}^p = (e_C^{n,4} + c_V^{p,4})(1 - f_{\mathrm{it}}^p) - (c_C^{n,4} + e_V^{p,4})f_{\mathrm{it}}^p \tag{581}$$

The electron emission rate and the hole capture rate for the state 1 are given by:

$$e_C^{n,1} = \sigma_n v_{\mathrm{th}}^n N_C \exp[-H(E_C - E_1)/kT + \Theta(F_{c,n})(|F|/F_{c,n})^{\rho_n} - E_B/kT] \tag{582}$$

$$c_V^{p,1} = \sigma_p v_{\mathrm{th}}^p p \exp[-H(E_V - E_1)/kT + \Theta(F_{c,p})(|F|/F_{c,p})^{\rho_p} - E_B/kT] \tag{583}$$

where:

- σ_n and σ_p are the electron and hole capture cross-sections (by default, $\sigma_n = 1.08 \times 10^{-15}\,\mathrm{cm}^2$ and $\sigma_p = 1.24 \times 10^{-14}\,\mathrm{cm}^2$).

- v_{th}^n and v_{th}^p are the electron and hole thermal velocity (by default, $v_{\mathrm{th}}^n = 1.5 \times 10^7\,\mathrm{cm/s}$ and $v_{\mathrm{th}}^p = 1.2 \times 10^7\,\mathrm{cm/s}$).

- F is the insulator electric field.

- $F_{c,n}$ and $F_{c,p}$ are the critical electric field (by default, $F_{c,n} = -1\,\mathrm{V/cm}$ and $F_{c,p} = 2.83 \times 10^6\,\mathrm{V/cm}$).

- ρ_n and ρ_p are the exponents of the field-dependent term (by default, $\rho_n = 2$ and $\rho_p = 2$).

- $H(x) = x\Theta(x)$.

When the energy-dependent hole distribution is available (hSHEDistribution is activated in the semiconductor region), you can use the following expression for $c_V^{p,1}$ instead of Eq. 583:

$$c_V^{p,1} = 2g_v\sigma_p\int_0^\infty v(\varepsilon)g(\varepsilon)f(\varepsilon)\exp[-H(E_V - E_1 - \varepsilon)/kT + \Theta(F_{c,p})(|F|/F_{c,p})^{\rho_p} - E_B/kT]d\varepsilon \quad (584)$$

The electron capture rate, the electron emission rate, the hole capture rate, and the hole emission rate for state 2 and state 4 are given by:

$$c_C^{n,i} = \sigma_n v_{th}^n n\exp[-H(E_i - E_C)/kT] \quad (585)$$

$$e_C^{n,i} = \sigma_n v_{th}^n N_C\exp[-H(E_C - E_i)/kT] \quad (586)$$

$$c_V^{p,i} = \sigma_p v_{th}^p p\exp[-H(E_V - E_i)/kT] \quad (587)$$

$$e_V^{p,i} = \sigma_p v_{th}^p N_V\exp[-H(E_i - E_V)/kT] \quad (588)$$

where $i = 2$ or 4.

Using Two-Stage NBTI Model

You can activate the two-stage NBTI model by specifying the NBTI command in the interface-specific Physics section of the command file. For example:

```
Physics ( MaterialInterface = "Silicon/Oxide" ) {
   NBTI (
      Conc = 5.0e12                        # N_0 [/cm^2]
      NumberOfSamples = 1000               # N_sample [1]
      hSHEDistribution | -hSHEDistribution   # (off by default)
   )
}
```

where Conc represents the density of the precursor N_0, and NumberOfSamples represents the number of random samples N_{sample}. Sentaurus Device generates N_{sample} random configurations for each interface vertex. Then, the interface charge density is obtained from the ensemble average as follows:

$$Q = Q_{ox} + Q_{it} = qN_0\langle s_2 + s_4\rangle + qN_0\langle s_4 f_{it}^p\rangle \quad (589)$$

where:

$$\langle x \rangle = \frac{1}{N_{\text{sample}}} \sum_{j=1}^{N_{\text{sample}}} x^j \tag{590}$$

During transient simulation, state occupation probabilities will change following the kinetic equations, which will change the interface charge density. It is assumed that $s_1 = 1$ at the beginning. In addition, you can restart NBTI degradation simulations by loading the saved data.

When the `hSHEDistribution` keyword is specified in the `NBTI` command (off by default), $c_V^{p,1}$ is computed from Eq. 584 instead of Eq. 583.

> **NOTE** You need to specify `hSHEDistribution` in the `Physics` section to compute the hole distribution function (see Using Spherical Harmonics Expansion Method on page 750).

You can plot the density of charge and the density of each state as follows:

```
Plot {
   InterfaceNBTICharge   # [1/cm^2]
   InterfaceNBTIState1   # [1/cm^2]
   InterfaceNBTIState2   # [1/cm^2]
   InterfaceNBTIState3   # [1/cm^2]
   InterfaceNBTIState4   # [1/cm^2]
}
```

The model parameters are defined in the interface-specific `NBTI` parameter set.

Extended Nonradiative Multiphonon Model

The extended nonradiative multiphonon (eNMP) model [3] can be used to investigate degradation related to NBTI. The model accounts for the behavior of oxide defects (traps) that can have four internal states, two of which are metastable.

As with the two-stage NBTI degradation model, the eNMP model uses a random sampling technique to obtain the average behavior of multiple sample defects (N_{sample}) at each interface vertex. The sample defects are considered to have random insulator positions, and distributed energy levels and activation energies.

Each sample defect is assumed to be located at a distance x_t from the interface, where x_t is distributed randomly between a minimum and maximum location:

$$x_{t,min} < x_t < x_{t,max} \tag{591}$$

NOTE   The implementation treats the average charge associated with the sample defects as an interface charge.

eNMP Model Description

The eNMP model considers a special trap having four internal states:

- s_1 : Neutral stable state
- s_2 : Positive stable state
- $s_{1'}$: Neutral metastable state
- $s_{2'}$: Positive metastable state

The model describes the transitions between these states according to the diagram in Figure 21, in which the k_{ij} terms represent the transition rates between the states.
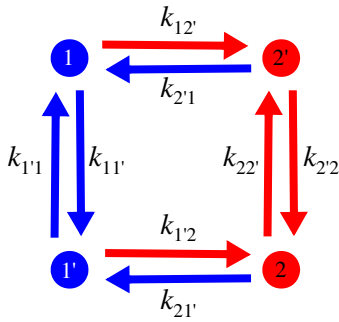
Figure 21   State diagram for the eNMP model

The state occupation probabilities s_i satisfy the normalization condition:

$$s_1 + s_{1'} + s_2 + s_{2'} = 1 \tag{592}$$

The rate equations for the transitions are given by:

$$\dot{s}_1 = -s_1(k_{11'} + k_{12'}) + s_{1'}k_{1'1} + s_{2'}k_{2'1} \tag{593}$$

$$\dot{s}_2 = -s_2(k_{21'} + k_{22'}) + s_{1'}k_{1'2} + s_{2'}k_{2'2} \tag{594}$$

$$\dot{s}_{1'} = -s_{1'}(k_{1'1} + k_{1'2}) + s_1 k_{11'} + s_2 k_{21'} \tag{595}$$

$$\dot{s}_{2'} = -s_{2'}(k_{2'1} + k_{2'2}) + s_1 k_{12'} + s_2 k_{22'} \tag{596}$$

The eight transition rates are given by the following expressions:

$$k_{12'} = (1 + R_1)^{3/2} \sigma_p v_{th}^p p \exp(-\varepsilon_{12'}/kT) \tag{597}$$

$$k_{2'1} = (1 + R_1)^{3/2} \sigma_p v_{th}^p N_V \exp(-\varepsilon_{12'}/kT) \exp(-(E_t - E_V - \varepsilon_{T2'})/kT) \tag{598}$$

$$k_{1'2} = (1 + R_{1'})^{3/2} \sigma_p v_{th}^p p \exp(-\varepsilon_{1'2}/kT) \tag{599}$$

$$k_{21'} = (1 + R_{1'})^{3/2} \sigma_p v_{th}^p N_V \exp(-\varepsilon_{1'2}/kT) \exp(-(E_t' - E_V)/kT) \tag{600}$$

$$k_{11'} = \nu_0 \exp(-(\varepsilon_{1'1} + E_t' - E_t)/kT) \tag{601}$$

$$k_{1'1} = \nu_0 \exp(-\varepsilon_{1'1}/kT) \tag{602}$$

$$k_{22'} = \nu_0 \exp(-(\varepsilon_{2'2} + \varepsilon_{T2'})/kT) \tag{603}$$

$$k_{2'2} = \nu_0 \exp(-\varepsilon_{2'2}/kT) \tag{604}$$

with:

$$\varepsilon_{12'} = \frac{(S_1 \hbar \omega_1)}{(1 + R_1)^2} + \frac{R_1}{1 + R_1}(E_V - E_t + \varepsilon_{T2'}) \tag{605}$$

$$\varepsilon_{1'2} = \frac{(S_{1'} \hbar \omega_{1'})}{(1 + R_{1'})^2} + \frac{R_{1'}}{1 + R_{1'}}(E_V - E_t') \tag{606}$$

For an insulator defect located a distance x_t from the interface:

$$\sigma_p = \sigma_{p0} \exp(-x_t/x_0) \tag{607}$$

$$E_t - E_V = E_{t0} - E_{V0} + qx_t|F| = \Delta E_t + qx_t|F| \tag{608}$$

$$E_t' - E_V = E_{t0}' - E_{V0} + qx_t|F| = \Delta E_t' + qx_t|F| \tag{609}$$

In these expressions:

- σ_{p0} is the hole-capture cross section, and $\exp(-x_t/x_0)$ accounts for the trap depth of tunneling.

- ΔE_t and $\Delta E_t'$ are the energy levels of the defect in the neutral stable state and the neutral metastable state, respectively, relative to the valence band energy in the absence of an electric field.

- F is the insulator electric field.

- v_{th}^p is the hole thermal velocity.

- ε_{ij} represent the transition energies between states.

- $\varepsilon_{T2'}$ is the energy of the positive metastable state relative to the positive stable state.

- ω_i are vibrational frequencies.

- $R_1 = \omega_1/\omega_{2'}$ and $R_{1'} = \omega_{1'}/\omega_2$.

- $S_i \hbar \omega_i$ are relaxation energies, where S_i are known as Huang–Rhys factors.

- ν_0 is the attempt frequency.

Using the eNMP Model

You can activate the eNMP model in an interface-specific `Physics` section of the command file with the keyword `eNMP`. The command syntax and options are:

```
Physics (MaterialInterface="<mat1>/<mat2>" | RegionInterface="<reg1>/reg2>") {
   eNMP (
      NumberOfSamples = <N_sample>              # Typically, 1000
      Conc = <N_0>                              # 1/cm^2, for example, 5e12
      [ SFactor="<dataset_name-or-pmi_model_name>" ]
      [ <eNMPTransitionRates_pmi_model_name> [StateCharge=<1 | -1>] ]
   )
}
```

where `Conc` represents the density of the precursor N_0. By default, the precursor concentration is constant over the interface. However, if `SFactor` is specified, the precursor concentration is obtained from a dataset (or a PMI user field that is read from the file specified with `PMIUserFields` in the `File` section of the command file), or from a space factor PMI written by users (see Space Factor on page 1190). If `SFactor` is specified without specifying `Conc`, the `SFactor` interface values are used directly. If `SFactor` is specified in addition to `Conc`, the `SFactor` values are normalized by the largest `SFactor` value and multiplied by `Conc`.

The `NumberOfSamples` keyword represents the number of random samples, N_{sample}. Sentaurus Device generates N_{sample} random defects for each interface vertex. Then, the interface charge density is obtained from the ensemble average of the charge states:

$$Q = qN_0 \langle s_2 + s_{2'} \rangle \tag{610}$$

where:

$$\langle x \rangle = \frac{1}{N_{\text{sample}}} \sum_{j=1}^{N_{\text{sample}}} x^j \tag{611}$$

During transient simulations, the state occupation changes according to the rate equations (Eq. 593 to Eq. 596), which will change the interface charge density. It is assumed that $s_1 = 1$ at the beginning, with all other states unoccupied.

eNMP Quantities Available for Plotting

Plots of the interface charge density and the density of each state can be specified in the `Plot` section of the command file:

```
Plot {
    InterfaceeNMPCharge
    InterfaceeNMPState1
    InterfaceeNMPState2
    InterfaceeNMPState1p
    InterfaceeNMPState2p
}
```

You can also obtain the plots of the capture and emission times:

```
Plot {
    eNMPCaptureTime
    eNMPEmissionTime
}
```

For this purpose, Sentaurus Device uses the first passage times given in [3]:

$$\frac{1}{\tau_{\text{cap}}} = \frac{1}{\tau_{\text{cap}}^{1'}} + \frac{1}{\tau_{\text{cap}}^{2'}} \tag{612}$$

$$\frac{1}{\tau_{\text{em}}} = \frac{1}{\tau_{\text{em}}^{1'}} + \frac{1}{\tau_{\text{em}}^{2'}} \tag{613}$$

where:

$$\frac{1}{\tau_{cap}^{1'}} = \frac{k_{11'}k_{1'2}}{k_{11'} + k_{1'2} + k_{1'1}} \qquad (614)$$

$$\frac{1}{\tau_{cap}^{2'}} = \frac{k_{12'}k_{2'2}}{k_{12'} + k_{2'2} + k_{2'1}} \qquad (615)$$

$$\frac{1}{\tau_{em}^{1'}} = \frac{k_{21'}k_{1'1}}{k_{21'} + k_{1'1} + k_{1'2}} \qquad (616)$$

$$\frac{1}{\tau_{em}^{2'}} = \frac{k_{22'}k_{2'1}}{k_{22'} + k_{2'1} + k_{2'2}} \qquad (617)$$

eNMP Model Parameters

The parameters used in the eNMP model are defined in the interface-specific `eNMP` parameter set. Table 103 to Table 106 on page 519 list the default parameter values for silicon–oxide interfaces.

Table 103   eNMP parameters that follow a Gaussian distribution: Default coefficients for silicon–oxide interfaces

Symbol	Parameter name	Mean	Standard deviation	Unit
ΔE_t	Et	-0.5	0.1	eV
$\Delta E_t'$	Etp	0.5	0.1	eV
R_1	R	0.6	0.1	1
$R_{1'}$	Rp	0.6	0.1	1
$S_1\hbar\omega_1$	ES	1.0	0.1	eV
$S_{1'}\hbar\omega_{1'}$	ESp	1.0	0.1	eV
$\varepsilon_{T2'}$	ET2p	0.5	0.1	eV
$\varepsilon_{1'1}$	E1p1	1.0	0.1	eV
$\varepsilon_{2'2}$	E2p2	0.5	0.1	eV

Table 104   eNMP parameters that follow a uniform distribution: Default coefficients for silicon–oxide interfaces

Symbol	Parameter name	Minimum Value	Maximum Value	Unit
x_t	xt	0.0	8.0	Å

Table 105   eNMP parameters that have separate values for electrons and holes: Default coefficients for silicon–oxide interfaces

Symbol	Parameter name	Electrons	Holes	Unit
σ_0	Xsec	1.0×10^{-15}	1.0×10^{-15}	cm^2
v_{th}	Vth	1.5×10^{7}	1.2×10^{7}	cm/s
x_0	x0	0.5	0.5	Å

Table 106   eNMP parameters that have a single value: Default coefficients for silicon–oxide interfaces

Symbol	Parameter name	Value	Unit
v_0	nu0	1.0×10^{13}	s^{-1}

eNMP Transition Rates PMI Model

An eNMP transition rates PMI model (see eNMP Transition Rates on page 1207) created by users can be utilized to calculate the transition rates for the eNMP model. This PMI allows for the possibility of either a positive or negative state charge, and provides additional dependencies that are not included in the built-in eNMP model.

Hot-Carrier Stress Degradation Model

The hot-carrier stress (HCS) degradation model is based on work in [15], and can be used as a general degradation model for MOS-based devices.

The HCS degradation model includes different mechanisms that contribute to bond breakage and the formation of interface traps [11][16][17]:

- Single-particle (SP) processes, where a single particle is responsible for bond breakage
- Multiple-particle (MP) processes, where the combined actions of several particles contribute to bond breakage
- Field-enhanced thermal (TH) processes, where thermal interactions with the lattice contribute to bond breakage

Sentaurus Device includes both an electron version of the model (eHCSDegradation) and a hole version of the model (hHCSDegradation).

The model and its usage are described in the following sections.

Model Description

The model equations are presented here. Details can be found in [15]. The equations presented apply to both the eHCSDegradation and hHCSDegradation models.

Single-Particle and Multiple-Particle Interface-Trap Densities

For the SP case, the interface trap density as a function of time and activation energy is given by

$$N_{it,SP}(\boldsymbol{r}, t, E_{SP}) = P_{SP}N_0[1 - e^{-k_{SP}(\boldsymbol{r}, E_{SP})t}] \tag{618}$$

where:

- P_{SP} is the probability for defect generation by SP processes.
- N_0 is the maximum number of interface bonds.
- E_{SP} is the activation energy for SP processes.
- $k_{SP}(\boldsymbol{r}, E_{SP})$ is the reaction rate for SP processes.

For the MP case, the interface trap density is given by:

$$N_{it,MP}(\boldsymbol{r}, t, E_{MP}) = P_{MP}N_0\left[\frac{P_{emi}}{P_{pass}}\left(\frac{P_u}{P_d}\right)^{N_1}(1 - e^{-P_{emi}t})\right]^{1/2} \tag{619}$$

where:

- P_{MP} is the probability for defect generation by MP processes.
- N_1 is the number of energy levels in the oscillator that models the bond.

The emission and passivation probabilities P_{emi} and P_{pass} are modeled as Arrhenius laws:

$$P_{emi} = \nu_{emi}e^{-E_{emi}/(k_B T)} \tag{620}$$

$$P_{pass} = \nu_{pass}e^{-E_{pass}/(k_B T)} \tag{621}$$

where:

- ν_{emi} and ν_{pass} are the emission and passivation frequencies, respectively.
- E_{emi} and E_{pass} are the emission and passivation energies, respectively.

The oscillator excitation and de-excitation probability rates are given by:

$$P_u = k_{ph}e^{-E_{ph}/(k_B T)} + k_{MP}(r, E_{MP}) \tag{622}$$

$$P_d = k_{ph} + k_{MP}(r, E_{MP}) \tag{623}$$

where:

- E_{ph} and k_{ph} are the phonon energy and the reaction rate, respectively.
- E_{MP} is the activation energy for MP processes.
- $k_{MP}(r, E_{MP})$ is the reaction rate for MP processes.

The reaction rates for SP and MP processes are given by scattering-rate integrals:

$$k_{SP}(r, E_{SP}) = \int_{E_{SP}}^{\infty} f(r, E)g(E)v(E)\sigma_{SP}(E)dE \tag{624}$$

$$k_{MP}(r, E_{MP}) = \int_{E_{MP}}^{\infty} f(r, E)g(E)v(E)\sigma_{MP}(E)dE \tag{625}$$

where:

- $f(r, E)$ is the carrier distribution function.
- $g(E)$ is the total density-of-states.
- $v(E)$ is the magnitude of the carrier velocity.
- $\sigma_{SP}(E)$ and $\sigma_{MP}(E)$ are the SP and MP reaction cross-sections.

The reaction cross-sections are given by:

$$\sigma_{SP}(E) = \sigma_{SP0}\left(\frac{E - E_{SP}}{k_B T}\right)^{p_{SP}} \tag{626}$$

$$\sigma_{MP}(E) = \sigma_{MP0}\left(\frac{E - E_{MP}}{k_B T}\right)^{p_{MP}} \tag{627}$$

where:

- p_{SP} and p_{MP} are exponents characterizing the SP and MP processes.
- σ_{SP0} and σ_{MP0} are fitting parameters.

Field-Enhanced Thermal Degradation

The interface-trap density due to field-enhanced thermal degradation is given by:

$$N_{it,TH}(\boldsymbol{r}, t, E_{TH}) = P_{TH} N_0 [1 - e^{-k_{TH}(E_{TH})t}] \tag{628}$$

where:

- P_{TH} is the probability for defect generation by thermal processes.
- The reaction rate for bond breakage k_{TH} is given by:

$$k_{TH}(\boldsymbol{r}, E_{TH}) = \nu_{TH} e^{-E_{TH}/(k_B T)} \tag{629}$$

$$E_{TH} = E_{TH0} - p E_{ox} \tag{630}$$

where:

- ν_{TH} is the lattice collision frequency.
- E_{TH0} is the activation energy for thermal processes in the absence of oxide field E_{ox}.
- p is the effective dipole moment.

Carrier Distribution Function

There are two options for obtaining the carrier distribution function $f(\boldsymbol{r}, E)$ used in the calculation of the scattering-rate integrals (Eq. 624 and Eq. 625):

- From the spherical harmonics expansion (SHE) method
- From an approximate analytic formulation

Spherical Harmonics Expansion Option

The SHE method computes the microscopic carrier-energy distribution function by solving the lowest-order SHE of the Boltzmann transport equation. When the carrier distribution function is available through the SHE method, it can optionally be used directly in the evaluation of Eq. 624 and Eq. 625. In this case, the band structure quantities $g(E)$ and $v(E)$ used in these equations are the same as those used in the SHE calculations.

NOTE   If the carrier distribution function is available through the SHE method, the SHE temperature will be used instead of the carrier temperature in the model equations, if the hydrodynamic model is not used.

Approximate Analytic Option

A method for obtaining an approximate carrier distribution function [15] is available. In this case, $f(\boldsymbol{r}, E)$ is modeled using an analytic non-Maxwellian formulation:

$$f_0(\boldsymbol{r}, E) = \frac{1}{A(\boldsymbol{r})} \exp\left[-\alpha(\boldsymbol{r})\frac{\gamma(E)}{k_{\mathrm{B}} T_c(\boldsymbol{r})}\right] \qquad (631)$$

$$\gamma(E) = \frac{E(1 + \delta E)}{1 + \beta E} \qquad (632)$$

where:

- $T_c(\boldsymbol{r})$ is the carrier temperature (T_n for `eHCSDegradation` and T_p for `hHCSDegradation`).
- δ and β are fitting parameters.
- $A(\boldsymbol{r})$ and $\alpha(\boldsymbol{r})$ are position-dependent parametric factors that are determined by requiring that:

$$c(\boldsymbol{r}) = \int_0^{E_{\max}} f_0(\boldsymbol{r}, E) g(E) dE \qquad (633)$$

$$T_c(\boldsymbol{r}) = \frac{2}{3 k_{\mathrm{B}}} \frac{\int_0^{E_{\max}} E(f_0(\boldsymbol{r}, E) g(E) dE)}{c(\boldsymbol{r})} \qquad (634)$$

where $c(\boldsymbol{r})$ is the electron concentration for `eHCSDegradation` and the hole concentration for `hHCSDegradation`. $E_{\max} = 10 \text{ eV}$ is used as the upper integration limit.

Bond Dispersion

The reaction rates given by Eq. 624, Eq. 625, and Eq. 629 are for a discrete activation energy. As an option, these rates can be modified to account for bond dispersion by assuming a distribution function for the activation energies:

$$g_{\mathrm{A},j}(E) = \frac{1}{\sigma_g} \frac{\exp\left(\frac{E_j - E}{\sigma_g}\right)}{\left[1 + \exp\left(\frac{E_j - E}{\sigma_g}\right)\right]^2} \qquad (635)$$

where σ_g is a dispersion width and $j = SP$, MP, or TH. As an alternative to calculating the scattering-rate integrals for every activation energy, the reaction rates are approximated at energies close to their peak values with the following expressions:

$$k_{SP}(\boldsymbol{r}, E) = k_{SP}(\boldsymbol{r}, E_{SP})e^{-(E - E_{SP})/(\lambda k_B T_c)} \tag{636}$$

$$k_{MP}(\boldsymbol{r}, E) = k_{MP}(\boldsymbol{r}, E_{MP})e^{-(E - E_{MP})/(\lambda k_B T_c)} \tag{637}$$

$$k_{TH}(\boldsymbol{r}, E) = k_{TH}(\boldsymbol{r}, E_{TH})e^{-(E - E_{TH})/(k_B T)} \tag{638}$$

Then, the interface-trap generation rates for each process will be calculated from:

$$N_{it,j}(\boldsymbol{r}, t) = \int_{E_j - m\sigma_g}^{E_j + m\sigma_g} g_{A,j}(E)N_{it,j}(\boldsymbol{r}, t, E)dE \tag{639}$$

Finally, the total interface-trap generation rate is taken as the sum of the separate processes:

$$N_{it}(\boldsymbol{r}, t) = N_{it,SP}(\boldsymbol{r}, t) + N_{it,MP}(\boldsymbol{r}, t) + N_{it,TH}(\boldsymbol{r}, t) \tag{640}$$

Using the HCS Degradation Model

You can include the HCS degradation model in a transient simulation by specifying the `eHCSDegradation` option, or the `hHCSDegradation` option, or both options as part of a `Traps` specification for the interface of interest. The syntax and options for these models are:

```
Physics (MaterialInterface = "Silicon/Oxide") {
   Traps (
      (eHCSDegradation( [SHE] [BondDispersion])

      # Specify appropriate parameters for the generated traps.
      Acceptor Level EnergyMid=0 fromMidBandGap
      )

      (hHCSDegradation( [SHE] [BondDispersion])

      # Specify appropriate parameters for the generated traps.
      Donor Level EnergyMid=0 fromMidBandGap
      )
   )
}
```

Notes regarding this specification:

- If the `SHE` option is selected, the distribution function and the band-structure quantities are obtained from the SHE method specified in the `Physics` section, for example:

  ```
  Physics (Material = "Silicon") {
      eSHEDistribution(FullBand)
  }
  ```

- If `SHE` is not selected, an approximate distribution function is used as described in . In this case, the band-structure quantities used in the calculations will be taken from the SHE full-band structure files.

- `BondDispersion` is used by default. Use `-BondDispersion` to switch off this option.

- If using `FixedCharge` traps, negative charge will be created with the `eHCSDegradation` model, and positive charge will be created with the `hHCSDegradation` model.

Parameters used in the model can be accessed through the `HCSDegradation` parameter set in the parameter file. Since this model describes interface trap generation, these parameters will only be recognized if they are part of a `MaterialInterface` or `RegionInterface` specification. Table 107 lists the default parameter values for silicon–oxide interfaces.

Table 107 HCS degradation model: Default coefficients for silicon–oxide interfaces

Symbol	Parameter name	Electrons	Holes	Unit
P_{SP}	Prsp	1.0	1.0	1
P_{MP}	Prmp	1.0	1.0	1
P_{TH}	Prth	1.0	1.0	1
N_0	N0	1.0×10^{12}	1.0×10^{12}	cm^{-2}
k_{ph}	kph	1.0×10^{8}	1.0×10^{8}	s^{-1}
E_{ph}	Eph	0.25	0.25	eV
E_{emi}	Eemi	0.26	0.26	eV
E_{pass}	Epass	0.2	0.2	eV
E_{TH0}	Eth0	1.9	1.9	eV
N_l	Nlev	10	10	1
ν_{emi}	nu_emi	1.0×10^{12}	1.0×10^{12}	s^{-1}
ν_{pass}	nu_pass	1.0×10^{12}	1.0×10^{12}	s^{-1}
ν_{th}	nu_th	1.0×10^{13}	1.0×10^{13}	s^{-1}
p	p	15.5	15.5	eÅ
E_{SP}	Esp	3.1	3.1	eV

Table 107 HCS degradation model: Default coefficients for silicon–oxide interfaces

Symbol	Parameter name	Electrons	Holes	Unit
E_{MP}	Emp	0.25	0.25	eV
p_{SP}	psp	11	11	1
p_{MP}	pmp	0.1	0.1	1
σ_{SP0}	Xsecsp	3.0×10^{-29}	3.0×10^{-29}	cm^2
σ_{MP0}	Xsecmp	1.0×10^{-24}	1.0×10^{-24}	cm^2
σ_g	sigmag	0.100	0.100	eV
λ	lambda	0.17	0.17	1
m	m	3	3	1
δ	delta	1.0	1.0	eV^{-1}
β	beta	0.15	0.15	eV^{-1}

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CHAPTER 20   Organic Devices

This chapter describes the organic models available in Sentaurus Device.

The electrical conduction process in organic materials is different from crystal lattice semiconductors. However, similar concepts in semiconductor transport theory can be used in treating the conduction process in organic materials.

Introduction to Organic Device Simulation

An organic material or semiconductor is formed from molecule chains, and the primary transport of carriers (electrons and holes) is through a *hopping* process. The lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO) energy levels in organic materials are analogous to the conduction and valence bands, respectively. In addition, excitons need to be considered since these bound electron–hole pairs contribute to the distribution of electron and hole populations. Traps are also central to organic transport, and these need to be taken into account appropriately.

Therefore, a combination of semiconductor models and organic physics models is required to model reasonably the physical transport processes of organic devices within the framework of Sentaurus Device. The models needed in a typical organic device simulation are:

- The Poole–Frenkel mobility model is used to model the hopping transport of the carriers (electrons and holes). This model is dependent on electric field and temperature. Note that it is common for electrons to have two orders of magnitude higher mobility than holes (see Poole–Frenkel Mobility (Organic Material Mobility) on page 382).

- Organic–organic heterointerface physics requires special treatment for the ballistic transport of carriers and bulk excitons across heterointerfaces with energy barriers (see Gaussian Transport Across Organic Heterointerfaces on page 766).

- Gaussian density-of-states (DOS) approximates the effective DOS for electrons and holes in disordered organic materials and semiconductors (see Gaussian Density-of-States for Organic Semiconductors on page 264).

- The traps model must be initialized with the appropriate capture cross sections and densities (see Chapter 17 on page 449).

- The Langevin bimolecular recombination model is used to model the recombination process of carriers and the generation process of singlet excitons (see Bimolecular Recombination on page 444).

■ A singlet exciton equation is introduced to model the diffusion process, the generation from bimolecular recombination, the loss from decay, and the optical emissions of singlet excitons. Note that only Frenkel excitons (electron–hole pairs existing on the same molecule) participate in the optical process in organic materials (see Singlet Exciton Equation on page 235).

The organic device simulator is based on the work of Kozłowski [1], and other useful papers are available [2]–[10].

Many acronyms are used to describe organic device layers and transport mechanisms (see Table 108).

Table 108   Commonly used acronyms for organic transport

Acronym	Definition
EBL	Electron blocking layer
EML	Emission layer
ETL	Electron transport layer
HOMO	Highest occupied molecular orbital
HTL	Hole transport layer
LUMO	Lowest unoccupied molecular orbital
SCL	Space charge limited
TCL	Trapped charge limited
TSL	Thermally stimulated luminescence

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CHAPTER 21   Optical Generation

> *This chapter describes various methods that are used to compute the optical generation rate when an optical wave penetrates into the device, is absorbed, and produces electron–hole pairs.*

The methods include simple optical beam absorption, the raytracing method, the transfer matrix method, the finite-difference time-domain, the beam propagation method, and loading external profiles from file. Different types of refractive index and absorption models, parameter ramping, and optical AC analysis are also described.

Overview

A unified interface for optical generation computation is available to provide a consistent simulation setup irrespective of the underlying optical solver methods. This allows for a gradual refinement of results and a balance of accuracy versus computation time in the course of a simulation, while only the solver-specific parameters have to change. Several approaches for computing the optical generation exist that are independent of the chosen optical solver:

- Compute the optical generation resulting from a monochromatic optical source.
- Compute the optical generation resulting from an illumination spectrum.
- Set a constant value for the optical generation rate either per region or globally.
- Read an optical generation profile from file.
- Compute the optical generation as a sum of the above contributions, possibly with different optical solvers or different solver-specific settings or excitation parameters.

For each of the contributions listed, a separate scaling factor can be specified. For transient simulations, it is possible to apply a time-dependent scaling factor that can be used, for example, to model the response to a light pulse or any other time-dependent light signal. This feature can also be used to improve convergence if the optical generation rate is very high. The unified interface also allows you to save the computed optical generation rate to a file for reuse in other simulations.

The optical generation resulting from a monochromatic optical source or an illumination spectrum is determined as the product of the absorbed photon density, which is computed by the optical solver, and the quantum yield. Several models for the quantum yield are available ranging from a constant scaling factor to a spatially varying quantum yield based on the band gap of the underlying material and the excitation wavelength of the optical source.

In the following sections, the different approaches for computing the optical generation and their corresponding parameters are described.

Specifying the Type of Optical Generation Computation

In the `OpticalGeneration` section of the command file, at least one of the following methods to compute the optical generation must be specified; otherwise, the optical generation is not computed and is set to zero everywhere:

- `ComputeFromMonochromaticSource` activates optical generation computation with a single wavelength that is either specified in the `Excitation` section or as a ramping variable.

- `ComputeFromSpectrum` allows the sum of optical generation to be computed from an input spectrum of wavelengths.

- `ReadFromFile` imports the optical generation profile.

- `SetConstant` enables you to set a background constant optical generation in the specified region or material.

> **NOTE** If the keyword `Scaling` is used in the above optical generation methods, the scaling applies only to quasistationary simulations. To scale transient simulations, see Specifying Time Dependency for Transient Simulations on page 547.

If several methods are specified, the total optical generation rate is given by the sum of the contributions computed with each method. The general syntax is:

```
Physics {
   ...
   Optics (
      OpticalGeneration (
         ...
         ComputeFromMonochromaticSource (...)
         ComputeFromSpectrum (...)
         ReadFromFile (...)
         SetConstant ( ... Value = <float> )
      )
      Excitation (...)
      OpticalSolver (...)
      ComplexRefractiveIndex (...)
   )
}
```

Each method can have its own options such as a scaling factor or a particular time-dependency specification used in transient simulations. An example setup where the optical generation read

from a file is scaled by a factor of 1.1 and a Gaussian time dependency is assumed for the monochromatic source is:

```
OpticalGeneration (
   ...
   ComputeFromMonochromaticSource (
      ...
      TimeDependence (
         WaveTime = (<t1>, <t2>)
         WaveTSigma = <float>
      )
   )
   ReadFromFile (
      ...
      Scaling = 1.1
   )
)
```

Note that both `Scaling` and `TimeDependence` can also be specified directly in the `OpticalGeneration` section if the same parameters will apply to all methods. If `TimeDependence` is specified directly in the `OpticalGeneration` section as well as in a source-specific section such as `ComputeFromMonochromaticSource`, the latter takes precedence. For an overview of all available options, see Table 247 on page 1443.

By default, the optical generation rate is calculated for every semiconductor region. However, you can suppress the computation of the optical generation rate for a specific region or material by specifying the keyword `-OpticalGeneration` in the corresponding region or material `Physics` section:

```
Physics ( region="coating" ) { Optics ( -OpticalGeneration ) }

Physics ( material="InP" ) { Optics ( -OpticalGeneration ) }
```

To visualize the optical intensity and generation, the keywords `OpticalIntensity` and `OpticalGeneration` must be added to the `Plot` section:

```
Plot {
   ...
   OpticalIntensity
   OpticalGeneration
}
```

Specifying `OpticalGeneration` in the `Plot` section plots not only the total optical generation that enters the electrical equations, but also the contributions from the different methods of optical generation computation. See Appendix F on page 1339 for the corresponding data names.

Optical Generation From Monochromatic Source

Specifying `ComputeFromMonochromaticSource (...)` in the `OpticalGeneration` section activates the computation of the optical generation assuming a monochromatic light source. Details of the light source such as angle of incidence, wavelength, and intensity, and the optical solver used to model it must be set in the `Excitation` section and `OpticalSolver` section, respectively (see Specifying the Optical Solver on page 554 and Setting the Excitation Parameters on page 560).

Together with the possibility of ramping parameters (see Controlling Computation of Optical Problem in Solve Section on page 572), for example, the wavelength of the incident light, this model can be used to simulate the optical generation rate as a function of wavelength.

Illumination Spectrum

The optical generation resulting from a spectral illumination source, which is sometimes also known as *white light generation*, can be modeled in Sentaurus Device by superimposing the spectrally resolved generation rates. To this end, `ComputeFromSpectrum (...)` must be listed in the `OpticalGeneration` section. The illumination spectrum is then read from a text file whose name must be specified in the `File` section:

```
File {
    ...
    IlluminationSpectrum = "illumination_spectrum.txt"
}
Physics {
    ...
    Optics (
        ...
        OpticalGeneration (
            ...
            ComputeFromSpectrum ( ... )
        )
    )
}
```

In its simplest form, the illumination spectrum file has a two-column format. The first column contains the wavelength in μm and the second column contains the intensity in W/cm^2. The characters # and * mark the beginning of a comment.

As a default, the integrated generation rate resulting from the illumination spectrum is only computed once, that is, the first time the optical problem is solved and remains constant

thereafter. However, it is possible to force its recomputation on every occasion by specifying the keyword `RefreshEveryTime` in the `ComputeFromSpectrum` section.

When the optical problem remains constant, that is, the absorbed photon density does not change, but the quantum yield is expected to vary (see Quantum Yield Models on page 544), specify the keyword `KeepSpectralData` in the `ComputeFromSpectrum` section. With this keyword, the spectral information of the last optical solution is kept in memory and only the quantum yield, which is needed to compute the optical generation rate and the optical absorption heat (see Optical Absorption Heat on page 545), is updated during the simulation.

Plotting spectral results requires the specification of a file name in the `File` section using the keyword `SpectralPlot` as well as the specification of the keyword `KeepSpectralData` in the `ComputeFromSpectrum` section. A file with extension `.tdr` is used to save spatial fields such as optical generation for each entry of the spectrum. Other results from the optical solver, for example, reflection, transmission, and absorption in the case of the TMM solver, as a function of the spectrum parameters are saved in a file with the extension `.plt`. The quantities saved in the `.plt` file are subject to the optical solver used in the simulation. To control the file name and when to plot, the same syntax in the `Solve` section applies to `SpectralPlot` as well as to `Plot`. See When to Plot on page 123 and Appendix G on page 1377.

In simulations that contain only a monochromatic source, the results from the optical solver are written to the current file. However, if a spectral source is present, the values should reflect the result of both the monochromatic source and the spectral source. Therefore, relative quantities (that is, unitless quantities) such as reflection are represented by a weighted average over all entries of the illumination spectrum and the monochromatic source if present. The weight is given by the corresponding number of incident photons. On the other hand, absolute quantities are represented by a simple sum over all spectral entries and the monochromatic source if present.

> **NOTE** The default for saving spectral plots is to write consecutive plots into one file. However, to write consecutive plots into several enumerated files, specify `SpectralPlot(-collected)=<string>`.

Multidimensional Illumination Spectra

Often, illumination spectra depend on additional parameters, which may be related to an experimental setup that users want to model. For example, the intensity of the incident light may depend on not only the wavelength but also the angle of incidence. To account for such simulation setups, Sentaurus Device supports multidimensional illumination spectra. The format of a corresponding illumination spectrum file is:

```
# some comment
* another comment # and so on
Optics/Excitation/Wavelength [um] theta [deg] phi [deg] intensity [W*cm^-2]
0.62 0 30 0.1
```

```
0.86 0 30 0.2
1.1 0 30 0.3
```

The header contains optional comment lines and a line defining the parameters assigned to each column. A parameter name or path is followed by its corresponding unit; if no unit is specified, the default unit of 1 is assumed. Listed parameters can refer either directly to existing parameters of the `Optics` section in Sentaurus Device or to user-defined parameters. The latter comes into play when using illumination spectra in combination with loading absorbed photon density or optical generation profiles from file. See Loading Solution of Optical Problem From File on page 640 for details.

> **NOTE** The parameter `Intensity` is mandatory in every illumination spectrum file. However, the order of columns is arbitrary. Parameter names are case insensitive.

For multidimensional illumination spectrum files, the active columns must be selected in the command file. All other columns are ignored in the simulation. The required syntax in the `OpticalGeneration` section is:

```
ComputeFromSpectrum (
   ...
   Select (
      Parameter = ("Optics/Excitation/Wavelength" "Theta")
   )
)
```

The parameter `Intensity` is selected by default and does not need to be specified.

Enhanced Spectrum Control

Being able to filter a given spectrum, based on a user-supplied condition, adds functionality to the computation of the optical generation resulting from a spectral illumination source. Specifying a static condition can be used to select a limited spectral range of interest or a subset of a multidimensional spectrum. The latter improves the handling of several spectra (for example, different standard spectra at various resolutions, and measured spectra) since they can be compiled in a single file and still be addressed separately.

A condition is called *dynamic* if it changes during the simulation. For example, a dynamic condition may include the excitation wavelength, which is ramped in a `Quasistationary` statement. Dynamic conditions can be used to ramp through different spectra or to superimpose a fixed spectrum with a varying spectrum.

To specify a condition, a Tcl-compatible expression enclosed in double quotation marks must be provided in the `Select` section:

```
ComputeFromSpectrum (
   ...
   Select (
      Parameter = ("Wavelength" "Theta")
      Condition = "$wavelength > 0.3 && $wavelength < 1.2"
   )
)
```

Identifiers preceded by a dollar sign (`$`) such as `wavelength` in the above example are considered to be variables referring to the respective column in the illumination spectrum file. Sentaurus Device extracts a subset of the spectrum by applying the condition expression to each row of the spectrum defined in the file. Before the expression is passed to the global Tcl interpreter of Sentaurus Device for evaluation, variables are substituted with their corresponding row-specific values. If the expression evaluates to true, the row is considered to be an active entry of the spectrum used in the `ComputeFromSpectrum` computation; otherwise, it is ignored.

> **NOTE** By default, duplicate entries of the spectrum are ignored. However, specifying the keyword `AllowDuplicates` in the `Select` section will retain such entries.

> **NOTE** Identifiers such as Sentaurus Device parameter names and variable names referring to the respective column in the illumination spectrum file are treated as case insensitive in the `Parameter` list and the `Condition` statement of the `Select` section.

Assuming a spectrum file containing different spectra distinguished by their names of the form:

```
wavelength [um] intensity [W*cm^-2] spectrum [1]
0.2 0.0012 "AM1.5g"
0.3 0.0034 "AM1.5g"
...
0.2 0.0056 "AM0"
...
```

a single spectrum can be selected by specifying the following in the `ComputeFromSpectrum` section:

```
Select (
   Parameter = ("Wavelength" "Spectrum")
   Condition = "$Spectrum == \"AM1.5g\" "
)
```

> **NOTE** Double quotation marks in the Tcl expression must be escaped to avoid
> conflicts with the parser of the Sentaurus Device command file.

For a condition to change during the simulation, it must reference an internal variable of
Sentaurus Device that is ramped in a `Quasistationary` statement. Sentaurus Device
interprets identifiers without a preceding $ in the condition expression as internal parameters.
If necessary due to ambiguity, internal parameters also may be specified using their full path
such as `Optics/Excitation/Wavelength`. Specifying an identifier that cannot be matched
with an internal parameter results in an error.

To select a subspectrum based on a dynamic condition, assume the following spectrum file:

```
wavelength [um] intensity [W*cm^-2] centralWavelength [nm]
0.2 0.0012 300
0.3 0.0034 300
...
0.3 0.0056 400
0.4 0.0068 400
...
```

The following command file syntax shows how to ramp through the various spectra identified
by their central wavelength:

```
Physics {
  Optics (
    OpticalGeneration (
      ComputeFromSpectrum (
        Select (
          Parameter = ("Wavelength" "centralWavelength")
          Condition = "abs( Wavelength - $centralWavelength*1e-3 ) < 1e-6"
        )
      )
    )
  )
}

Solve {
  Quasistationary (
    Goal { modelParameter = "Wavelength" value = 1.2 }
  ) { Coupled {Poisson Electron Hole} }
}
```

> **NOTE** In the condition expression, it is the responsibility of the user to rescale
> the spectrum variables if necessary when comparing them to internal
> parameters having a fixed unit. Despite the fact that the units of the
> spectrum variables are known to Sentaurus Device, it is unclear whether
> they are related to internal parameters as the names of spectrum
> variables are arbitrary.

> **NOTE** When comparing floating-point numbers for equality in a condition expression, it is recommended that you check that the absolute value of their difference is smaller than a user-specified epsilon as shown in the examples. This avoids any unexpected precision issues resulting from numeric operations or reading floating-point numbers from file.

For more flexibility, the `Select` section contains an auxiliary keyword `Var`, which holds a floating-point value. It has no impact on the optical generation computation as such, but it can be ramped in a `Quasistationary` statement like any other internal parameter that supports ramping. Therefore, the keyword `Var` allows you to create dynamic conditions without affecting the results of any other optical generation contributions defined in the `OpticalGeneration` section such as `ComputeFromMonochromaticSource`. This is demonstrated by the following syntax, which is based on the above example where Sentaurus Device ramps through various spectra, but it contains a fixed monochromatic source:

```
Physics {
   Optics (
      Excitation (
         Wavelength = 0.6
      )
      OpticalSolver ( ... )
      OpticalGeneration (
         ComputeFromMonochromaticSource ( ... )
         ComputeFromSpectrum (
            Select (
               Parameter = ("Wavelength" "centralWavelength")
               Condition = "abs( Var - $centralWavelength*1e-3 ) < 1e-6"
            )
         )
      )
   )
}

Solve {
   Quasistationary (
      Goal { modelParameter = "Var" value = 1.2 }
   ) { Coupled {Poisson Electron Hole} }
}
```

The keyword `Var` can be plotted by specifying `ModelParameter="Physics/Optics/ OpticalGeneration/ComputeFromSpectrum/Select/Var"` in the `CurrentPlot` section of the command file.

Loading and Saving Optical Generation From and to File

Sometimes, solving the optical problem may require long computation times, in which case, it can be useful to save the solution to a file and to load the optical generation or absorbed photon density profile in later simulations whose optical properties remain constant. In the following example, optical generation is used as a synonym for absorbed photon density. The command file syntax for saving the optical generation rate to a file is:

```
File {
   OpticalGenerationOutput = <filename>
}
```

For loading the optical generation rate from a file, the syntax is:

```
File {
   OpticalGenerationInput = <filename>
}

Physics {
   Optics (
      OpticalGeneration (
         ReadFromFile (
            DatasetName = AbsorbedPhotonDensity | OpticalGeneration
         )
      )
   )
}
```

If the input file to be loaded contains both an optical generation and an absorbed photon density profile, the keyword `DatasetName` controls which one to use. By default, the absorbed photon density is used. The optical generation profile to be loaded also may be defined on a mixed-element grid that is different from the one used in the device simulation, or on a tensor grid resulting from an EMW simulation. In that case, the profile is interpolated automatically onto the simulation grid upon loading. For more details on how to control the interpolation, including the truncation and shifting of the interpolation domain, see Controlling Interpolation When Loading Optical Generation Profiles on page 659.

Further options of the `ReadFromFile` section can be found in Table 247 on page 1443. Similar but more powerful functionality is provided by the feature `FromFile` (see Loading Solution of Optical Problem From File on page 640).

Constant Optical Generation

Assigning a constant optical generation rate to a certain region or material is achieved by specifying a value for a particular region or material as shown here:

```
Physics (Region = <name of region>) {
   ...
   Optics (
      OpticalGeneration (
         SetConstant (
            Value = <float>
         )
      )
   )
}

Physics (Material = <name of material>) {
   ...
   Optics (
      OpticalGeneration (
         SetConstant (
            Value = <float>
         )
      )
   )
}
```

If all semiconductor regions are supposed to have the same optical generation rate, its value is best specified in the global `Physics` section as follows:

```
Physics {
   ...
   Optics (
      OpticalGeneration (
         SetConstant (
            Value = <float>
         )
      )
   )
}
```

NOTE   The constant optical generation model is functionally equivalent to the constant carrier generation model presented in Constant Carrier Generation on page 412.

Quantum Yield Models

The quantum yield model describes how many of the absorbed photons are converted to generated electron–hole pairs. The simplest model, `QuantumYield(Unity)`, assumes that all absorbed photons result in generated charge carriers irrespective of the band gap or other properties of the underlying material. This corresponds to a global quantum yield factor of one, which is the default value, except for nonsemiconductor regions where it is always set to zero even if photons are actually absorbed.

A more realistic model, `QuantumYield(Stepfunction(...))`, takes the band gap into account. If the excitation energy is greater than or equal to the bandgap energy E_g, the quantum yield is set to one; otherwise, it is set to zero. The bandgap energy used can be set directly by specifying a value for `Energy` in eV or, alternatively, a corresponding `Wavelength` in micrometers. Another option is `Bandgap`, which uses the temperature-dependent bandgap energy as given in Bandgap and Electron-Affinity Models on page 250 (Eq. 159, p. 250). To include bandgap narrowing effects in the form of Eq. 164, p. 251, the keyword `EffectiveBandgap` must be specified.

In the presence of free carrier absorption (FCA), which is activated in Sentaurus Device by specifying `CarrierDep(Imag)` in the `ComplexRefractiveIndex` section of the command file, the spatially varying quantum yield factor is reduced according to the ratio of free carrier absorption, α_{FCA}, to total absorption, α_{tot}:

$$\eta_G = \eta_{G_\Theta}\left(1 - \frac{\alpha_{FCA}}{\alpha_{tot}}\right) \tag{641}$$

where α_{FCA} and α_{tot} are determined by the `ComplexRefractiveIndex` specification in the parameter file, given the following relation between the absorption coefficient and the extinction coefficient:

$$\alpha = \frac{4\pi k}{\lambda} \tag{642}$$

The change of the extinction coefficient due to free carrier absorption is represented by Δk_{carr} (see Carrier Dependency on page 580). The prefactor η_{G_Θ} can be set to 1 by specifying the keyword `EffectiveAbsorption` in the `QuantumYield` section, or it can represent a step function: If the photon energy is sufficiently large to allow for interband optical absorption, it is 1, or otherwise 0. The latter requires the specification of a `Stepfunction` section, which takes precedence over `EffectiveAbsorption` if both are specified.

The command file syntax for specifying quantum yield models is:

```
Physics {
   Optics (
      OpticalGeneration (
         ...
         QuantumYield = <float>
         QuantumYield ( Unity )
         QuantumYield (
            EffectiveAbsorption
            StepFunction ( Wavelength = <float> #[um]
                           # OR
                           Energy = <float>      #[eV]
            )
            StepFunction ( Bandgap | EffectiveBandgap )
         )
      )
   )
}
```

For more sophisticated quantum yield models, Sentaurus Device offers a PMI interface (see). All quantum yield models also can be specified in a region or material `Physics` section. The resulting quantum yield can be plotted by specifying `QuantumYield` in the `Plot` section.

> **NOTE** By default, the optical absorption due to `ComputeFromSpectrum` is computed only once; any further changes in the quantum yield are neglected. To account for varying quantum yield, it is necessary to recompute the corresponding optical absorption using `RefreshEveryTime` in the `ComputeFromSpectrum` section. However, this will impact simulator performance depending on the size of the spectrum and the chosen optical solver.

Optical Absorption Heat

The absorbed photon energy E_{ph} is distributed among different processes by quantum yield factors. The following two channels are accounted for:

- Thermalization to the band gap (interband absorption): When a photon is absorbed across the band gap in a semiconductor, it is absorbed to create an electron–hole pair. The excess energy (photon energy minus the band gap) of the new electron–hole pair is assumed to thermalize, resulting eventually in lattice heating.

- Complete thermalization (intraband absorption): In the case of the photon energy being smaller than the band gap, the photon can be absorbed to increase the energy of a carrier. The excess energy relaxes eventually, contributing to lattice heating.

In both processes, it is assumed that the eventual lattice heating occurs in the locality of photon absorption. The corresponding energy equation reads as:

$$E_{ph} = \eta_{T_{Eg}}(E_{ph} - E_g) + \eta_G E_g + \eta_{T_0} E_{ph} \qquad (643)$$

where the energy contributions of the first term and the third term are dissipated into the lattice through thermalization. The energy of the second term is consumed for the generation of an electron–hole pair.

In general, $\eta_{T_{Eg}} = \eta_G$ since it is assumed that every photon generates a charge carrier, while the residual energy $E_{ph} - E_g$ is dissipated into the lattice. Therefore, ignoring free carrier absorption, if the chosen quantum yield model evaluates to 1, $\eta_{T_{Eg}} = \eta_G = 1$ and $\eta_{T_0} = 0$. If the quantum yield model evaluates to 0, $\eta_{T_{Eg}} = \eta_G = 0$ and $\eta_{T_0} = 1$.

Distinguishing between $\eta_{T_{Eg}}$ and η_G allows for the control of multiple-generation processes as well. For example, in the UV spectrum, it is possible that $E_{ph} > 2E_g$, and so more than one charge carrier can be generated per absorbed photon. To model multiple-generation processes, the `OpticalQuantumYield` PMI (see Optical Quantum Yield on page 1183) must be used where all quantum yield factors can be specified independently for each vertex.

Supporting several optical absorption processes affects the value of η_G as can be seen from Eq. 643. It no longer depends on the local effective bandgap energy only. Factoring in free carrier absorption means that photons absorbed through this process do not contribute to the optical generation rate, which is used in the drift-diffusion equations. In general, the quantum yield factors are independent as long as the energy equation is fulfilled locally.

The quantum yield factor η_G is given by Eq. 641, and the quantum yield factor attributed to complete thermalization is computed as:

$$\eta_{T_0} = 1 - \eta_G \qquad (644)$$

The quantum yield factor $\eta_{T_{Eg}}$ is set to η_G unless it is specified explicitly using the `OpticalQuantumYield` PMI.

> **NOTE** If η_G is set to a constant value in the command file, η_{T_0} is still given by Eq. 644 to ensure energy balance.

Specifying `OpticalAbsorptionHeat` and `ThermalizationYield` in the `Plot` section of the command file results in the following quantities being written to the plot file for each vertex:

- `OpticalAbsorptionHeat`: $(\eta_{T_{Eg}}(E_{ph} - E_g) + \eta_{T_0} E_{ph})N_{ph}$
- `OpticalAbsorptionHeat(Bandgap)`: $\eta_{T_{Eg}}(E_{ph} - E_g)N_{ph}$
- `OpticalAbsorptionHeat(Vacuum)`: $\eta_{T_0} E_{ph} N_{ph}$

- `ThermalizationYield(Bandgap)`: $\eta_{T_{E_g}}$
- `ThermalizationYield(Vacuum)`: η_{T_0}

where N_{ph} represents the number of absorbed photons.

> **NOTE** `OpticalAbsorptionHeat` is not calculated for optical absorption that is loaded using `ReadFromFile` or for constant optical generation specified by `SetConstant` because the corresponding wavelength of the light source is unknown.

Specifying Time Dependency for Transient Simulations

To model the electrical response of a light pulse, incident on a device, a description of the light signal over time can be specified either globally or separately for each type of optical generation computation. For the former, `TimeDependence (...)` is listed directly in the `OpticalGeneration` section, while for the latter, it is given as an argument of the chosen type of optical generation computation. If `TimeDependence` is specified both globally and for a specific type of optical generation computation such as `ComputeFromMonochromaticSource`, the latter takes precedence. `TimeDependence` can only be specified in the global `Physics` section and not for a particular region or material.

The given time dependency essentially scales the optical generation rate, resulting from a stationary solution of the optical problem as a function of time. The time dependency is only taken into account inside a `Transient` statement and the corresponding scaling factor for the different types of optical generation computation is automatically written to the `Current` file under the name `TimeDependence(Ft)`. If the optical generation needs to be scaled inside a `Quasistationary`, the keyword `Scaling` in the `OpticalGeneration` section can be used. However, this scaling factor does not apply inside a `Transient` statement. Instead, `Scaling` can be set directly in the respective `TimeDependence` section.

Different types of time dependency are available:

- Linear time dependency
- Gaussian time dependency
- Exponential time dependency
- Cosine time dependency
- Arbitrary time dependency read from a file

> **NOTE** If no time dependency has been specified, a scaling factor of 1 is used inside a `Transient` statement irrespective of any other scaling factors set in the `OpticalGeneration` section.

In addition, each of the above time dependencies can be extended to a periodic signal of the respective type. For the analytic time dependencies, you can specify a time interval `WaveTime= (<t1>, <t2>)`. Before `<t1>`, the optical generation rate undergoes an increase from zero characterized by the type of analytic time dependency. After `<t2>`, the optical generation rate experiences a corresponding decrease.

By default, Sentaurus Device adds turning points (see Time-Stepping on page 89) to the `Transient` statement at several characteristic time points of the light pulse to help convergence and to ensure it is resolved even if the time step of the `Transient` statement is larger than the entire pulse width. For details about optical turning points, see Optical Turning Points on page 552.

The linear time function as shown in Figure 22 is expressed as:

$$F(t) = \begin{cases} \max(0, m(t - t_1) + 1) & , t < t_1 \\ 1 & , t_1 \leq t \leq t_2 \\ \max(0, m(t_2 - t) + 1) & , t > t_2 \end{cases} \tag{645}$$

where m is given by `WaveTSlope`. Alternatively, `WaveTLin` can be specified, which is the inverse of m, that is, it corresponds to the rise time $t_{\text{lin}} = t_1 - t_0$ in seconds.
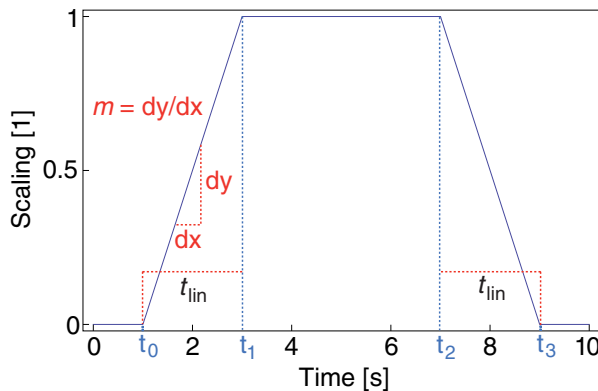
Figure 22   Rise and decay times based on a linear function

The Gaussian time function as shown in Figure 23 on page 549 is expressed as:

$$F(t) = \begin{cases} \exp\left(-\left(\frac{t_1 - t}{\sigma}\right)^2\right) & , t < t_1 \\ 1 & , t_1 \leq t \leq t_2 \\ \exp\left(-\left(\frac{t - t_2}{\sigma}\right)^2\right) & , t > t_2 \end{cases} \tag{646}$$

where σ is defined by `WaveTSigma`.
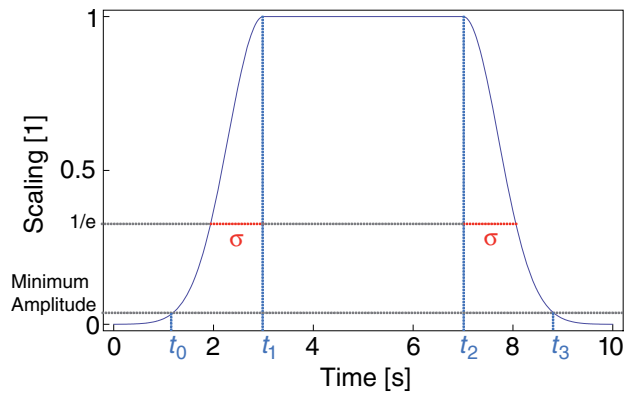
Figure 23   Rise and decay times based on a Gaussian function

The exponential time function as shown in Figure 24 is expressed as:

$$
F(t) = \begin{cases} \exp\left(\dfrac{t - t_1}{t_{\text{exp}}}\right) & , t < t_1 \\ \\ 1 & , t_1 \le t \le t_2 \\ \\ \exp\left(\dfrac{t_2 - t}{t_{\text{exp}}}\right) & , t > t_2 \end{cases} \tag{647}
$$

where t_{exp} is defined by `WaveTExp`.
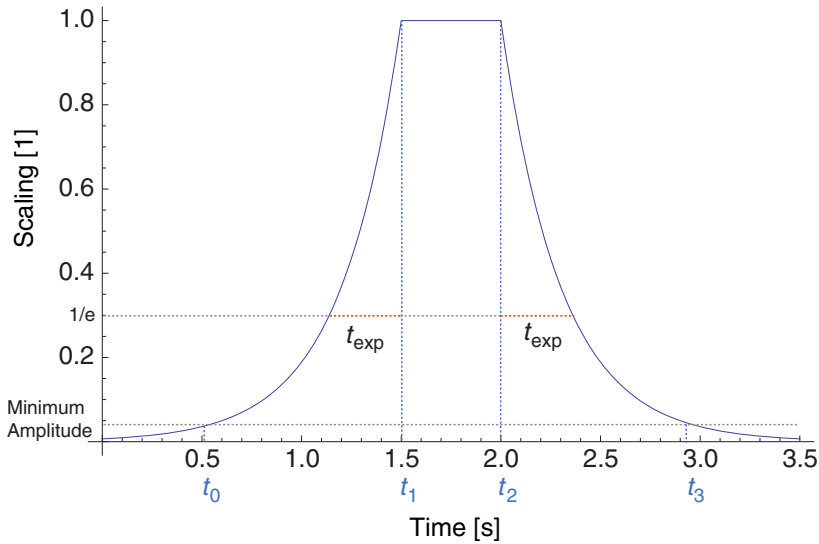
Figure 24   Rise and decay times based on an exponential function

The cosine time function as shown in Figure 25 is expressed as:

$$
F(t) = \begin{cases}
0 & t \le t_1 - t_{\cos} \vee t \ge t_2 + t_{\cos} \\
\frac{1}{2} \cdot \left(1 + \cos\left(\pi \dfrac{t - t_1}{t_{\cos}}\right)\right) & t_1 - t_{\cos} < t < t_1 \\
1 & t_1 \le t \le t_2 \\
\frac{1}{2} \cdot \left(1 + \cos\left(\pi \dfrac{t - t_2}{t_{\cos}}\right)\right) & t_2 < t < t_2 + t_{\cos}
\end{cases}
\tag{648}
$$

where $t_{\cos}$ is defined by `WaveTCos`.
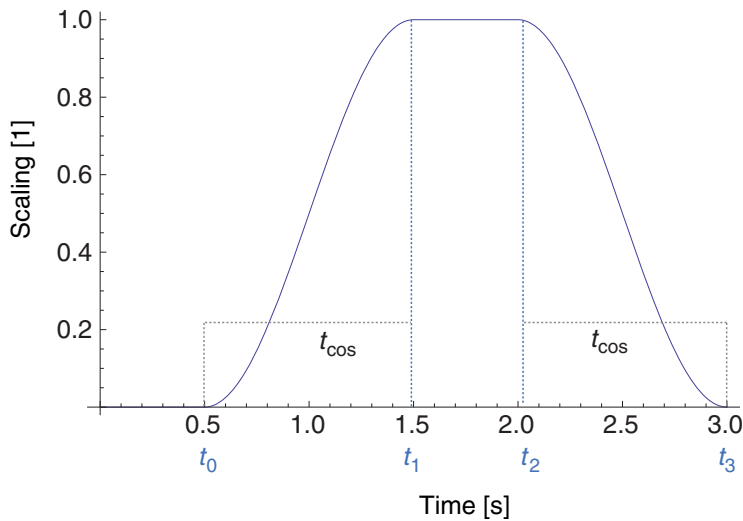
Figure 25   Rise and decay times based on a cosine function

If no time interval is specified, $t_1 = t_2 = 0$ is assumed. The analytic time dependencies are selected by specifying a value for the corresponding parameters as shown in Table 109.

Table 109   Selection of analytic time dependency

Time dependency	Required keyword
Linear	`WaveTSlope or WaveTLin`
Gaussian	`WaveTSigma`
Exponential	`WaveTExp`
Cosine	`WaveTCos`

An arbitrary time dependency can be applied by defining a time function whose interpolation points are given in a file with a whitespace-separated, two-column format. The first column contains the time points in seconds and the second column contains the corresponding function values. Linear interpolation is used to obtain function values between the interpolation points.

This type of time dependency can be activated using the following syntax:

```
File {
   OptGenTransientScaling= <filename>   # file containing interpolation points
}

Physics {
   Optics (
      OpticalGeneration (
         TimeDependence ( FromFile )
      )
   )
}
```

To transform any of the above time dependencies into a periodic signal, its period in seconds must be specified using the keyword `WaveTPeriod`. The specified signal is repeated infinitely, unless the number of periods is set explicitly with the keyword `WavePeriods`.

For linear and Gaussian time dependency, an additional temporal offset can be defined to essentially control the relative location of the signal within the period as illustrated in Figure 26.
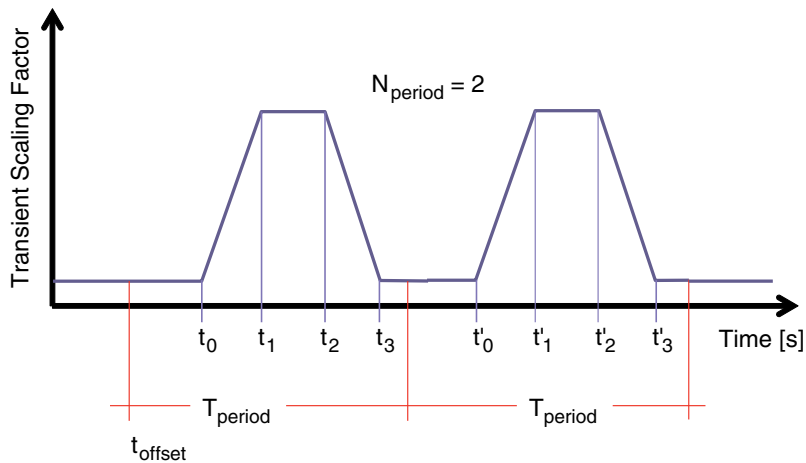
Figure 26   Extension of a predefined time dependency to a periodic signal where T_{period}, N_{period}, and t_{offset} correspond to WaveTPeriod, WavePeriods, and WaveTPeriodOffset

The syntax for the linear periodic signal shown in Figure 26 is:

```
Physics {
   Optics (
      OpticalGeneration (
         TimeDependence (
            WaveTime = (t1, t2)
            WaveTSlope = m
```

```
            WaveTPeriod = Tperiod
            WavePeriods = Nperiod
            WaveTPeriodOffset = toffset
        )
      )
    )
  }
```

Optical Turning Points

Typically, you specify turning points as described in Time-Stepping on page 89 in the `Transient` statement to limit the advancing time step. Controlling time-stepping based on knowledge about the device physics and its characteristics can improve the convergence behavior. Light pulses in transient simulations have a strong impact on device characteristics and, therefore, corresponding optical turning points are added by default. The default optical turning points also guarantee that a light pulse is resolved to a certain degree, independent of the advancing time step before the start time of the pulse. You can switch off the default optical turning points or change their parameters in the command file.

In contrast to general turning points described in Time-Stepping on page 89, optical turning points are specified in the `OpticalTurningPoints` section within the `TimeDependence` section with the definition of the light pulse.

The predefined optical turning points correspond to the time points t_0, t_1, t_2, and t_3 shown in Figure 22 on page 548 to Figure 26 on page 551, for which the advancing time step can be limited using the keywords `DtRiseStart`, `DtRiseEnd`, `DtFallStart`, and `DtFallEnd`, respectively. In addition, the time step can be limited for the ranges $[t_0 t_1]$, $[t_1 t_2]$, and $[t_2 t_3]$ that are associated with the keywords `DtRise`, `DtPlateau`, and `DtFall`. You can limit the maximum time step in these ranges separately using the aforementioned keywords or set the same maximum time step for all three time ranges using the keyword `Dt`. If both `Dt` and a range-specific keyword such as `DtPlateau` are specified, the value of the range-specific keyword is used.

> **NOTE**   Limiting the maximum time step within a range, using `DtRise`, `DtPlateau`, or `DtFall`, has an effect only if the time-stepping is such that the calculated time step used to advance from the last time point t_i before a range is not larger than $t_3 - t_i$. In other words, limiting the time step becomes active only if the regular time-stepping enters the predefined range. See Time-Stepping on page 89 for details about the behavior of turning points.

Specifying a time step equal to 0 switches off the corresponding optical turning point or range.

NOTE The points $t_0 - t_3$ are enabled by default; whereas, the ranges must be enabled explicitly by specifying a limiting time step greater than 0. To switch off all optical turning points and ranges, specify `-OpticalTurningPoints` in the respective `TimeDependence` section.

For analytic light signals with asymptotically decaying tails such as a Gaussian, the time points t_0 and t_3 are not naturally defined. By default, they are chosen to be the time points where the signal amplitude is equal to 0.01. However, by setting `MinAmplitude` in the `OpticalTurningPoints` section to a different value, you can shift the time points t_0 and t_3 in either direction.

For time-dependence `FromFile`, only the time points t_0 and t_3 and a single range $[t_0 t_3]$ are supported, which are active by default. The limiting time step for the range can be set with the keyword `Dt`. The time points t_0 and t_3 are associated with the first and last time points given in the `OptGenTransientScaling` file specified in the `File` section.

The following example demonstrates the syntax for optical turning points (an overview of the various parameters and corresponding default values is given in Table 248 on page 1445):

```
Physics {
  Optics (
    OpticalGeneration (
      TimeDependence (
        WaveTime = (t₁, t₂)
        WaveTSigma = σ
        OpticalTurningPoints (
          DtRiseStart = 1e-4        # [s]
          DtFallEnd = 0             # switch off turning point t₃
          MinAmplitude = 0.005
          DtPlateau = 1e-3          # [s]
          DtFall = 2e-4             # [s]
        )
      )
    )
  )
}
```

Solving the Optical Problem

`ComputeFromMonochromaticSource` and `ComputeFromSpectrum` require the solution of the optical problem for a given excitation to obtain the optical generation rate. Several optical solvers are available and the choice for a specific method is determined usually by the optimum combination of accuracy of results and computation time.

Besides selecting a certain optical solver and specifying its particular parameters, it is necessary to define the excitation parameters, to choose an appropriate refractive index model, and to control when a solution is computed in the `Solve` section. These steps are explained in the following sections.

Specifying the Optical Solver

The following optical solvers are supported:

- Transfer matrix method (TMM)
- Finite-difference time-domain (FDTD)
- Raytracing (RT)
- Beam propagation method (BPM)
- Loading solution of optical problem from file
- Optical beam absorption method
- Composite method

> **NOTE** By default, the log of the optical solver is written to standard output and the simulation log file as part of the general simulation log. However, depending on the specific setup, the optical solver log can be verbose and affect the overall readability of the simulation log. To avoid this behavior, you can either:
>
> - Set `Verbosity=0` in the `Optics` section to completely suppress any logging activity of the optical solver except for warning and error messages.
>
> - Redirect the log of the optical solver to a separate log file by specifying the keyword `OpticsOutput` in the global `File` section.

Transfer Matrix Method

The TMM solver is selected using the following syntax:

```
Physics {
   ...
   Optics (
      ...
      OpticalSolver (
         TMM (
            <TMM options>
         )
      )
```

```
      )
   }
```

The TMM-specific options, such as the parameters for the extraction of the layer stack, are described in Using Transfer Matrix Method on page 630.

Finite-Difference Time-Domain Method

In contrast to the TMM solver, the FDTD-specific parameters, such as boundary conditions and extractors, are defined in a separate command file that is set in the `File` section with the keyword `OpticalSolverInput`. To provide some basic control of the FDTD solver from within Sentaurus Device, excitation parameters such as `Wavelength`, `Theta`, and `Phi`, as well as the polarization `Psi`, are overwritten by their counterparts in the `Excitation` section of the Sentaurus Device command file if specified.

> **NOTE**   The `Psi` keyword in EMW corresponds to the `PolarizationAngle` keyword in Sentaurus Device.

> **NOTE**   The FDTD solver in Sentaurus Device supports both the 2D and 3D excitation specification of EMW as outlined in Sentaurus™ Device Electromagnetic Wave Solver User Guide, Specifying Direction and Polarization on page 47.

The syntax for activating the FDTD solver requires as input the name of the command file of the FDTD solver. The general syntax is:

```
File {
   OpticalSolverInput= <EMW_command_file>
}

Physics {
   Optics (
      OpticalSolver (
         FDTD ( ... )
      )
   )
}
```

The FDTD algorithm is based on a tensor mesh, which can be generated independently before the device simulation. Another option is to build the tensor mesh during the simulation before the call to EMW. The main advantage of the latter option is that the tensor grid can be adjusted to a possibly changing excitation wavelength in a `Quasistationary` statement. Since the accuracy and stability of the FDTD method crucially depend on the discretization with respect to the wavelength, this feature becomes important when a large range of the light spectrum is scanned (see Illumination Spectrum on page 536 and Parameter Ramping on page 573).

To activate this feature, `GenerateMesh (...)` must be specified in the `FDTD` section and a common base name (that is, file name excluding suffix) for the boundary file and the Sentaurus Mesh command file must be defined in the `File` section using the keyword `MesherInput`. Sentaurus Mesh is then called with the specified base name prepended by the basename of the `Plot` file given in the `File` section of the Sentaurus Device command file. The resulting tensor grid file is detected automatically and replaces the grid file in the user-provided EMW command file.

By default, a tensor mesh is generated before the first call to EMW and remains in use during further calls to the solver. However, if the excitation wavelength varies and the initially built tensor mesh no longer fulfills the requirements, two options exist that control the update of the mesh.

Using the keyword `ForEachWavelength` in the `GenerateMesh` section triggers the computation of a new tensor mesh whenever the wavelength changes compared to the previous solution of the FDTD solver. Internally, the wavelength specified in the user-provided Sentaurus Mesh command file is replaced with the current value.

Since the slope of the complex refractive index as a function of wavelength can vary from almost zero to high values, depending on the wavelength interval, it is possible to limit the mesh generation according to a list of strictly monotonically increasing wavelengths. If the current wavelength enters a new interval, the mesh is updated and remains in use until the wavelength moves beyond the interval boundaries. The syntax for such a use case is:

```
FDTD (
   ...
   GenerateMesh (
      Wavelength = ( 0.35 0.55 0.7 0.8 ) # wavelength in [µm]
   )
)
```

For the command file syntax and options of the FDTD solver, refer to the *Sentaurus™ Device Electromagnetic Wave Solver User Guide*.

Raytracing

More details about the raytracer can be found in . The raytracer requires the use of the complex refractive index model, and various excitation variables can be ramped. These rampable excitation variables are `Intensity`, `Wavelength`, `Theta`, `Phi`, and `PolarizationAngle` or `Polarization`.

The required syntax is:

```
Physics {...
   Optics (
      ComplexRefractiveIndex(...)
```

```
        OpticalGeneration(...)
        OpticalSolver(
           RayTracing(...)
        )
        Excitation(...)
    )
}
```

where the `RayTracing` section contains:

```
RayTracing(
   # Setting keywords of raytracer
   # ----------------------------
   CompactMemoryOption
   MonteCarlo
   OmitReflectedRays
   OmitWeakerRays
   RedistributeStoppedRays

   PolarizationVector = vector
   PolarizationVector = Random
   DepthLimit = integer
   MinIntensity = float              # fraction, relative value
   RetraceCRIchange = float          # fractional change to retrace rays
   VirtualRegions { "string" "string" ... }
   VirtualRegions {}
   ExternalMaterialCRIFile = "string"
   WeightedOpticalGeneration

   # Defining starting rays:
   # -----------------------
   RayDistribution( ... )
   RectangularWindow (
      RectangleV1 = vector           # vertex 1 of rectangular window [um]
      RectangleV2 = vector           # vertex 2 of rectangular window [um]
      RectangleV3 = vector           # vertex 3 needed only for 3D [um]
      # number of rays = LengthDiscretization * WidthDiscretization
      LengthDiscretization = integer  # longer side
      WidthDiscretization = integer   # shorter side needed only for 3D
      RayDirection = vector
   )

   UserWindow (
      NumberOfRays = integer         # number of rays in file
      RaysFromFile = "filename.txt"  # position(um) direction area(cm^2)
      PolarizationVector = ReadFromExcitation
   )
)
```

Some comments about the RT syntax:

- The keyword `RetraceCRIchange` specifies the fractional change of the complex refractive index (either the real or imaginary part) from its previous state that will force a total recomputation of raytracing.

- Starting rays for raytracing can be set using `RectangularWindow` or `UserWindow`. Details can be found in Window of Starting Rays on page 600. Only one of the windows can be chosen but not both.

- Starting rays also can be set using the illumination window (see Illumination Window on page 562) and the `RayDistribution` section (see Distribution Window of Rays on page 602).

- Raytracing in cylindrical coordinates is also possible (see Cylindrical Coordinates for Raytracing on page 603).

Beam Propagation Method

The BPM solver is selected using the following syntax:

```
Physics {
   Optics (
      OpticalSolver (
         BPM (
            <BPM options>
         )
      )
   )
}
```

The BPM-specific options, such as the specific excitation type or the discretization parameters, are described in Using Beam Propagation Method on page 649.

Loading Solution of Optical Problem From File

The solution of the optical problem, which can be either an absorbed photon density profile or an optical generation profile, also can be loaded from a file. In contrast to using `OpticalGeneration ( ReadFromFile ( ... ) )`, the optical solver `FromFile` offers more flexibility for simulation setups that involve an illumination spectrum or parameter ramping.

The required syntax is:

```
File {
   OpticalSolverInput = "<file name or file name pattern>"
}

Physics {
   Optics (
      OpticalGeneration (
         ComputeFromMonochromaticSource ()
      )
      OpticalSolver (
         FromFile (
            <FromFile options>
         )
      )
   )
}
```

The use of the optical solver `FromFile` is described in Loading Solution of Optical Problem From File on page 640.

Optical Beam Absorption Method

The following syntax is used to select the optical beam absorption method as the optical solver:

```
Physics {
   Optics (
      OpticalSolver (
         OptBeam (
            <OptBeam options>
         )
      )
   )
}
```

The `OptBeam`-specific options, such as the parameters for the extraction of the layer stack, are described in Using Optical Beam Absorption Method on page 646.

Composite Method

The following syntax is used to select the composite method as the optical solver:

```
Physics {
   Optics (
      OpticalSolver (
         Composite (
```

```
            <Composite options>
          )
        )
      )
   }
```

The `Composite` solver itself is not a numeric method to solve an optical problem. Instead, it coordinates the execution of other solvers that might depend on each other and sums their results to yield a general solution. As such, it requires the specification of at least another optical device instance. For details about this solution approach, see Composite Method on page 656.

Setting the Excitation Parameters

The `Excitation` section is common to all optical solvers and mainly specifies a plane wave excitation. It contains the following keywords:

- `Intensity` [W/cm^2]
- `Wavelength` [μm]
- `Theta` [deg]
- `Phi` [deg]
- `PolarizationAngle` [deg] or `Polarization`

In combination with the optical solvers `TMM`, `OptBeam`, and `FromFile`, an additional `Window` section is required to specify the parameters of the illumination window, which is described in Illumination Window on page 562.

> **NOTE** For the optical solver `FromFile`, the requirement of a `Window` section only applies when one-dimensional profiles are loaded.

The propagation direction is defined by the angles with the positive z-axis and x-axis, respectively. In two dimensions, the propagation direction is well-defined by specifying `Theta` only, where `Theta` corresponds to the angle between the propagation direction and the positive y-axis. However, in three dimensions, the propagation direction is defined by `Theta` and `Phi`:

- `Theta` is the angle between the positive z-axis and the propagation direction.
- `Phi` is the angle between the positive x-axis and the projection of the propagation direction on the xy plane as shown in Figure 27 on page 561.

For vectorial methods, such as the FDTD solver, the polarization is set using the keyword `PolarizationAngle`, which represents the angle between the H-field and the $z \times \hat{k}$ axis, where $\hat{k}$ is the unit wavevector (see Sentaurus™ Device Electromagnetic Wave Solver User Guide, Plane Waves on page 46).

For the TMM and RT solvers, the conventions for polarization are as follows:

- In two dimensions, the keyword `Polarization` is a real number in the interval [0,1], where `Polarization=0` refers to TM, and `Polarization=1` refers to TE excitations, respectively. If the keyword `PolarizationAngle` is specified, it takes precedence over the keyword `Polarization`. A simple relationship between `PolarizationAngle` and `Polarization` can be established: $\text{Polarization} = \sin^2(\text{PolarizationAngle})$.

- In three dimensions, the polarization vector is defined by rotating the $z \times \hat{k}$ vector counterclockwise, about the wave direction, by an angle defined by `PolarizationAngle` when looking in the propagation direction.

    NOTE   For the RT solver, specifying the `PolarizationVector` explicitly overrides the keywords `Polarization` and `PolarizationAngle`.
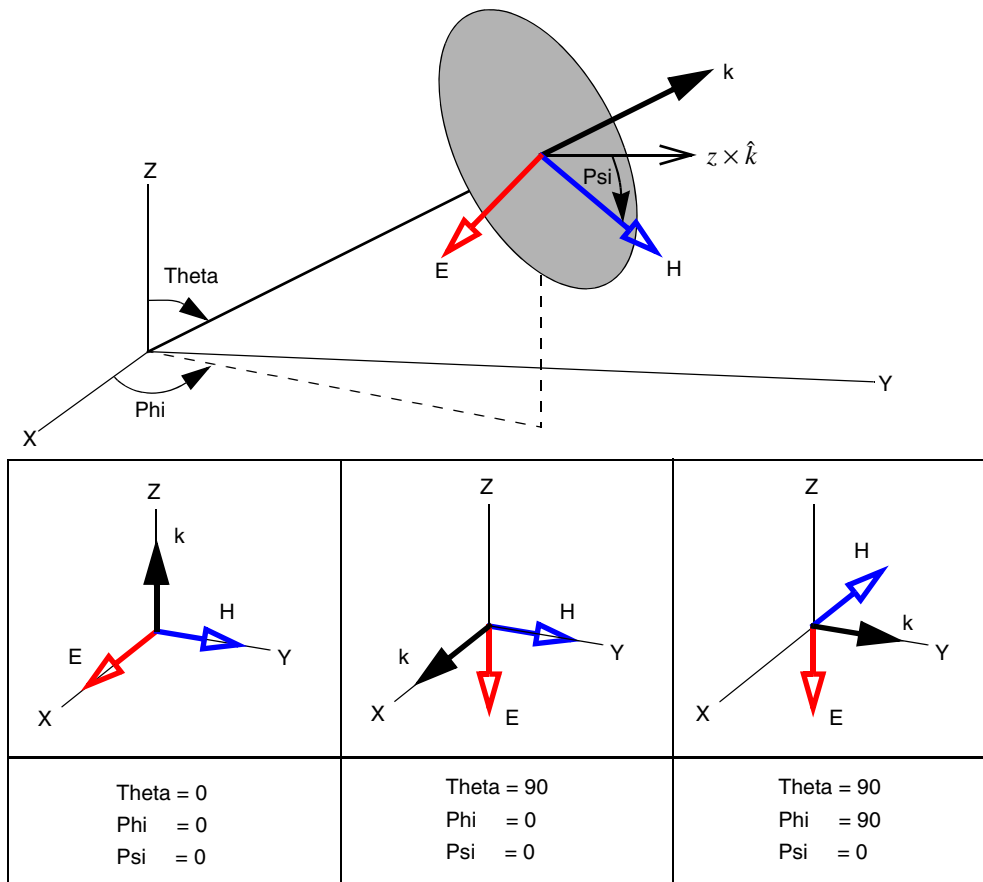
Figure 27   Definition of coordinate system for 3D plane wave excitation and examples of parameters of 3D plane wave

Illumination Window

The concept of an illumination window to confine the light that is incident on the surface of a device structure plays an important role in various simulation setups for photo-diode devices, such as photodetectors, solar cells, and image sensors. Sentaurus Device supports a flexible user interface for the specification of one or more illumination windows, which also allows you to move these windows during a simulation by ramping the corresponding parameters. This common interface is currently available for the TMM, FromFile (only for loading 1D profiles), OptBeam, and RayTracing (see Using the Raytracer on page 596) solvers, while different solver-specific implementations exist for BPM (see Using Beam Propagation Method on page 649) solvers.

The illumination window is described using a local coordinate system specified by the global location of its origin and the x- and y-directions given as vectors or in terms of rotation angles as illustrated in Figure 28.

Within this local coordinate system, several window shapes can be defined using relative quantities such as width and height, together with an origin anchor for a line in 2D or a rectangular window in 3D. Alternatively, or for shapes that do not support relative quantities, absolute coordinates are used to characterize the shape of the window. For example, a polygon would be defined by specifying a series of vertices in the local 2D coordinate system.
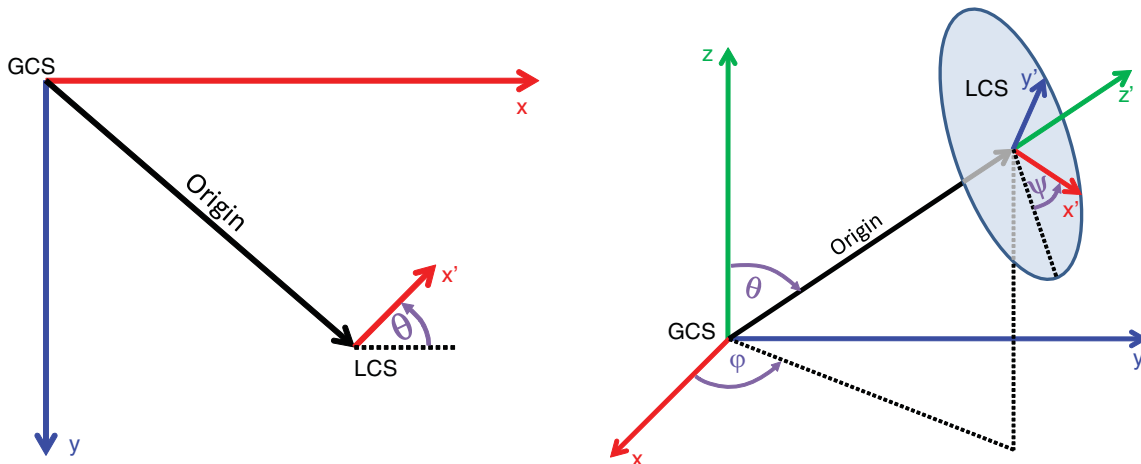
Figure 28   Coordinate system used in the illumination window for (*left*) two dimensions and (*right*) three dimensions

The following window shapes are supported:

■   Line (in 2D only)

■   Rectangle (in 3D only)

■   Polygon (in 3D only)

■   Circle (in 3D only)

You can define more than one illumination window. The specification of an optional name tag allows you to refer to the respective window when ramping one of its parameters. It is also helpful for identifying results for a specific window in the current file. If two windows overlap, the solutions of the corresponding windows will be added in the intersection.

The global location of the origin of the local coordinate system is specified with the keyword `Origin`, whose default is `(0, 0, 0)`. To specify its orientation, the directions of the coordinate axes can be defined using the vectors `XDirection` and `YDirection`. In 2D, only `XDirection` needs to be specified.

Alternatively, you can set three rotation angles `theta` (angle with z-axis), `phi` (angle between x-axis and projection of window normal n on xy plane), and `psi` (angle between local x-axis and the vector $\hat{z} \wedge \hat{n}$), which define the vector `RotationAngles` in three dimensions as shown in Figure 28 on page 562. For two dimensions, only the first angle of the vector `RotationAngles` is used, which means a rotation of the angle from the local +y'-axis to the local +x'-axis. The local origin can be defined within each `Window` using the keyword `Origin=<vector>`. The `RotationAngles` are compatible with the optical solvers `TMM`, `Raytracing`, `Optbeam`, and `FromFile`. In general, the direction of excitation defined in (`Theta`, `Phi`) of the `Excitation` section is independent of the angles defined by `RotationAngles`.

If the location of a window in the local coordinate system is not specified by its corresponding vertex coordinates, its placement is determined by the bounding box of the window shape and a cardinal direction such as `North`, `South`, `NorthWest`, and so on, or `Center` defining which point of the bounding box coincides with the local origin. The cardinal direction is specified using the keyword `OriginAnchor`.

The illumination window is specified in the `Excitation` section as follows:

```
Physics {
  Optics (
    Excitation (
      Window (
        <Window options>
      )
    )
  )
}
```

The following examples introduce the supported window shapes and show different ways of specifying them. Depending on the simulation setup, one specification may be more convenient than others, for example, if the window needs to be moved by using the parameter ramping feature.

Line

Line normal to y-axis at y=-10, xmin=-5, xmax=5:

```
Window (
   Origin = (0,-10)
   OriginAnchor = Center # Default
   Line ( Dx = 10 )
)
```

Line normal to y-axis at y=-10, xmin=5, xmax=500:

```
Window (
   Origin = (5,-10)
   OriginAnchor = West
   Line ( Dx = 545 )
)
```

or alternatively:

```
Window (
   Origin = (0,-10)
   XDirection = (1, 0, 0) # Default
   Line (
      X1 = 5
      X2 = 500
   )
)
```

Two lines normal to y-axis at y=-10, with xmin1=5, xmax1=10, and xmin2=15, xmax2=20:

```
Window ("W1") (
   Origin = (5, -10)
   OriginAnchor = West
   Line ( Dx = 5 )
)

Window ("W2") (
   Origin = (15, -10)
   OriginAnchor = West
   Line ( Dx = 5 )
)
```

Rectangle

Rectangle normal to z-axis at z=10, with width=10 and height=5, centered at x=0 and y=0:

```
Window (
   Origin = (0, 0, 10)
   OriginAnchor = Center # Default
   Rectangle (
      Dx = 10
      Dy = 5
   )
)
```

or alternatively:

```
Window (
   Origin = (0, 0, 10)
   Rectangle (
      Corner1 = (-5, -2.5)
      Corner2 = (5, 2.5)
   )
)
```

Polygon

Triangle in xz plane at y=4, and corners at (0, 0, 0), (1, 0, 0), and (0, 0, 1):

```
Window (
   Origin = (0, 4, 0)
   XDirection = (1, 0, 0) # Default
   YDirection = (0, 0, 1)
   Polygon( (0, 0), (1, 0), (0, 1) )
)
```

NOTE More complex polygon specifications also are supported by specifying
several polygon loops, which may or may not intersect. In this case, the
vertices of each loop must be enclosed in extra parentheses within the
`Polygon` section.

Circle

Circle in xy plane with center at (5, 4, -10) and radius 3:

```
Window (
   Origin = (5, 4, -10)
   XDirection = (1, 0, 0) # Default
   YDirection = (0, 1, 0) # Default
   Circle ( Radius = 3 )
)
```

Common Illumination Configurations

The following examples show the specification of the `Excitation` section for the most common case of normal incident light from the top of the device structure in the UCS and the DF–ISE coordinate system in two and three dimensions.

DF–ISE coordinate system in two dimensions:

```
Excitation (
   ...
   Window (
     Origin = (0, <ymin of device>)
     Line ( x1 = <xmin> x2 = <xmax> )    # Extent of illumination window
   )
)
```

UCS in two dimensions:

```
Excitation (
   ...
   Theta = 90                           # Illumination from top in +x direction
   Window (
     Origin= (<xmin of device>, 0)
     xDirection= (0, 1)                  # Local x' points in global +y direction
     Line (x1=<ymin> x2=<ymax> )        # Extent of illumination window
   )
)
```

DF–ISE coordinate system in three dimensions:

```
Excitation (
   ...
   Theta = 180                          # Illumination from top in -z direction
   Window (
     Origin = (0, 0, <zmax of device>)
     Rectangle (
       # Extent of illumination window
       corner1 = (<xmin>, <ymin>) corner2 = (<xmax>, <ymax> )
     )
   )
)
```

UCS in three dimensions:

```
Excitation (
   ...
   Theta = 90                               # Illumination from top in +x direction
   Window (
     Origin = (<xmin of device>, 0, 0)
```

```
            xDirection = (0, 0, 1)          # Local x' points in global +z direction
            yDirection = (0, 1, 0)          # Local y' points in global +y direction
            Rectangle (
               # Extent of illumination window
               corner1 = (<zmin>, <ymin>) corner2 = (<zmax>, <ymax> )
            )
         )
      )
```

NOTE   In these examples, keywords whose default values are correct for the
given use case have been omitted to demonstrate the minimum required
specification.

Moving Windows Using Parameter Ramping

The following syntax demonstrates how illumination windows can be moved and resized
during a simulation using the parameter ramping framework:

```
Physics {
   Optics (
      Excitation (
         Window("L1") (
            Origin = (-0.5, -0.1, 0)
            XDirection = (1,0,0) # Default
            Line(
               x1 = -0.5
               x2 = 0.5
            )
         )
         Window("L2") (
            Origin = (0.5, -0.1, 0)
            OriginAnchor = Center # Default
            XDirection = (1,0,0) # Default
            Line( Dx = 1 )
         )
      )
   )
}

Solve{
   Optics
   Quasistationary (
      InitialStep=0.2 MaxStep=0.2 MinStep=0.2
      Goal { ModelParameter="Optics/Excitation/Window(L2)/Line/Dx" value=0.2 }
   ) { Optics }

   Quasistationary (
      InitialStep=0.2 MaxStep=0.2 MinStep=0.2
```

```
        Goal { ModelParameter="Optics/Excitation/Window(L2)/Origin[0]"
        value=0.9 }
        Goal { ModelParameter="Optics/Excitation/Window(L2)/Origin[1]"
        value=0.5 }
        Goal { ModelParameter="Optics/OpticalSolver/TMM/
        LayerStackExtraction(L2)/Position[0]" value=0.9 }
    ) { Optics }
}
```

For more details on ramping parameters, including the ramping of vector parameters, see Parameter Ramping on page 573.

Spatial Intensity Function Excitation

With the illumination window feature (see Illumination Window on page 562), you can define a spatial profile within each illumination window. The intensity profile corresponds to a modified Gaussian profile with the shape shown in Figure 29.
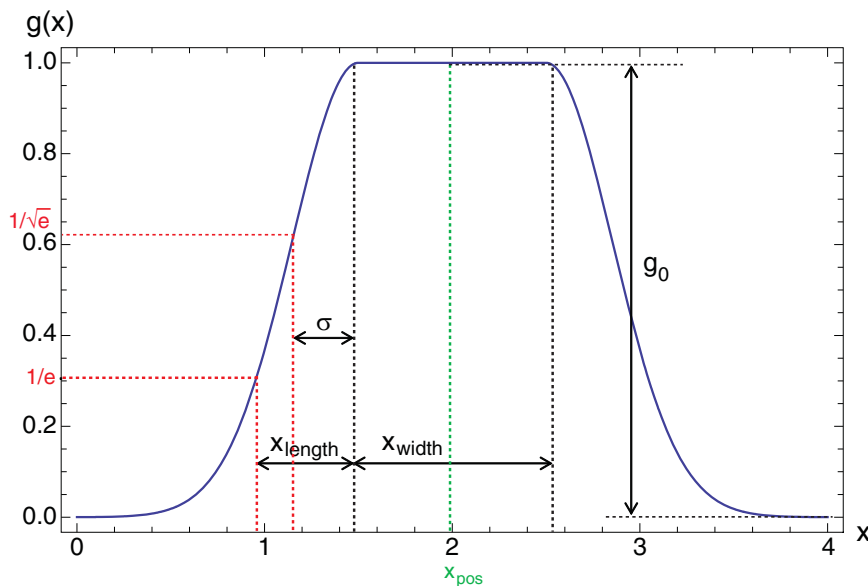
Figure 29   Gaussian spatial intensity distribution, showing the definition of key parameters

There is a top plateau, with both ends decaying with symmetric Gaussian functions. Its peak value is normalized to 1.0. Mathematically, the spatial shape is defined by:

$$g_x(x) = \begin{cases} \exp\left(-\dfrac{\left(\left|x - x_{\text{pos}}\right| - \dfrac{x_{\text{width}}}{2}\right)^2}{2\sigma^2}\right) & , \left|x - x_{\text{pos}}\right| > \dfrac{x_{\text{width}}}{2} \\ 1 & , \text{otherwise} \end{cases} \tag{649}$$

where σ (Sigma) is the Gaussian width, x_{pos} (PeakPosition) is the center peak position of the function, and x_{width} (PeakWidth) is the width of the center plateau. To add flexibility, you can add g_0 (Scaling) as a scaling factor to the final expression:

$$g(x) = g_0 \cdot g_x(x) \tag{650}$$

This modified spatial Gaussian function can be applied to the different supported types of illumination window: line, rectangle, polygon, and circle (see Illumination Window on page 562). In two dimensions, the product of two modified Gaussian functions is:

$$g(x, y) = g_0 \cdot g_x(x) \cdot g_y(y) \tag{651}$$

The syntax of the spatial intensity function is embedded within the syntax of the illumination window:

```
Optics (
   Excitation (...
      Wavelength = 0.5
      Intensity = 100    * [W/cm2]
      Window(
         IntensityDistribution(
            Gaussian(
               Sigma = (<float>,<float>) | Length = (<float>,<float>)
               PeakPosition = (<float>,<float>)
               PeakWidth = (<float>,<float>)
               Scaling = <float>
            )
         )
         Rectangle(dx = 1, dy = 2)
      )
   )
)
```

Comments about the syntax:

- The `IntensityDistribution` section is specified within the illumination window (`Window`). It follows the local coordinate system of the window, that is, `PeakPosition` is taken with reference to the origin of the local coordinate of the window.

- Either `Sigma` or `Length` must be specified. If `Length` is specified, `Sigma` is calculated using the formula: $\sigma = x_{\text{length}}/\sqrt{2}$.

- The parameters are input as a single floating-point number (for one dimension) or a vector (for two dimensions). For example, `Sigma=0.05` for a 1D Gaussian and `Sigma=(0.03,0.04)` for a 2D Gaussian.

- The `IntensityDistribution` section works with the raytracing, `TMM`, `OptBeam`, and `FromFile` optical solvers.

> **NOTE**   For 1D solvers such as `TMM` and `OptBeam`, the spatial intensity profile is simply overlaid onto the 1D field distribution; it is not an indication of a more accurate solution.

Choosing Refractive Index Model

The complex refractive index model as described in Complex Refractive Index Model on page 578 is available for all optical solvers. It must be specified in the `Optics` section when using the unified interface for optical generation computation.

Extracting the Layer Stack

The optical solvers `TMM` (see Transfer Matrix Method on page 625) and `OptBeam` (see Optical Beam Absorption Method on page 644) require the extraction of a layer stack from the actual device structure as they are based on 1D algorithms whose solution is extended to the dimension of the simulation grid. Both the extension of the solution and the extraction of the layer stack are bound to the illumination window (see Illumination Window on page 562), which determines the domain of the device structure being represented by the 1D optical problem.

The layer stack extraction algorithm works by extracting all grid elements along a line normal to the corresponding illumination window starting from a user-specified position within the window. The direction of extraction, that is, positive or negative, is derived from the propagation direction of the incident light as specified in the `Excitation` section.

By default, all elements belonging to the same region will form a single layer, which is part of the entire stack. This assumes that the material properties do not vary within the region. If this is not the case or not a good approximation, you can create a separate layer for each extracted

element by selecting the option `ElementWise` instead of `RegionWise` for the keyword `Mode` in the `LayerStackExtraction` section. As this can lead to a large number of layers whose difference in material properties may be insignificant for the solution of the optical solver, yet impact its performance, a threshold value can be specified to control the creation of the layer stack from the extracted grid elements.

All elements whose relative difference in the refractive index or extinction coefficient, compared with the previous layer, is lower than the threshold are merged into one layer. In doing so, the refractive index and the extinction coefficient are treated separately, both deviations must be lower than the specified threshold. The material properties of this merged layer are obtained by averaging the corresponding element properties. The thickness of each element computed by the distance between the intersection points of the extraction line with the corresponding element is summed to yield the total thickness of the representative layer of the stack.

The threshold can be specified using the keyword `ComplexRefractiveIndexThreshold` in the `LayerStackExtraction` section.

Options are available for defining the starting point of the extraction line:

- Exact position in the global coordinate system using the keyword `Position`.
- Position within the bounding box of the window designated by a cardinal direction.
- Position within the bounding box of the window specified as a point in the local coordinate system of the illumination window.

The last two options require the specification of the keyword `WindowPosition`. Its argument can be either one of `North`, `South`, `NorthWest`, and so on, and `Center` or a 2D point, for example, `WindowPosition = (1.5, 2)`.

The following is an example for a `LayerStackExtraction` section used by the TMM solver:

```
Physics {
  Optics (
    OpticalSolver (
      TMM (
        LayerStackExtraction (
          WindowName = "L1"
          Position = (-0.5, -0.1, 0)
          Mode = ElementWise # Default RegionWise
        )
      )
    )
  )
}
```

The keyword `WindowName` is required if more than one illumination window exists. Its argument specifies to which illumination window the `LayerStackExtraction` refers.

> **NOTE** If the starting point of the extraction line is outside of the device structure, the extracted layer stack will contain a layer representing the space between the starting point of the extraction line and the surface of the device structure. In general, the material properties of vacuum are assigned to this layer. For optical solvers that support user-defined bulk media on the top and the bottom of the layer stack using the `Medium` statement, the material properties of the top medium if specified are used except that the extinction coefficient `k` is set to 0. For more details about user-defined bulk media, see Using Transfer Matrix Method on page 630.

Controlling Computation of Optical Problem in Solve Section

Specifying the keyword `Optics` in the `Solve` section triggers the solution of the optical problem. For example, the following is sufficient to compute the optical generation and the optical intensity:

```
Physics {
   Optics (
      OpticalGeneration ( ... )
   )
}

Solve { Optics }
```

If only the keyword `Optics` is specified in the `Solve` section, either directly or within a `Quasistationary` or `Transient` statement, and no other equations are solved, the simulation is classified as an optics standalone simulation. In general, such simulations do not require the specification of contacts in the grid file. In optics standalone simulations, it is possible to switch on the creation of double points at region interfaces independent of the type of interface. In other words, a heterojunction interface is treated in the same way as a semiconductor–insulator interface. This feature is enabled by specifying the keyword `Discontinuity` in the `Physics` section (see Discontinuous Interfaces on page 231).

The `Solve` section of a typical transient device simulation reads as follows:

```
Solve {
   Optics
   Poisson
   Coupled { Poisson Electron Hole }
```

```
    Transient (
       InitialTime = 0
       FinalTime = 3e-6
    ) { Coupled { Poisson Electron Hole } }
}
```

In this example, the optical generation rate is computed at the beginning when the optical problem is solved and is used afterwards in the electronic equations. To recompute the optical generation at a later point, the `Optics` statement can be listed wherever a `Coupled` statement is allowed.

The optical generation depends on the solution of the optical problem and, therefore, has an implicit dependency on all quantities that serve as input to the optical equation. Internally, an automatic update scheme ensures that, whenever the optical generation rate is read, all its underlying variables are up-to-date. Otherwise, it will be recomputed. This mechanism can be switched off by specifying `-AutomaticUpdate` in the `OpticalGeneration` section. By default, `AutomaticUpdate` is switched on.

Parameter Ramping

Sentaurus Device can be used to ramp the values of physical parameters (see Ramping Physical Parameter Values on page 78). For example, it is possible to sweep the wavelength of the incident light to extract the spectral dependency of a certain output characteristic conveniently. Ramping model parameters of the unified interface for optical generation computation works the same way except that instead of using the expression `Parameter = "<parameter name>"`, it uses the keyword `ModelParameter = "<parameter name or path>"`.

The value of `ModelParameter` can be either the parameter name itself such as `"Wavelength"` if it is unambiguous or the parameter name including its full path:

```
Solve {
   Quasistationary (
      Goal {
         [ Device = <device> ]
         [ Material = <material> | MaterialInterface = <interface> |
           Region = <region> | RegionInterface = <interface> ]
         ModelParameter = "Optics/Excitation/Wavelength" Value = <float>
      }
   ){ Optics }
}
```

Specifying the device and location (material, material interface, region, or region interface where applicable) is optional. However, `ModelParameter` and its `Value` must always be specified.

Similarly, the corresponding `CurrentPlot` section reads as follows:

```
CurrentPlot {
   [ Device = <device> ]
   [ Material = <material> | MaterialInterface = <interface> |
   Region = <region> | RegionInterface = <interface> ]
   ModelParameter = "Optics/Excitation/Wavelength"
}
```

Parameters whose value type is a vector of floating-point numbers support ramping of the individual vector components.

For example, to ramp the x- and y-components of the illumination window origin, the following syntax is required:

```
Quasistationary (
   InitialStep=0.2 MaxStep=0.2 MinStep=0.2
   Plot { Range = ( 0., 1 ) Intervals = 5 }
   Goal { ModelParameter="Optics/Excitation/Window(L2)/Origin[0]" value=0.9 }
   Goal { ModelParameter="Optics/Excitation/Window(L2)/Origin[1]" value=0.5 }
) {
   Optics
}
```

NOTE   When ramping parameters that reside in sections that can occur multiple times, such as the `Window` section, an identifying section name or tag in parentheses must follow the section name in the parameter path as shown in the example above.

Table 110 lists the parameters that can be ramped using the unified interface for optical generation computation.

Table 110   Parameters that can be ramped

Parameter path	Parameter name
`Optics/OpticalGeneration`	`Scaling`
`Optics/OpticalGeneration/ComputeFromMonochromaticSource`	`Scaling`
`Optics/OpticalGeneration/ReadFromFile`	`Scaling`
`Optics/OpticalGeneration/ComputeFromSpectrum`	`Scaling`
`Optics/OpticalGeneration/SetConstant`	`Value`

Table 110   Parameters that can be ramped (Continued)

Parameter path	Parameter name
`Optics/Excitation`	`Wavelength, Intensity, Theta, Phi, PolarizationAngle, Polarization`
`Optics/Excitation/Window`	All parameters that are not of type string or identifier.
`Optics/OpticalSolver/<SolverName>`	Except for raytracing, all parameters that are not of type string or identifier.

A list of parameter names that can be ramped in the command file is printed when the following command is executed:

```
sdevice --parameter-names <command file>
```

Accurate Absorbed Photon Density for 1D Optical Solvers

In 1D optical solvers such as `TMM`, `OptBeam`, and `FromFile`, the 1D absorbed photon density (APD) is superimposed onto the projected volume from an illumination window that extends into the 2D or 3D device geometry.

While the sampled APD at each vertex is exact for the 1D solver, the integration with `CurrentPlot` simply multiplies the box method volume, and this can result in inaccuracy due to the following:

- If the mesh is coarse, the projected volume from an illumination window intersects the box method volumes partially at the fringes.
- Depending on where the vertices are located, the box method–integrated APD can be smaller or larger than the true integrated value.

Such inaccuracies can lead to nonconservation of particles or energy because an incorrectly integrated APD produces an incorrect optically generated current.

To reduce the mesh dependency of the integrated APD values for 1D optical solvers, a virtual wireframe is constructed over the projected volume from an illumination window to compute a discrete Riemann integral of the APD. In the transverse plane of the illumination window, the wireframe is chosen automatically with either a discretization of 10 nm or a limit of 200 transverse wireframe cells. In the propagation direction, the wireframe is first divided into layers and, then within each layer, a further discretization of `NumberOfCellsPerLayer` is used for refinement.

The number of layers for the `TMM` and `OptBeam` solvers is fixed at the number of extraction layers, while the `FromFile` optical solver allows you to specify the number of layers.

`NumberOfCellsPerLayer` can be controlled by all three optical solvers. Although a denser wireframe provides a more accurate integrated APD, it also slows down the simulation since the APD must be sampled at every wireframe point in the propagation direction.

After the accurate integrated APD has been computed, it is used to compute a weighting factor for the APD on the mesh vertices such that, when `CurrentPlot` multiplies the box method volume to obtain the integrated values, you can retrieve the correct integrated APD. The vertices within the projected volume from an illumination window are divided into the center zone and the fringe zone:

- The center zone vertices have edges that connect only to vertices within the projected window volume.

- The fringe zone vertices have edges that cross the boundary of the projected window volume.

> **NOTE** The weighting factor is applied only to the fringe zone vertices, so you might see a distorted APD value at those vertices.

Numerically, the weighting factor is computed in each layer and is defined as:

$$W_{\text{layer}(k)} = \frac{\displaystyle\int_{\text{layer}(k)} f_{\text{APD}}(\text{wireframe})dv - \sum_{\text{centerzone}} F_{\text{APD}}(v_i) \cdot \text{box}(v_i)}{\displaystyle\sum_{\text{fringezone}} F_{\text{APD}}(v_i) \cdot \text{box}(v_i)} \tag{652}$$

After this computation, the weighting factor is applied to the APD of the fringe zone vertices:

$$F'_{\text{APD}}(v_i) = W_{\text{layer}(k)} \cdot F_{\text{APD}}(v_i) \tag{653}$$

However, there can be instances whereby the center zone box-integrated APD is greater than the wireframe-integrated APD. In such cases, the weighting factor is computed as

$$W_{\text{layer}(k)} = \frac{\displaystyle\int_{\text{layer}(k)} f_{\text{APD}}(\text{wireframe})dv}{\displaystyle\sum_{\text{centerzone}} F_{\text{APD}}(v_i) \cdot \text{box}(v_i) + \sum_{\text{fringezone}} F_{\text{APD}}(v_i) \cdot \text{box}(v_i)} \tag{654}$$

and it is applied to modify the APD of all center and fringe zone vertices.

This new methodology can be activated selectively in different illumination windows as follows:

```
Physics {...
   Optics (...
      Excitation (...
         Window("win_1") (...
```

```
            # To switch off, add '-' in front or leave blank.
            -WeightedAPDintegration
         )
         Window("win_2") (...
            # To switch on, use this keyword
            WeightedAPDintegration
         )
      )
   )
}
```

The syntax for controlling the wireframe density is:

```
Physics {...
   Optics (...
      Excitation (...
         Window(...) (...
            # Various options available
            WeightedAPDintegration(
               PrintInfo
               NumberOfCellsPerLayer = <int>                  # default is 10000
               NumberOfTransverseCellsPerDirection = <int>   # default is 200
               Mode = Auto                              # or Full, default is Auto
            )
         )
      )
   OpticalSolver(...
         FromFile(...
            # Default value is the number of regions but is limited to 20
            WeightedAPDintegrationlayers = <int>
            WeightedAPDIntegrationSetBoundaries = (<float>, <float>, ...)
         )
      )
   )
}
```

Some comments about this syntax:

■   To speed up the wireframe integration of APD, you probe strategic points (three points in two dimensions and five points in three dimensions) in each delta projection window (the illumination window area multiplied by the wireframe cell thickness) to determine whether to perform the full transverse numeric integration or to use a precomputed volume. The keyword `Mode=Auto` allows for a quick assessment and should be used when the projected illumination window is expected to stay within the device domain.

■   For the `TMM` and `OptBeam` optical solvers, the number of layers is set to be the same as that from the `LayerStackExtraction` section. For the `FromFile` optical solver, you can set the number of layers using `WeightedAPDIntegrationLayers`, which divides the total propagation length into equal layer thicknesses. Alternatively, if the structure contains

important thin layers, you can specify the boundaries of each layer using `WeightedAPDIntegrationSetBoundaries`. These boundaries are measured from the illumination window in the direction of propagation, so they must be positive numbers. Otherwise, the default for the number of layers is the number of significant regions, that is, regions whose volumes are at least 10% of the total volume of the device.

- You can control the discretization of the wireframe with the following keywords:

  - `NumberOfCellsPerLayer` controls the discretization in the direction of propagation.

  - `NumberOfTransverseCellsPerDirection` controls the discretization of the illumination window in the 2D plane containing the window.

  NOTE   The plane of the window might not necessarily align with the standard xy, yz, or xz planes.

Complex Refractive Index Model

The complex refractive index model in Sentaurus Device allows you to define the refractive index and the extinction coefficient depending on mole fraction, wavelength, temperature, carrier density, and local material gain. In addition, it provides a flexible interface that can be used to add new complex refractive index models as a function of almost any internally available variable.

This complex refractive index model is designed primarily for use in LED simulations, the unified interface for optical generation computation, the raytracer, the TMM, and the FDTD optical solvers. It is also supported by other tools besides Sentaurus Device, such as Sentaurus Device Electromagnetic Wave Solver (EMW) and Sentaurus Mesh, allowing for a consistent source of optical material parameters across the entire tool flow. A common Sentaurus Device parameter file can be shared and only the syntax for activating the different models may slightly change from tool to tool to comply with the respective command file syntax.

Physical Model

The complex refractive index $\tilde{n}$ can be written as:

$$\tilde{n} = n + i \cdot k \tag{655}$$

with:

$$n = n_0 + \Delta n_\lambda + \Delta n_T + \Delta n_{\text{carr}} + \Delta n_{\text{gain}} \tag{656}$$

$$k = k_0 + \Delta k_\lambda + \Delta k_{\text{carr}} \tag{657}$$

The real part n is composed of the base refractive index n_0, and the correction terms Δn_λ, Δn_T, Δn_{carr}, and Δn_{gain}. The correction terms include the dependency on wavelength, temperature, carrier density, and gain.

The imaginary part k is composed of the base extinction coefficient k_0, and the correction terms Δk_λ and Δk_{carr}. The correction terms include the dependency on wavelength and carrier density. The absorption coefficient α is computed from k and wavelength λ according to:

$$\alpha = \frac{4\pi}{\lambda} \cdot k \tag{658}$$

Wavelength Dependency

The complex refractive index model offers three ways to take wavelength dependency into account:

- An analytic formula considers a linear and square dependency on the wavelength λ:

$$\Delta n_\lambda = C_{n,\lambda} \cdot \lambda + D_{n,\lambda} \cdot \lambda^2$$
$$\Delta k_\lambda = C_{k,\lambda} \cdot \lambda + D_{k,\lambda} \cdot \lambda^2 \tag{659}$$

  The parameters $C_{n,\lambda}$, $D_{n,\lambda}$, $C_{k,\lambda}$, and $D_{k,\lambda}$ are adjusted in the `ComplexRefractiveIndex` section of the parameter file (see Table 113 on page 583).

- Tabulated values can be read from the parameter file. The table contains three columns specifying wavelength λ, refractive index n', and the extinction coefficient k'. Thereby, n' and k' represent $n_0 + \Delta n_\lambda$ and $k_0 + \Delta k_\lambda$, respectively. The character * is used to insert a comment. The row is terminated by a semicolon. For wavelengths not listed in the table, the refractive index and the extinction coefficient are obtained using linear interpolation or spline interpolation. At least two rows are required for linear interpolation. To form a cubic spline from the table entries, at least four rows are needed.

- Tabulated values can be read from an external file. The file holds a table that is structured as described in the previous point. The name of the file is specified in the `ComplexRefractiveIndex` section of the parameter file.

Temperature Dependency

The temperature dependency of the real part of the complex refractive index follows the relation according to:

$$\Delta n_T = n_0 \cdot C_{n,T} \cdot (T - T_{\text{par}}) \tag{660}$$

The parameters $C_{n,T}$ and T_{par} can be adjusted in the `ComplexRefractiveIndex` section of the parameter file (see Table 116 on page 583).

Carrier Dependency

The change in the real part of the complex refractive index due to free carrier absorption is modeled according to [1]:

$$\Delta n_{\text{carr}} = -C_{n,\,\text{carr}} \cdot \frac{q^2 \lambda^2}{8\pi^2 c^2 \varepsilon_0 n_0} \cdot \left(\frac{n}{m_n} + \frac{p}{m_p} \right) \tag{661}$$

where:

- $C_{n,\,\text{carr}}$ is a fitting parameter.
- q is the elementary charge.
- λ is the wavelength.
- c is the speed of light in free space.
- ε_0 is the permittivity.

Furthermore, n and p are the electron and hole densities, and m_n and m_p are the effective masses of electron and hole, which are computed according to the specification of the eDOSMass and hDOSMass sections in the parameter file. If only optics is solved, for example Solve {Optics} is specified in the command file, then n and p correspond to the respective doping concentrations.

To account for the change of the extinction coefficient due to free carrier absorption, a model is available that assumes linear dependency on carrier concentration and power-law dependency on wavelength:

$$\Delta k_{\text{carr}} = \frac{10^{-4}}{4\pi} \cdot \left(\left(\frac{\lambda}{\mu m} \right)^{\Gamma_{k,\,\text{carr},\,n}} \frac{C_{k,\,\text{carr},\,n}}{\text{cm}^2} \cdot \frac{n}{\text{cm}^{-3}} + \left(\frac{\lambda}{\mu m} \right)^{\Gamma_{k,\,\text{carr},\,p}} \frac{C_{k,\,\text{carr},\,p}}{\text{cm}^2} \cdot \frac{p}{\text{cm}^{-3}} \right) \tag{662}$$

where:

- $C_{k,\,\text{carr},n}$, $C_{k,\,\text{carr},p}$, $\Gamma_{k,\,\text{carr},n}$, $\Gamma_{k,\,\text{carr},p}$ are fitting parameters.
- λ is the wavelength in μm.
- n and p are the electron and hole densities in units of cm^{-3}.

For linear dependency on wavelength, $C_{k,\,\text{carr},n}$ and $C_{k,\,\text{carr},p}$ are given in units of cm^{-2}.

An alternative formulation found in the literature [2][3] reads as follows:

$$\Delta\alpha_{\text{FCA}} = An\lambda^B + Cp\lambda^D \tag{663}$$

where the free carrier absorption coefficient $\Delta\alpha_{\text{FCA}}$ is given in units of cm^{-1}, the wavelength is given in nanometers, and the carrier concentrations are given in cm^{-3}.

The fitting parameters A, B, C, and D in Eq. 663 are related to the corresponding fitting parameters in Eq. 662 by the following expressions:

$$\Gamma_{k,\,\mathrm{carr},\,n} = B + 1 \tag{664}$$

$$C_{k,\,\mathrm{carr},\,n} = 10^{3B}A \tag{665}$$

$$\Gamma_{k,\,\mathrm{carr},\,p} = D + 1 \tag{666}$$

$$C_{k,\,\mathrm{carr},\,p} = 10^{3D}C \tag{667}$$

The parameters $C_{n,\,\mathrm{carr}}$, $C_{k,\,\mathrm{carr},\,n}$, $C_{k,\,\mathrm{carr},\,p}$, $\Gamma_{k,\,\mathrm{carr},n}$, and $\Gamma_{k,\,\mathrm{carr},p}$ are adjusted in the `ComplexRefractiveIndex` section of the parameter file (see Table 117 on page 584).

Gain Dependency

The complex refractive index model offers two formulas to take into account the gain dependency:

- The linear model is given by:

$$\Delta n_{\mathrm{gain}} = C_{n,\,\mathrm{gain}} \cdot \left(\frac{n+p}{2N_{\mathrm{par}}} - 1 \right) \tag{668}$$

- The logarithmic model reads:

$$\Delta n_{\mathrm{gain}} = C_{n,\,\mathrm{gain}} \cdot \ln\left(\frac{n+p}{2N_{\mathrm{par}}} \right) \tag{669}$$

The parameters $C_{n,\,\mathrm{gain}}$ and N_{par} are adjusted in the `ComplexRefractiveIndex` section of the parameter file (see Table 118 on page 584).

Using Complex Refractive Index

The complex refractive index model is activated by using the `ComplexRefractiveIndex` statement in the `Optics` section of the `Physics` section. When using the unified interface for optical generation computation, `ComplexRefractiveIndex` can be specified globally, per region or per material. Otherwise, support is only available for global specification.

Table 283 on page 1466 lists the available keywords, which allow you to select the dependencies that change the complex refractive index, for example:

```
Physics {
   Optics (
      ComplexRefractiveIndex (
         WavelengthDep (real imag)
         TemperatureDep (real)
         CarrierDep (real imag)
         GainDep (real(log))
      )
   )
}
```

All parameters valid for the `ComplexRefractiveIndex` section of the parameter file are summarized in Table 111 to Table 118 on page 584. They can be specified for mole-dependent materials using the standard Sentaurus Device technique with linear interpolation on specified mole intervals.

Interpolation for mole-dependent tables is more complex due to the 2D nature of the problem (interpolation with respect to mole fraction and wavelength) and the sharp discontinuities near the absorption edges. Therefore, if `Formula = 1–3`, the complex refractive index at a given wavelength and mole fraction is computed by interpolating its value with respect to the wavelength for the lower and upper limits of the mole-fraction interval and subsequently with respect to the mole fraction. Optionally, the latter interpolation can be linear or piecewise constant. By default, mole-fraction interpolation for `NumericalTable` is switched off, and Sentaurus Device will exit with an error if the complex refractive index is requested at a mole fraction for which no `NumericalTable` is defined.

Table 111   Base parameters

Symbol	Parameter name	Unit
n_0	n0	1
k_0	k0	1

The keyword `Formula` is used in the parameter file to select one of the three models that are available to describe the wavelength dependency.

Table 112   Model selection for wavelength dependency

Keyword	Value	Description
Formula	=0	Use analytic formula (default).
	=1	Read tabulated values from parameter file.
	=2	Read tabulated values from external file.

Table 113   Parameters used to described wavelength dependency

Symbol	Parameter name	Unit
$C_{n,\lambda}$	Cn_lambda	μm^{-1}
$D_{n,\lambda}$	Dn_lambda	μm^{-2}
$C_{k,\lambda}$	Ck_lambda	μm^{-1}
$D_{k,\lambda}$	Dk_lambda	μm^{-2}

Table 114 lists the different interpolation methods available for `NumericalTable`, where *logarithmic interpolation* refers to taking the natural logarithm of the coordinates, performing linear interpolation, and exponentiating the results. If a value must be interpolated in an interval where one or both of the coordinates at the interval boundaries is smaller than or equal to zero, linear interpolation is used instead.

Table 114   Specifying interpolation method for NumericalTable

Keyword	Value	Description
TableInterpolation	=Linear	Use linear interpolation.
	=Logarithmic	Use logarithmic interpolation.
	=PositiveSpline	Use cubic spline interpolation. If interpolated values are negative, set them to zero (default).
	=Spline	Use cubic spline interpolation.

Table 115 lists the different interpolation methods available for interpolation of mole fraction–dependent `NumericalTable`.

Table 115   Specifying interpolation method for mole fraction–dependent NumericalTable

Keyword	Value	Description
MolefractionTableInterpolation	=Linear	
	=Off	Default
	=PiecewiseConstant	

Table 116   Parameters used to describe temperature dependency

Symbol	Parameter name	Unit
$C_{n,T}$	Cn_temp	K^{-1}
T_{par}	Tpar	K

Table 117   Parameters used to describe carrier dependency

Symbol	Parameter name	Unit	Description
$C_{n,\,\mathrm{carr}}$	`Cn_carr`	1	
$C_{k,\,\mathrm{carr},\,n}$, $C_{k,\,\mathrm{carr},\,p}$	`Ck_carr`	cm^2	Values for electrons and holes are separated by a comma.
$\Gamma_{k,\,\mathrm{carr},\,n}$, $\Gamma_{k,\,\mathrm{carr},\,p}$	`Gamma_k_carr`	1	Values for electrons and holes are separated by a comma.

Table 118   Parameters used to described gain dependency

Symbol	Parameter name	Unit
$C_{n,\,\mathrm{gain}}$	`Cn_gain`	1
N_{par}	`Npar`	cm^{-3}

An example of the `ComplexRefractiveIndex` section in the parameter file is:

```
ComplexRefractiveIndex {
    * Complex refractive index model: n_complex = n + i*k (unitless)
    * Base refractive index and extinction coefficient
    n_0 = 3.45    # [1]
    k_0 = 0.00    # [1]

    * Wavelength dependence
    * Example for analytical formula:
    Formula = 0
    Cn_lambda = 0.0000e+00    # [um^-1]
    Dn_lambda = 0.0000e+00    # [um^-2]
    Ck_lambda = 0.0000e+00    # [um^-1]
    Dk_lambda = 0.0000e+00    # [um^-2]
    * Example for reading values from parameter file:
    Formula = 1
    TableInterpolation = Spline
    NumericalTable
    ( * wavelength [um]   n [1]   k [1]
       0.30    5.003    4.130;
       0.31    5.010    3.552;
       0.32    5.023    3.259;
       0.33    5.053    3.009;
    )
    * Example for reading values from external file:
    Formula = 2
    NumericalTable = "GaAs.txt"

    * Temperature dependence (real):
```

```
          Cn_temp = 2.0000e-04       # [K^-1]
          Tpar = 3.0000e+02          # [K]

          * Carrier dependence (real)
          Cn_carr = 1                           # [1]
          * Carrier dependence (imag)
          Ck_carr = 0.0000e+00 , 0.0000e+00   # [cm^2]

          * Gain dependence (real)
          Cn_gain = 0.0000e+00       # [cm^3]
          Npar = 1.0000e+18          # [cm^-3]
      }
```

The following `ComplexRefractiveIndex` section demonstrates the use of mole fraction–dependent `NumericalTables`:

```
ComplexRefractiveIndex {
   Formula = 1
   TableInterpolation = Linear
   MolefractionTableInterpolation = Linear
   Xmax(0)=0.0
   NumericalTable(0)
   ( * wavelength [um]    n [1]    k [1]
      0.30      5.003      4.130;
      0.31      5.010      3.552;
      0.32      5.023      3.259;
      0.33      5.053      3.009;
   )
   Xmax(1)=0.25
   NumericalTable(1)
   ( * wavelength [um]    n [1]    k [1]
      0.20      5.003      4.130;
      0.29      4.010      2.552;
      0.34      4.023      1.259;
      0.49      4.053      2.009;
   )
   Xmax(2)=0.6
   NumericalTable(2)
   ( * wavelength [um]    n [1]    k [1]
      0.25      3.123      0.130;
      0.27      3.410      0.552;
      0.29      3.523      0.259;
      0.43      3.753      0.009;
   )
}
```

The complex refractive index is plotted when the keyword `ComplexRefractiveIndex` is defined in the `Plot` section.

> **NOTE** `TableODB` is no longer supported. A wavelength table of complex refractive indices can be input using the `ComplexRefractiveIndex - NumericalTable` section instead.

The complex refractive index model is available for the following optical solvers:

- Transfer matrix method for optical generation computation (see Transfer Matrix Method on page 625).

- Raytracing (see Raytracing on page 593).

Complex Refractive Index Model Interface

The complex refractive index model interface (CRIMI) allows the addition of new complex refractive index models as a function of almost any internally available variable. These models must be implemented as C++ functions, and Sentaurus Device loads the functions at runtime using the dynamic loader. No access to the Sentaurus Device source code is necessary. The concept is similar to that of the physical model interface (see Chapter 38 on page 1043); however, it is not limited to Sentaurus Device.

The generated shared object containing the model implementation can be used together with Sentaurus Device Electromagnetic Wave Solver (see Sentaurus™ Device Electromagnetic Wave Solver User Guide, Complex Refractive Index Model Interface on page 34) and Sentaurus Mesh (see Sentaurus™ Mesh User Guide, Computing Cell Size Automatically (EMW Applications) on page 95).

Three main steps are required for integrating user-defined models:

- First, a C++ class implementing the complex refractive index model must be written.

- Second, a shared object must be created that can be loaded at runtime.

- Third, the model must be activated in the command file.

These steps are described in the following sections in more detail.

C++ Application Programming Interface (API)

For each complex refractive index model, two C++ subroutines must be implemented: one to compute the refractive index and another to compute the extinction coefficient. More specifically, a C++ class must be implemented that is derived from a base class declared in the header file `CRIModels.h`. In addition, a so-called virtual constructor function, which allocates an instance of the derived class, and a virtual destructor function, which de-allocates it, must be provided.

The public interface of the base class from which a model-specific class must be derived is declared in the header file `CRIModels.h` as:

```
class CRI_Model : public CRI_Model_Interface {
   public:
      CRI_Model(const CRI_Environment& env);
      virtual ~CRI_Model();
      //definition of complex refractive index
      struct ComplexRefractiveIndexConstituentsReal {
         double n0;
         double dn_lambda;
         double dn_temp;
         double dn_carr;
         double dn_gain;
      };

      struct ComplexRefractiveIndexConstituentsImag {
         double k0;
         double dk_lambda;
         double dk_carr;
      };

      //methods to be implemented by user

      //definition of complex refractive index in terms of its constituents
      virtual void Compute_n(ComplexRefractiveIndexConstituentsReal& data);
      virtual void Compute_k(ComplexRefractiveIndexConstituentsImag& data);

      //direct definition of complex refractive index
      virtual void Compute_n(double& n) = 0;
      virtual void Compute_k(double& k) = 0;
};
```

The CRIMI provides a *basic interface* where only the actual value of the refractive index and the extinction coefficient can be overridden as well as an *advanced interface*. In the advanced interface, the total values are computed automatically from its constituents, and it has the advantage that the user-specified constituents can be visualized instead of its default values. If carrier dependency is modeled with a CRIMI and quantum yield or temperature or both should be consistent, the advanced interface must be used. If a CRIMI is used in a thermal simulation where free carrier absorption plays a role, using the advanced interface is mandatory. For more details, see Quantum Yield Models on page 544.

The arguments of the `Compute` functions indicate that they are passed as references to the respective functions. They carry the values corresponding to the model specification in the `ComplexRefractiveIndex` section in the command file. When implementing a user-defined complex refractive index model, the values for `n` and `k` (in the case of the basic interface) or the members of `struct ComplexRefractiveIndexConstituentsReal` and `struct`

`ComplexRefractiveIndexConstituentsImag` must be overwritten in the function body. Otherwise, the original values remain unchanged, which can be useful if, for example, only a new model for either the real or the imaginary part of the complex refractive index must be implemented or if only a specific constituent needs to be modified.

Often, a complex refractive index model is based on several material-specific parameters. For each region or material, these parameters can be defined in special sections of the parameter file that carry the model name as given in the command file. The parameters are best initialized in the constructor as it is called once for every region. For this purpose, the member function called `InitParameter` is used, which has two arguments. The first argument is the name of the parameter as listed in the parameter file, and the second argument is its default value. The latter is used if no value is assigned to the parameter for a particular region or material. The supported value types for user-defined parameters are integer, floating-point number, and string.

The following example shows how to initialize a parameter called `Gamma` in the constructor:

```
Constant_CRI_Model::Constant_CRI_Model(const CRI_Environment& env) :
CRI_Model(env) {

    Gamma = InitParameter("Gamma", 1.5);

}
```

where `Gamma` was declared as a data member of type `double` in the class `Constant_CRI_Model`.

In addition to the implementation of the two class member functions `Compute_n` and `Compute_k`, the virtual constructor function and destructor function must be defined as:

```
extern "C" {

    opto_n_cri::CRI_Model*
    new_CRI_Model(const opto_n_cri::CRI_Environment& env)
    {
        return new opto_n_cri::Constant_CRI_Model(env);
    }

    void
    delete_CRI_Model(opto_n_cri::CRI_Model* cri_model)
    {
        delete cri_model;
    }

}
```

In the above sample functions, it is assumed that the name of the user-provided derived class is `Constant_CRI_Model`.

Runtime Support

The base class of `CRI_Model` is derived from another class called `CRI_Model_Interface`, which adds several functions that extend the possibilities for defining new complex refractive index models. Among them are functions that query basic properties of the model such as its name, for which region and material it is called and which models have been specified in the command file. Another group of functions allows you to read the values of the most common variables on which the complex refractive index depends, namely, wavelength, carrier densities, and temperature as well as the default values for the various contributions to the complex refractive index. For most models, this set of functions should be sufficient.

For advanced models, it may be necessary to have access to additional internal variables to model the dependencies correctly. To this end, three interface functions are available that allow you to query, to register, and to read the internal variables available. A specific variable can only be read in the `Compute` functions if it has been registered in the constructor. The internal name of the corresponding variable can be obtained from the function `GetAvailableVariables`, which returns a vector of strings containing the names of all supported variables.

The remaining functions offer support for mole fraction–dependent models and for direct access of the `NumericalTables` defined in the parameter file.

The signatures of the runtime support functions discussed here can be found in the header file `CRIModels.h` and are briefly described below. Corresponding type declarations are contained in the header file `ExportedTypes.h` in the same installation directory. These header files are located in `$STROOT/tcad/$STRELEASE/lib/opto/include/`.

General utility functions:

- `std::string Name() const`: Returns the name of the `CRIModel` as specified in the command file.
- `std::string ReadRegionName() const`: Returns the name of the region to which the vertex belongs.
- `std::string ReadMaterialName() const`: Returns the name of the material to which the vertex belongs.
- `bool WithModel(ComplexRefractiveIndexModelType model) const`: Returns `true` if `model` is activated for the region to which the vertex belongs; otherwise, `false`. For each `model`, a corresponding specification in the `ComplexRefractiveIndex` section of the command file exists (see Using Complex Refractive Index on page 581).

Functions for reading the values of the most common variables on which the complex refractive index depends:

- `double ReadWavelength() const`: Returns wavelength in [μm].

- `double ReadTemperature() const`: Returns temperature in [K].

- `double Read_eDensity() const`: Returns electron density in [cm^{-3}].

- `double Read_hDensity() const`: Returns hole density in [cm^{-3}].

- `double ReadQW_eDensity() const`: Returns quantum-well electron density corresponding to the bound states of the well in [cm^{-3}].

- `double ReadQW_hDensity() const`: Returns quantum-well hole density corresponding to the bound states of the well in [cm^{-3}].

Functions for accessing additional internal variables to model the dependencies correctly:

- `const std::vector<std::string>& GetAvailableVariables() const`: Returns a vector of strings containing all internal variable names.

- `void RegisterVariableToRead(std::string variable_name)`: Use variable name string from previous call to `GetAvailableVariables()` to register a variable for reading in the function body of the `Compute` functions. This is performed typically in the constructor.

- `double ReadVariableValue(std::string variable_name) const`: Returns current value of variable selected by specifying variable name string from previous call to `GetAvailableVariables()` as argument.

The following C++ code sample shows the use of the three functions for accessing additional internal variables listed above:

```
Constant_CRI_Model::Constant_CRI_Model(const CRI_Environment& env) :
CRI_Model(env) {
   // print out available variables
   const std::vector<std::string>& variables = GetAvailableVariables();
   std::cout << "Available variables: ";
   for(size_t i=0;i<variables.size();++i){
      std::cout << variables[i] << " ";
   }std::cout << std::endl;

   RegisterVariableToRead("my_dn");
}

void Constant_CRI_Model::Compute_n(double& n) {
   double my_dataset_val = ReadVariableValue("my_dn");
   n = Read_n();
   n += my_dataset_val;
}
```

In the above code sample, the dataset `my_dn` is registered in the constructor as a readable variable and, in the `Compute` function, its value is added to the default refractive index given by the specified models such as `WavelengthDep` in the `ComplexRefractiveIndex` section. The `for` loop in the constructor is optional and allows you to query the exact names of the datasets, which are needed as arguments to the `ReadVariableValue` function.

Functions for reading the real and imaginary parts of the complex refractive index as well as its corresponding constituents computed according to the command file and parameter file specification:

- `double Read_n() const`: Returns the real part of the complex refractive index.

- `double Read_k() const`: Returns the imaginary part of the complex refractive index.

- `double Read_n0() const`: Returns the base refractive index given in Eq. 656, p. 578.

- `double Read_k0() const`: Returns the base extinction coefficient given in Eq. 657, p. 578.

- `double Read_d_n_lambda() const`: Returns the change in refractive index due to its wavelength dependency.

- `double Read_d_k_lambda() const`: Returns the change in extinction coefficient due to its wavelength dependency.

- `double Read_d_n_temp() const`: Returns the change in refractive index due to its temperature dependency.

- `double Read_d_n_carr() const`: Returns the change in refractive index due to its carrier dependency.

- `double Read_d_k_carr() const`: Returns the change in extinction coefficient due to its carrier dependency.

- `double Read_d_n_gain() const`: Returns the change in extinction coefficient due to its gain dependency.

Functions for retrieving information about mole fraction–dependent models and for direct access of the `NumericalTables` defined in the parameter file:

- `int ReadNumberOfMoleFractionIntervals() const`: Returns the number of mole-fraction intervals defined in the `ComplexRefractiveIndex` section of the parameter file.

- `double ReadxMoleFractionUpperLimit(int interval) const`: Returns upper limit of x-mole fraction interval specified as an argument.

- `double ReadNumericalTableValue_n(int interval = 0) const`: Returns the refractive index for the current wavelength and the mole-fraction interval specified as an argument.

- `double ReadNumericalTableValue_k(int interval = 0) const`: Returns the extinction coefficient for the current wavelength and the mole-fraction interval specified as an argument.

- `NumericalTable<double>* ReadNumericalTable(int interval = 0) const`: Returns the numeric table for the mole-fraction interval specified as an argument. This function may be useful if a custom table interpolation algorithm must be implemented.

Shared Object Code

Sentaurus Device assumes that the shared object code corresponding to a CRI model can be found in the file `modelname.so.arch`. The base name of this file must be identical to the name of the CRI model. The extension `.arch` depends on the hardware architecture.

The script `cmi`, which is also a part of the CMI (see Compact Models User Guide, Chapter 4 on page 125), can be used to produce the shared object files (see Compact Models User Guide, Runtime Support on page 150).

Command File of Sentaurus Device

To load CRI models into Sentaurus Device, the `PMIPath` search path must be defined in the `File` section of the command file. The value of `PMIPath` consists of a sequence of directories, for example:

```
File {
    PMIPath = ". /home/joe/lib /home/mary/sdevice/lib"
}
```

For each CRI model, which appears in the `ComplexRefractiveIndex` section, the given directories are searched for a corresponding shared object file `modelname.so.arch`.

A CRI model can be activated in the `ComplexRefractiveIndex` section of the command file by specifying the name of the model as shown in the following example:

```
Physics {
    Optics (
        ComplexRefractiveIndex (
            CRIModel (Name = "modelname")
        )
    )
}
```

A CRI model name can only consist of alphanumeric characters and underscores (_). The first character must be either a letter or an underscore. All the CRI models can be specified regionwise or materialwise:

```
Physics (region = "Region.1") { ... }
Physics (material = "SiO2") { ... }
```

when using the unified interface for optical generation computation in Sentaurus Device; otherwise, only global specification is supported.

Raytracing

Sentaurus Device supports the simulation of photogeneration by raytracing in two and three dimensions for arbitrarily shaped structures, as well as body-of-revolution structures using 2D and cylindrical coordinates. The calculation of refraction, transmission, and reflection follows geometric optics, and special boundary conditions can be defined. A dual-grid setup can be used to speed up simulations that include raytracing.

Raytracer

In Sentaurus Device, the raytracer has been implemented based on linear polarization. It is optimized for speed and needs to be used in conjunction with the complex refractive index model (see Complex Refractive Index Model on page 578). Each region/material must have a complex refractive index section defined in the parameter file. If the refractive index is zero, it is set to a default value of 1.0.

The raytracer uses a recursive algorithm: It starts with a source ray and builds a binary tree that tracks the transmission and reflection of the ray. A reflection/transmission process occurs at interfaces with refractive index differences. This is best illustrated in Figure 30.

An incident ray impinges on the interface of two different refractive index (n_1 and n_2) regions, resulting in a reflected ray and a transmitted ray. The incident, reflected, and transmitted rays are denoted by the subscripts i, r, and t, respectively. Likewise, the incident, reflected, and transmitted angles are denoted by θ_i, θ_r, and θ_t, respectively. These angles can be derived from the concept of interface tangential phase-matching (commonly called Snell's law) using:

$$n_1 \sin \theta_i = n_2 \sin \theta_t \tag{670}$$

To define these angles, a plane of incidence must be clearly defined. It is apparent that the plane of incidence is the plane that contains both the normal to the interface and the vector of the ray.

When the plane of incidence is defined, the concept of TE and TM polarization can then be established.

A ray can be considered a plane wave traveling in a particular direction with its polarization vector perpendicular to the direction of propagation. The length of the polarization vector represents the amplitude, and the square of its length denotes the intensity. The TE polarization (s-wave) applies to the ray polarization vector component that is perpendicular to the plane of incidence. On the other hand, the TM polarization (p-wave) applies to the ray polarization vector component that is parallel to the plane of incidence.

In Figure 30, the TE and TM components of the ray polarization vector are denoted by E_{TE} and E_{TM}, respectively.
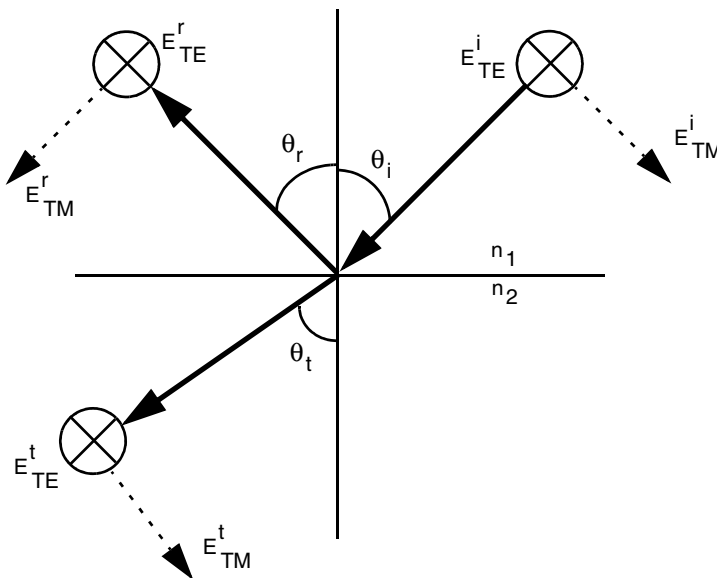
Figure 30   Incident ray splits into reflected and transmitted rays at an interface: the TE component of the polarization vector maintains the same direction, whereas the TM component changes direction

The TE and TM components of the ray polarization vector experience different reflection and transmission coefficients. These coefficients are:

Amplitude reflection coefficients:

$$r_{\mathrm{TE}} = \frac{k_{1z} - k_{2z}}{k_{1z} + k_{2z}} \tag{671}$$

$$r_{\mathrm{TM}} = \frac{\varepsilon_2 k_{1z} - \varepsilon_1 k_{2z}}{\varepsilon_2 k_{1z} + \varepsilon_1 k_{2z}} \tag{672}$$

Amplitude transmission coefficients:

$$t_{\mathrm{TE}} = \frac{2k_{1z}}{k_{1z} + k_{2z}} \tag{673}$$

$$t_{\mathrm{TM}} = \frac{2\varepsilon_2 k_{1z}}{\varepsilon_2 k_{1z} + \varepsilon_1 k_{2z}} \tag{674}$$

Power reflection coefficients:

$$R_{\mathrm{TE}} = |r_{\mathrm{TE}}|^2 \tag{675}$$

$$R_{\mathrm{TM}} = |r_{\mathrm{TM}}|^2 \tag{676}$$

Power transmission coefficients:

$$T_{\mathrm{TE}} = \frac{k_{2z}}{k_{1z}}|t_{\mathrm{TE}}|^2 \tag{677}$$

$$T_{\mathrm{TM}} = \frac{\varepsilon_1 k_{2z}}{\varepsilon_2 k_{1z}}|t_{\mathrm{TM}}|^2 \tag{678}$$

where:

$$k_0 = 2\pi/\lambda_0 \tag{679}$$

$$k_{1z} = n_1 k_0 \cos\theta_i \tag{680}$$

$$k_{2z} = n_2 k_0 \cos\theta_t \tag{681}$$

$$\varepsilon_1 = n_1^2 \tag{682}$$

$$\varepsilon_2 = n_2^2 \tag{683}$$

where λ_0 is the free space wavelength, and k_0 is the free space wave number. Note that for amplitude coefficients, $1 + r = t$. For power coefficients, $R + T = 1$. These relations can be verified easily by substituting the above definitions of the reflection and transmission coefficients of the respective TE and TM polarizations. For normal incidence when $\theta_i = \theta_t = 0$, $r_{\mathrm{TE}} = -r_{\mathrm{TM}}$, and $R_{\mathrm{TE}} = R_{\mathrm{TM}}$.

If the refractive index is complex, the reflection and transmission coefficients are also complex. In such cases, only the absolute value is taken into account.

The raytracer automatically computes the plane of incidence at each interface, decomposes the polarization vector into TE and TM components, and applies the respective reflection and transmission coefficients to these TE and TM components.

Ray Photon Absorption and Optical Generation

When there is an imaginary component (extinction coefficient), κ, to the complex refractive index, absorption of photons occurs. To convert the absorption coefficient to the necessary units, the following formula is used for power/intensity absorption:

$$\alpha(\lambda)[\text{cm}^{-1}] = \frac{4\pi\kappa}{\lambda} \tag{684}$$

In the complex refractive index model, the refractive index is defined element-wise. In each element, the intensity of the ray is reduced by an exponential factor defined by $\exp(-\alpha L)$ where L is the length of the ray in the element. Therefore, the photon absorption rate in each element is:

$$G^{\text{opt}}(x, y, z, t) = I(x, y, z)[1 - e^{-\alpha L}] \tag{685}$$

$I(x, y, z)$ is the rate intensity (units of s^{-1}) of the ray in the element. After all of the photon absorptions in the elements have been computed, the values are interpolated onto the neighboring vertices and are divided by its sustaining volume to obtain the final units of $\text{s}^{-1} \cdot \text{cm}^{-3}$. The absorption of photons occurs in all materials (including nonsemiconductor) with a positive extinction coefficient for raytracing. Depending on the quantum yield (see Quantum Yield Models on page 544), a fraction of this value is added to the carrier continuity equation as a generation rate so that correct accounting of particles is maintained.

Using the Raytracer

The raytracer must be invoked within the unified interface for optical generation computation (see Raytracing on page 556), and can have the following options:

- Raytracing used in simple optical generation.
- Monte Carlo raytracing.
- Multithreading for raytracing.
- Compact memory model for raytracing.
- User-defined and distribution windows of starting rays.
- Cylindrical coordinates for raytracing.
- Different boundary conditions for raytracing.
- Visualizing raytracing results.

Optical generation by raytracing is activated by the `RayTracing` statement in the `Physics` section. An example of optical generation by raytracing is:

```
Plot {...
   RayTrees
}

Physics {...
   Optics (
      ComplexRefractiveIndex(
         WavelengthDep(real imag)
         CarrierDep(real imag)
         GainDep(real)                        * or real(log)
         TemperatureDep(real)
         CRImodel (Name = "crimodelname")
      )
      OpticalGeneration(...)
      Excitation (...
         PolarizationAngle = 45              * deg
         Wavelength        = 0.5             * um
         Intensity         = 0.1             * W/cm2
         Window(
            Rectangle(dx = 1, dy = 2)
            IntensityDistribution(...)
         )
      )
      OpticalSolver (
         RayTracing(
            RayDistribution(...)
            MonteCarlo
            CompactMemoryOption    * reduced memory consumption
            MinIntensity = 1e-3    * fraction of start intensity to stop ray
            UseAverageMinIntensity * use average intensity of all starting rays
                                   * as reference for MinIntensity
            DepthLimit = 1000      * maximum number of interfaces to pass
            RetraceCRIchange = 0.1 * fractional change of CRI to retrace
         )
      )
   )
}
```

The complex refractive index model must be used in conjunction with the raytracer. Various dependencies of the complex refractive index can be included, and they are controlled by parameters in the `ComplexRefractiveIndex` section of the parameter file (see Complex Refractive Index Model on page 578). The CRI model can be defined regionwise or materialwise. The keyword `RetraceCRIchange` specifies the fractional change of the complex refractive index (either the real or imaginary part) from its previous state that will

force a total recomputation of raytracing. To force retracing at every ramping point, you can set `RetraceCRIchange` to a negative number.

The starting rays are defined by a rectangular window or a user-defined window (see Window of Starting Rays on page 600).

Terminating Raytracing

Raytracing offers different termination conditions:

- Raytracing is terminated if the ray intensity becomes less than n times (`MinIntensity` specifies n) the original intensity of each starting ray.

- `DepthLimit` specifies the maximum number of material boundaries that the ray can pass through.

- `UseAverageMinIntensity` activates the computation of an average value of all the starting rays, I_{avg}, and raytracing terminates when the ray intensity becomes less than $I_{avg} \times \text{MinIntensity}$. This is only useful with the spatial intensity excitation profile (see Spatial Intensity Function Excitation on page 568).

Monte Carlo Raytracing

In instances where rays are randomly scattered, for example on rough surfaces, a Monte Carlo–type raytracing is required, since you need to look at the aggregate solution of the raytracing process.

The concept of Monte Carlo raytracing follows that of the Monte Carlo method for carrier transport simulation. Suppose a ray impinges an interface. In the deterministic framework, the ray will split into a reflected part and a transmitted part at this interface. In the Monte Carlo framework, you track only one ray path and take the reflectivity as a probability constraint to decide if the ray is to be reflected or transmitted. As more rays impinge this material interface, the aggregate number of reflected rays will recover information about the reflectivity, and this is the crux of the Monte Carlo method. In a likewise manner, rough surface scattering gives an angular probability and, using the same strategy, the ensemble average of rays can model the physics of rough surface scattering.

As an example, the algorithm for the Monte Carlo raytracing at a regular material interface is:

- Compute the reflection and transmission coefficients, R and T, of the ray at the material interface.

- Generate a random number, r.

- If $r \leq R$, then choose to propagate the reflected ray only.
- If $r > R$, then choose to propagate the transmitted ray only.

In the case of special rays, such as those from the raytrace PMI, care must be taken to choose only a single propagating ray based on a new set of probabilistic rules.

The Monte Carlo raytracing has been implemented in both general raytracing and LED raytracing. The syntax is:

```
Physics {
   Optics (
      OpticalSolver (
         RayTracing (
            MonteCarlo
         )
      )
   )
}
```

> **NOTE**   Since only one ray path is chosen at each scattering event in the Monte Carlo method, the rays in the raytree will appear to have the same intensity values after scattering.

Multithreading for Raytracer

Each raytree traced from the list of starting rays is mutually exclusive, so that the raytracer is an excellent candidate for parallelization.

To activate the multithreading capability of the raytracer, include the following syntax in the `Math` section of the command file:

```
Math {
   Number_Of_Threads = 2    # or maximum
   StackSize = 20000000     # increase to, for example, 20 MB
}
```

> **NOTE**   Raytracing is a recursive process, so it can easily obliterate the default (1 MB) stack space if the level of the raytree becomes increasingly deep. This may lead to unexplained segmentation faults or abortion of the program. To resolve this issue, increase the stack space using the keyword `StackSize` in the `Math` section as shown in the above syntax. The other solution is to use the compact memory model as described next.

Compact Memory Model for Raytracer

The compact memory model for the raytracer does not store the raytree as it is being created, so it reduces the use of significant memory. Only essential information is tracked and stored, and this alleviates the amount of memory required. A reduced structure is used, and clever ways of extracting information in this reduced structure have been implemented without upsetting the multithreading feature of raytracing.

The compact memory model is activated as the default only for the unified interface for optical generation computation. The default is still switched off for the LED raytracing interface. A minus sign can be added in front of the keyword to deactivate it. If raytrees are requested to be plotted in the `Plot` statement, the compact memory model is switched off automatically, and a warning message appears in the log file to alert you of the changes. The command file syntax to switch off the compact memory option is:

```
Physics {...
   Optics( OpticalSolver(...
      RayTracing (
         -CompactMemoryOption
      )
   ))
}
```

Window of Starting Rays

Two mutually exclusive options for defining a set of starting rays are available: a user-defined set of rays or a distribution window. These can be defined within the `Physics-Optics-OpticalSolver-Raytracing` statement syntax:

```
UserWindow (
   NumberOfRays = integer          # number of rays in file
   RaysFromFile = "filename.txt"    # position(um) direction area(cm^2)
   PolarizationVector = Random | ReadFromExcitation | ReadFromFile
)

RayDistribution (WindowName= "windowname1" ...)
```

User-Defined Window of Rays

In the `UserWindow` section, you can enter your own set of starting rays using a text file. This means that you can choose the positions, directions, area, and polarization vector of each starting ray, thereby achieving greater flexibility.

The power (W) of each ray then is computed by multiplying the input area (cm^2 in 3D or cylindrical simulations, and cm in 2D simulations) by the input wave power (W/cm^2). Remarks are allowed but they must begin with a hash character (#). A sample of this file for 3D rays is:

```
filename.txt:
   # Position(x,y,z)[um]  Direction(x,y,z)[um]  Area[cm^2] Polarization(x,y,z)
   0.0    0.0    0.0      0.0    0.0    1.0      1.0e-5      1 0 0
   0.0    0.05   0.0      0.0    0.0    1.0      1.0e-5      0 1 0
   0.0    0.05   0.05     0.0    0.0    1.0      1.0e-5      0 1 0
   ...
```

> **NOTE** In 2D simulations, you must input the `Area` as a segment length (in cm). Consistent with 2D Sentaurus Device simulations, the third dimension is taken to be a default of $1\mu m$, which means that the actual area for each user ray is the user `Area` [cm] multiplied by $1\mu m$.

Different types of `PolarizationVector` can be chosen:

- `Random`: A random vector perpendicular to the ray direction is generated. In two dimensions, the generated random vector can be a 3D vector.

- `ReadFromFile`: The polarization vector is entered as the last three columns in the file.

- `ReadFromExcitation`: The polarization vector is constructed based on the information contained within the `Excitation` section. This is the default if the keyword `PolarizationVector` is omitted. The priority order for reading the polarization under this option is:
  (1) `OpticalSolver - RayTracing - PolarizationVector = (<float> <float> <float>)`
  (2) `OpticalSolver - RayTracing - PolarizationRandom`
  (3) `Excitation - PolarizationAngle = <float>`
  (4) `Excitation - Polarization = TE | TM | <float>`

If none of these options is found, `Excitation - PolarizationAngle=0` is used by default.

> **NOTE** If `PolarizationVector` is set to `ReadFromExcitation` or `Random`, the last three columns of the file that describe the polarization are ignored.

In 2D simulations, the TE polarization vector is (0,0,1) and the TM polarization vector is formed by the cross product of the ray's direction vector and (0,0,1), with reference to Figure 30 on page 594.

Table 119 Requirements for the parameters in the input file for the user ray

Parameter	2D simulation	Cylindrical simulation	3D simulation
Position [μm]	(x,y,0)	(x,y,0)	(x,y,z)
Direction	(x,y,0)	(x,y,0)	(x,y,z)
Units of user input `Area`	cm (internally will be multiplied by $1\,\mu$m)	cm^2	cm^2
Polarization vector (`ReadFromFile` only)	(x,y,z)	(x,y,z)	(x,y,z)

Distribution Window of Rays

When the illumination window (see Illumination Window on page 562) is defined for raytracing, a corresponding `RayDistribution` section must be created to define how the excitation parameters can be translated in a raytracing context:

```
Physics {
   Optics (
      Excitation(
         Window ("windowname1")(
            Origin = (xx,yy)
            OriginAnchor = Center | North | South | East | West | NorthEast |
               SouthEast | NorthWest | SouthWest
            RotationAngles = (phi, theta, psi)
            xDirection = (x,y,z)
            yDirection = (x,y,z)
            # You can define one of the following excitation shapes.
            # Rectangle, Circle, and Polygon are for three dimensions.
               Rectangle( ... )
               Line( ... )
               Circle( ... )
               Polygon( ... )
         )
         Window ("windowname2") (...)
         Window ("windowname3") (...)
      )
      OpticalSolver(
         Raytracing(
            RayDistribution(
               WindowName = "windowname1"
               Mode = Equidistant | MonteCarlo | AutoPopulate
               NumberOfRays = integer     # for Mode=MonteCarlo | AutoPopulate
               Dx = float                 # for Mode=Equidistant
               Dy = float                 # for Mode=Equidistant
               Scaling = float            # scaling factor
            )
```

```
              RayDistribution (WindowName="windowname2" ...)
              RayDistribution (WindowName="windowname3" ...)
           )
        )
     )
  }
```

Multiple excitation windows and `RayDistribution` windows can be created. The only restriction is that every `RayDistribution` section must have a matching `Excitation` section. Matching is through the user-specified window name. If no window name for the `RayDistribution` section is specified, the parameters in that window are applied to all excitation windows, except those with matching window names.

The shape of the excitation is defined in the `Excitation(...Window(...))` section, and the shape can be a `Line` for two dimensions, and a `Rectangle`, `Circle`, or `Polygon` for three dimensions.

There are different ways in which you can create a set of starting rays on the excitation shape:

- `Mode=Equidistant`: The starting positions of the rays are arranged in a regular grid with intervals defined by `Dx` and `Dy`. Then, the grid is superimposed onto the excitation shape to extract an appropriate set of starting rays.

- `Mode=MonteCarlo`: Random positions are generated with the excitation shape to form the set of starting rays.

- `Mode=AutoPopulate`: A uniform grid of variable grid size is superimposed onto the excitation shape. The grid size is varied until the maximum possible number of grid points that is less than `NumberOfRays` can be fitted into the shape, and the set of starting ray positions is extracted from the fitted grid vertices.

Cylindrical Coordinates for Raytracing

Body-of-revolution structures can be modeled optically in raytracing by tracing the rays in the 2D cut of the cylindrical structure and taking into account the reflection at the cylindrical axis and the ring volume of revolution.

To model body-of-revolution structures with raytracing:

1. Switch on the cylindrical coordinates in the `Math` section, and specify the location of the cylindrical axis. You can use either the keyword `xAxis` to specify the revolution around the y-axis (`xAxis=<float>`) or the keyword `yAxis` to specify the revolution around the x-axis (`yAxis=<float>`). The syntax is:

   ```
   Math {...
       Cylindrical(xAxis=<float>)       # default is xAxis=0
   }
   ```

2. Define the illumination window appropriately, so that it lies on the same side as the device from the cylindrical axis, and both the window and device do not intersect the cylindrical axis.

3. There is no need to define any special reflecting boundary at the cylindrical axis. Sentaurus Device automatically creates an internal virtual reflecting boundary at the cylindrical axis so that any rays impinging it will be reflected.

4. The `RayDistribution` illumination window supports cylindrical coordinates. All methods of generating cylindrical starting rays are possible: `AutoPopulate`, `Equidistant`, and `MonteCarlo`. If the Gaussian spatial intensity is specified, the Gaussian shape is superimposed on the cylindrical ring-area weighted power of each starting ray, only for the `AutoPopulate` and `Equidistant` options. There is no support for the Gaussian spatial intensity and cylindrical `MonteCarlo` starting rays.

5. The illumination window can be at a skewed angle from the cylindrical axis, as shown in Figure 31.

Assuming that the angle subtended between the illumination window and the cylindrical axis is θ, the conical ring area of revolution is:

$$\text{Area} = \pi(r_1 + r_2)(r_2 - r_1)\frac{1}{\sin\theta} \tag{686}$$

This area is multiplied to each starting ray to retrieve the power carried by it. As a check, when $\theta = 90°$, Eq. 686 reduces to that of a ring area.
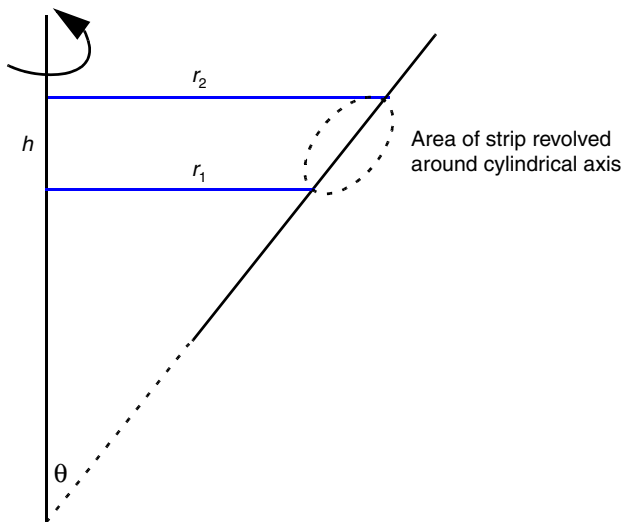
Figure 31   An illumination window subtended at an angle θ from the cylindrical axis, forming a conical surface of revolution

Boundary Condition for Raytracing

Special and spatially arbitrary boundary conditions can be specified in raytracing. There are two ways to define a boundary condition (BC) for raytracing by:

- Using special contacts.

  In the contact-based definition, the boundaries are drawn as contacts (see Specifying Electrical Boundary Conditions on page 67) and are labeled accordingly using Sentaurus Structure Editor. These contacts can be constructed specifically for setting a raytrace boundary condition, or they can coincide with an electrode or a thermode. To define clearly special raytrace boundary conditions, each line or surface contact defined must have a distinct name. This means that two parallel contacts must have different contact names, and intersecting contacts must also have different contact names. The contact is discretized into edges (2D) or faces (3D) after meshing.

- Using `Physics MaterialInterface` or `Physics RegionInterface`.

  In the `Physics MaterialInterface`– or `Physics RegionInterface`–based definition, the boundaries are defined at the interface between the material or region. As with typical Sentaurus Device operation, `RegionInterface` takes precedence over `MaterialInterface`. After meshing, the interface is discretized into edges (two dimensions) or faces (three dimensions).

A mixture of contact-based and physics interface definitions of BCs is allowed. However, the contact-based definition takes precedence over the physics interface–based definition if there is an overlap.

Each edge or face defined as a special contact can only associate itself to one type of boundary condition. The following boundary conditions are listed in the order of preference, that is, if two boundary conditions are specified for the same edge or face, the higher ranked one is chosen:

1. Fresnel BC.

2. Constant reflectivity/transmittivity BC.

3. Raytrace PMI BC.

4. Multilayer antireflective coating BC.

5. Diffuse surface BC, implemented as an installed PMI.

6. Periodic BC.

Fresnel Boundary Condition

The physics interface–based BC can quickly set many interfaces to a particular type of BC, especially if the material interface contains many region interfaces. What is missing is the disabling of a particular region interface from the general BC definition. Therefore, the Fresnel BC is introduced as a complement set to unset a particular region interface-based or contact-based BC. This can greatly simplify the command syntax input and enhance ease of use.

Furthermore, the Fresnel BC also can be used to *sense* the photon flux flowing through a particular interface when users activate the `PlotInterfaceFlux` feature (see Plotting Interface Flux on page 618).

The syntax for activating the Fresnel BC is:

```
RayTraceBC {                        Physics(RegionInterface="reg1/reg2") {
  { Name = "contact1"                 RaytraceBC (
    Fresnel                             Fresnel
  }                                   )
}                                   }
```

Constant Reflectivity and Transmittivity Boundary Condition

In the command file, constant reflectivity and transmittivity boundaries must be specified by the following syntax:

```
RayTraceBC {                        Physics (RegionInterface="regionname1/regionname2") {
  { Name = "ref_contact1"             RayTraceBC (
    Reflectivity = float                Reflectivity = float
  }                                     Transmittivity = float
  { Name = "ref_contact2"             )
    Reflectivity = float            }
    Transmittivity = float
  }
  ...
}
```

These are power reflection, R, and transmission, T, coefficients. It is not necessary for $R + T = 1$. If R is specified only, $T = 1 - R$. If T is specified only, $R = 1 - T$.

For total absorbing or radiative boundary conditions, set `Reflectivity = 0` and `Transmittivity = 0` (or `Transmittivity = 1`). Defining `Reflectivity = 1` ensures that rays are totally reflected at that boundary. In the 2D case, reflection occurs at the edge of the element. In the 3D case, reflection occurs at the face of the element. This versatile boundary condition feature enables you to use symmetry to reduce the simulation domain.

Examples of the boundary condition whereby `Reflectivity` has been set to 1.0 are shown in Figure 32 and Figure 33. In the 2D case, a star boundary is drawn within a device; in the 3D case, a rectangular boundary is drawn within the device.
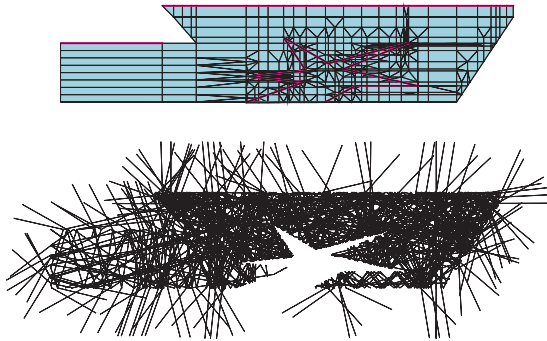
Figure 32   Applying the reflecting boundary condition in a 2D LED simulation; the boundary is drawn as a star inside the device
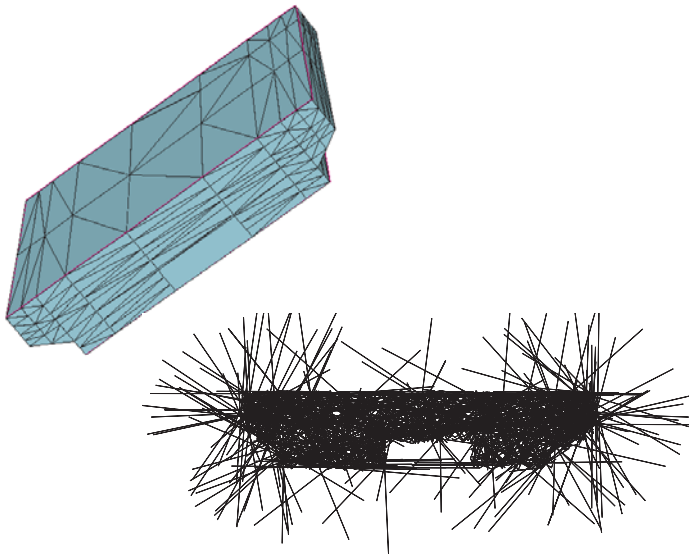
Figure 33   Applying the reflecting boundary condition in a 3D LED simulation; the boundary is drawn as a hollow rectangular waveguide inside the device

Raytrace PMI Boundary Condition

A special raytrace PMI BC can be defined. You can obtain useful information about the ray with this raytrace PMI and can modify some parameters of the ray. For details about this PMI and how it can be incorporated into the simulation, see Preprocessing for Newton Iterations and Newton Step Control on page 1246.

As with the standard PMI, you can create a PMI section in the parameter file where you can initialize the parameters of the PMI. Note that the parameter must be specified either regionwise or material-wise in accordance to the standard PMI framework.

To activate the PMI, specify the location of the PMI BC and include the following syntax in the `RayTraceBC` section of the command file:

```
RayTraceBC {...                       Physics (MaterialInterface="materialname1/materialname2") {
  { Name = "pmi_contact"                RayTraceBC (
    PMIModel = "pmi_modelname"            pmiModel = "modelname"
  }                                     )
}                                     }
```

> **NOTE** Care must be taken to ensure that your PMI code is thread safe since the raytracing algorithm is multithreaded. Use only local variables and avoid global variables in your PMI code (see Parallelization on page 1091).

Thin-Layer-Stack Boundary Condition

A thin-layer-stack boundary condition can be used to model interference effects in raytracing. The modeling of antireflective coatings used in solar cells is a typical example of the use of such boundary condition. The coatings are specified as special contacts and are treated as a boundary condition for the raytracer. The angle at which the ray is incident on the coating is passed as input to the TMM solver (the theory is described in Transfer Matrix Method on page 625), which returns the reflectance, transmittance, and absorbance for both parallel and perpendicular polarizations to the raytracer. The angle of refraction is calculated by the raytracer according to Snell's law, a direct implication of phase matching. This boundary condition is available for both 2D and 3D simulations.

The following command file excerpt, along with its demonstration in Figure 34 on page 609, shows the use of this boundary condition:

```
RayTraceBC {                          Physics (MaterialInterface="Gas/Silicon") {
  { Name="rayContact1" reflectivity=1.0 }   RayTraceBC (
  { Name="rayContact2"                        TMM (
    ReferenceMaterial = "Gas"                   ReferenceMaterial = "Gas"
    LayerStructure {                            LayerStructure {
      70e-3 "Nitride"; # um                       70e-3 "Nitride";  # um
      6e-3 "Oxide"     # um                        6e-3 "Oxide";     # um
    }                                           }
  }                                         )
}                                         )
                                        }
```

The first line in the `RayTraceBC` section above shows the definition of a constant reflectivity as a boundary condition (see Fresnel Boundary Condition on page 606). This option is usually chosen for the boundary of the simulation domain.

The other section defines a multilayer structure, for which the corresponding contact (`rayContact2`) in the grid file can be seen as a placeholder. Alternatively, you can use the `Physics` interface method of specifying such a special BC (as shown in the above syntax to the right). For each layer, the corresponding thickness ([µm]) and material name must be specified. For the calculation of transmittance and reflectance, the transfer matrix method reads the complex refractive index from the respective parameter file. An additional parameter file or a new set of parameters must be added by you in either of the following cases: (a) a layer contains a material that does not exist in the grid file or (b) the material properties of a layer differ from the properties of a region in the grid file with the same material.

To fix the orientation of the multilayer structure with respect to the specified contact in the grid file, a `ReferenceMaterial` or a `ReferenceRegion` that is adjacent to the contact must be specified. The topmost entry of the `LayerStructure` table corresponds to the layer that is adjacent to the `ReferenceMaterial` or `ReferenceRegion`.

> **NOTE** It is only possible to specify a `ReferenceMaterial` or `ReferenceRegion` if the material names or region names, respectively, on either side of the contact do not coincide.

The multilayer structure is allowed to have an arbitrary number of layers.
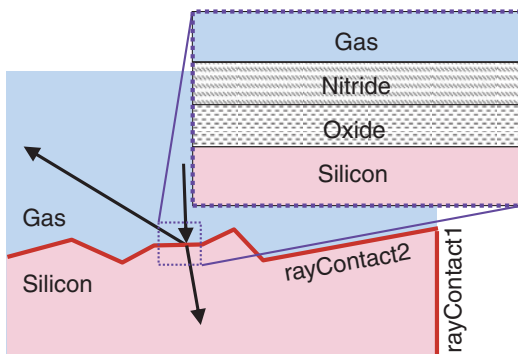
Figure 34   Illustration of thin-layer-stack boundary condition for simulation of an antireflection-coated solar cell

TMM Optical Generation in Raytracer

In modern thin-film solar-cell design, the multilayer thin film can be made of materials that can generate carriers by absorbing photons. To cater to such a phenomenon, the TMM contact in the raytracer has been modified to collect optical generations as rays traverse the TMM contact.

The collected optical generations can then be distributed into specific regions of the electrical grid.

In addition, to model the correct optical geometry, the thin-film layers must be drawn into the device structure. However, the raytracer treats the physics of thin film using a TMM contact, and these thin layers should effectively be ignored during the raytracing process. As such, you need to use `VirtualRegions` (see Virtual Regions in Raytracer on page 614) to ignore these thin layers in the raytracing process. The required syntax is:

```
RayTraceBC {...                      Physics (RegionInterface="regionname1/
  { Name="TMMcontact"                regionname2") {
    ReferenceMaterial = "Gas"          RayTraceBC (
    LayerStructure {...}                 TMM (
    MapOptGenToRegions {"thinlayer1"       ReferenceMaterial = "Gas"
                    "thinlayer2" ...}      LayerStructure {...}
    QuantumEfficiency = float              MapOptGenToRegions {"thinlayer1"
  }                                                        "thinlayer2" ...}
}                                          QuantumEfficiency = float
                                         )
                                       )
                                     }
```

```
  Physics {...
    Optics(...
      OpticalSolver(
        RayTracing (...
          VirtualRegions{"toppml" "nitride" "oxide" ...}
        )
      )
    )
  }
```

A few comments about the syntax:

■   `QuantumEfficiency` denotes the fraction of absorbed photons in the TMM BC that will be converted to optical generation. The keyword `QuantumYield` also can be specified in the unified raytracing interface. Therefore, the overall quantum yield of the TMM BC is a product of `QuantumEfficiency` and `QuantumYield`.

■   The region names in the `MapOptGenToRegion` section refer to regions in the electrical device grid. The `MapOptGenToRegions{...}` list and `VirtualRegions{...}` list are independent, and there is no need for a one-to-one correspondence. For example, you can have `VirtualRegions{r1,r2,r3}` and `MapOptGenToRegions{r2,r4}` whereby the entire optical generation from a TMM BC will be mapped onto regions `r2` and `r4` according to their volume ratio. The order of the region list is not relevant.

- For the optical generation mapping, a constant optical generation profile is assumed. The optical generation from a TMM BC is lumped into a constant value and distributed to different `MapOptGenToRegions` regions according to their volume ratios.

- The region names in the `VirtualRegions` section refer to regions in the optical device grid.

Diffuse Surface Boundary Condition

Rough surfaces can be modeled by diffuse surface boundary conditions. The available diffuse BC models are:

- Phong scattering model with distribution:

$$I/I_0 = \cos^\omega(\alpha + \gamma) \tag{687}$$

where ω is the order of the Phong model, α is the scattered angle with respect to the scattering surface, and γ is an offset angle for the lobe of the distribution.

- Lambert scattering model with distribution:

$$I/I_0 = \cos(\alpha + \gamma) \tag{688}$$

NOTE The Lambert scattering model is a special case of the Phong model.

- Gaussian scattering model with distribution:

$$I/I_0 = \exp\left(-\frac{(\alpha + \gamma)^2}{2\sigma^2}\right) \tag{689}$$

where σ^2 is the variance of the distribution.

- Random scattering model with uniform distribution.

Within Sentaurus Device, a random number $x \in [0, 1]$ is generated, and a mapping function is used to compute the scattering angle α. The mapping function is computed as follows:

The random number $x \in [0, 1]$ has a uniform distribution such that:

$$\int_0^1 f(x)dx = 1 \tag{690}$$

The scattering angle $\alpha \in [0, \pi/2]$ has a distribution function, $p(\alpha)$, which can be the Phong, Lambert, or Gaussian model.

3D Case

The mapping requirement is:

$$p(\alpha)2\pi R \sin\alpha d\alpha = f(x)dx \tag{691}$$

and the normalization requirement is:

$$\int_0^{\pi/2} 2\pi R p(\alpha) \sin\alpha d\alpha = 1 \tag{692}$$

2D Case

The mapping requirement is:

$$p(\alpha)Rd\alpha = f(x)dx \tag{693}$$

and the normalization requirement is:

$$\int_0^{\pi/2} p(\alpha)Rd\alpha = 1 \tag{694}$$

For the different scattering models, R must be derived based on the normalization conditions for 2D and 3D, respectively.

To find the inverse mapping of the random variable x to α, the integration of the probability density functions to α and x is performed, respectively:

$$\int_0^{\alpha} 2\pi R p(\alpha) \sin\alpha d\alpha = x \text{ for 3D} \tag{695}$$

and:

$$\int_0^{\alpha} p(\alpha)Rd\alpha = x \text{ for 2D} \tag{696}$$

Then, the objective would be to express α as a function of x. As an example, the inverse mapping function for the 3D Phong model is:

$$\alpha = \cos^{-1}[^{\omega+1}\!\sqrt{1-x}] \tag{697}$$

The inverse mapping functions of the other scattering models can be derived in a similar manner.

The diffuse surface BC has been implemented as an installed PMI and can be invoked by including the following syntax in the Sentaurus Device command file:

```
RayTraceBC {                               Physics(RegionInterface="region1/region2") {
  { Name = "rough_contact"                   RayTraceBC (
    PMImodel = pmi_rtDiffuseBC ( ... )         PMImodel = pmi_rtDiffuseBC ( ... )
  }                                          )
}                                          }
```

where ... stands for the following scattering model parameters:

```
model = "Phong"                 # "Lambert", "Random", "Gaussian"
phong_w = 200                   # w parameter of Phong model
gaussian_sigma = 0.1            # sigma parameter of Gaussian model
set_randomseed = 123            # 0 to 10000, or -1=do not set
debug = 0                       # 1=print debug message, 0=do not print,
                                # 99999 = interactive debug
ReflectionTransmissionTable = "wavelengthRTtable.txt"   # file input
pdfDimension = 2                # dimension of probability density function
reflectivity = 0.0             # reflectivity of rough surface
transmittivity = 1.0           # transmittivity of rough surface
```

Some comments about the parameter settings:

- You can set the specific reflectivity and transmittivity of the diffusive surface. However, if you still want to use the original reflectivity and transmittivity computed from the adjoining regions, set `reflectivity=-1` and `transmittivity=-1`.

- Setting a random seed allows for reproducibility of the simulation results.

- A useful `debug` option is included to ensure that the correct distribution is obtained.

- You can include the content of the `"wavelengthRTtable.txt"` file that contains a table of three columns: wavelength (μm), reflectivity, and transmittivity. These are power reflectivity and transmittivity values, and enable the reflectivities and transmittivities of the specific diffuse boundary to change according to the wavelength.

- The `pdfDimension` refers to the dimension of the probability density function (PDF), and this can be chosen to be different from the dimension of the device. If this keyword is not included, the `pdfDimension` is set to the dimension of the device.

> **NOTE** Instead of specifying the PMI parameters in the command file, you also can define them in the parameter file. To do so, in the command file, in the `RayTraceBC` section, set `PMIModel= "pmi_rtDiffuseBC"`. In the material parameter file, add a section `pmi_rtDiffuseBC {...}`, where ... corresponds to the scattering model parameters as previously described.

Periodic Boundary Condition

The periodic boundaries are limited to parallel X-, Y-, or Z-surfaces, so the device must have parallel surfaces in the direction of the periodicity. No special raytrace contacts need to be drawn onto the device, and you only need to specify the following syntax:

```
RayTraceBC {
   { Side="X" Periodic }
   { Side="Y" Periodic }
   { Side="Z" Periodic }
}
```

These periodic specifications are mutually exclusive, so you can specify a combination of any of them.

When the `PlotInterfaceFlux` feature (see Plotting Interface Flux on page 618) is activated, the corresponding entries describing the periodic fluxes are output to the plot file:

```
PeriodicFlux
   Xmin.FluxIn(region_name1)
   Xmin.FluxOut(region_name1)
   Xmax.FluxIn(region_name2)
   Xmax.FluxOut(region_name2)
   Ymin.FluxIn(region_name3)
   Ymin.FluxOut(region_name3)
   Ymax.FluxIn(region_name4)
   Ymax.FluxOut(region_name4)
   Zmin.FluxIn(region_name5)
   Zmin.FluxOut(region_name5)
   Zmax.FluxIn(region_name6)
   Zmax.FluxOut(region_name6)
```

NOTE   Only those regions that contain any of the periodic BCs will be included in the list.

Virtual Regions in Raytracer

This feature is a prelude to the TMM optical generation in the raytracer feature. Virtual regions can be defined in the raytracer such that rays ignore the presence of these regions during the raytracing process. In other words, when rays enter or leave a virtual region, no reflection or refraction occurs, and the ray is transmitted without change. This allows for additional flexibility in dual-grid simulations where some regions are important for electrical transport but insignificant for optics.

The syntax is:

```
Physics {...
   Optics(...
      OpticalSolver(
         RayTracing (...
            VirtualRegions{"nitride" "oxide" "layer555" ...}
         )
      )
   )
}
```

External Material in Raytracer

The default material surrounding a device is assumed to be air. In many cases, especially in LEDs, the device can be immersed in another material such as epoxy or some kind of phosphor. To correctly account for the directional, reflectivity, and transmittivity changes caused by such external material, a user-defined file of wavelength-dependent complex refractive indices can be entered. The syntax is:

```
Physics {
   Optics (
      OpticalSolver (
         Raytracing (
            ExternalMaterialCRIFile = "string"
         )
      )
   )
}
```

The external material CRI file should contain three columns: wavelength (μm), n, and k. A hash sign (#) is used to precede remarks. If the keyword `ExternalMaterialCRIFile` is not specified, the external medium is taken to be air with refractive index of 1.0.

Additional Options for Raytracing

Additional options enable better control of raytracing in Sentaurus Device:

- Omitting reflected rays when performing raytracing.
- Omitting weaker rays when performing raytracing.

The syntax for these options is:

```
Physics { ...
   Optics(...
```

```
        OpticalSolver(
           RayTracing (
              OmitReflectedRays
              OmitWeakerRays
           )
        )
     )
   }
```

Redistributing Power of Stopped Rays

When the raytracing terminates at a designated `DepthLimit` or `MinIntensity` value, there is still leftover power in those terminated rays. The sum of the powers contained in all these stopped rays can be redistributed into the raytree. The total power of the rays is:

$$P_{\text{Total}} = P_{\text{abs}} + P_{\text{escape}} + P_{\text{stopped}} \tag{698}$$

where P_{abs} is the absorbed power, P_{escape} is the power of the escaped rays (out of the device), and P_{stopped} is the power of the rays terminated by the `DepthLimit` or `MinIntensity` condition.

Rearranging the equation, the following expression is obtained:

$$P_{\text{Total}} = \frac{1}{\left(1 - \dfrac{P_{\text{stopped}}}{P_{\text{Total}}}\right)} (P_{\text{abs}} + P_{\text{escape}}) \tag{699}$$

Therefore, by multiplying a redistribution factor to P_{abs} and P_{escape}, the leftover power in the stopped rays can be accounted for. The syntax is:

```
Physics {...
   Optics(...
      OpticalSolver(
         RayTracing (...
            RedistributeStoppedRays
         )
      )
   )
}
```

In addition, this feature applies to LED raytracing.

> **NOTE** This feature does not work with Monte Carlo raytracing due to the fundamental assumption of the Monte Carlo method.

Weighted Interpolation for Raytrace Optical Generation

In raytracing, first optical absorption is computed elementwise, and then it is distributed evenly onto the associated vertices of the element. However, as a ray traverses an element, it can be closer to one particular corner or vertex of the element, in which case, distributing the optical absorption evenly onto all vertices of the element does not give a true picture. A better approximation is to use a weighted interpolation approach to distribute the optical absorption to vertices that are nearer to the center of each ray that traverses the element. The ray center is defined as the midpoint of the ray with respect to the optical absorption. This will improve the representation and accuracy of optical absorption profiles, and reduce the dependency on mesh size. The syntax is:

```
Physics{
   Optics(
      OpticalSolver(
         Raytracing(
            WeightedOpticalGeneration
         )
      )
   )
}
```

Visualizing Raytracing

The keyword `RayTrees` can be set in the `Plot` section to visualize raytracing using the TDR format. Thereby, an additional geometry is added to the plot file representing the ray paths. The following datasets are available for each ray element:

- `Depth`: Number of material boundaries that the ray has passed through.

- `Intensity`: Ray intensity.

- `Transmitted` (Boolean): True, as long as the ray is transmitted.

   NOTE   `RayTrees` cannot be plotted with the compact memory option.

Reporting Various Powers in Raytracing

Various powers are reported in the log file after a raytracing event, and the format is as follows:

```
Summary of RayTrace Total Photons and Powers:
                Input       Escaped     StoppedMinInt  StoppedDepth  AbsorbedBulk  AbsorbedBC
Photons [#/s]:  4.531E+11   1.333E+11   4.142E+07      0.000E+00     6.236E+10     2.574E+11
Powers [W]:     3.000E-07   8.826E-08   2.743E-11      0.000E+00     4.129E-08     1.704E-07
```

A brief summary of these powers is:

■ Input power is computed by multiplying the input wave power (units of W/cm^2) by the rectangular or circular window area where the starting rays have been defined.

■ In two dimensions, the length in the third dimension is taken as $1\ \mu m$, conforming to the rest of the Sentaurus Device 2D treatment. The total input power listed should correspond to the `Intensity` in the `Excitation` section multiplied by the actual area of the starting ray window. If an area factor has been defined in the simulation, this area factor also is multiplied into the result.

■ Escaped power refers to the sum of powers of the rays that are ejected from the device and are unable to re-enter the device.

■ StoppedMinInt power sums the powers of the rays terminated by the MinIntensity condition.

■ StoppedDepth power sums the powers of the rays terminated by the DepthLimit criteria.

■ AbsorbedBulk power refers to power absorbed in bulk regions.

■ AbsorbedBC power refers to power absorbed in the TMM contacts. This column is shown only if TMM contacts have been defined.

In the plot file, the raytrace photon rates and powers are listed under `RaytracePhoton` and `RaytracePower`, respectively. In addition, the ratio of the various powers and the input power are plotted under `RaytraceFraction`.

Plotting Interface Flux

The photon flux flowing through any interface can be tracked with the `PlotInterfaceFlux` feature. The tracking is made possible by recording the reflected, transmitted, and absorbed flux flowing through each interface or contact BC. Since photon flux is directional, there is a need to distinguish between the flux flowing from Region 1 to Region 2, or from Region 2 to Region 1, as shown in Figure 35.
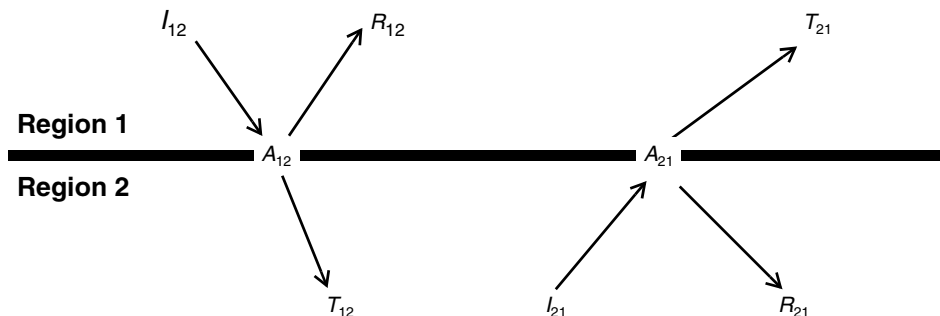
Figure 35   Distinguishing directional photon flux

Consider the photon fluxes (carried by rays) flowing from Region 1 to Region 2. For photon flux conservation:

$$I_{12} = R_{12} + T_{12} + A_{12} \tag{700}$$

where:

- I_{12} is the incident flux.
- R_{12} is the reflected flux.
- T_{12} is the transmitted flux.
- A_{12} is the flux absorbed at the interface.

The reverse is true for flux flowing from Region 2 to Region 1. At each interface, the summation of R_{12}, T_{12}, A_{12}, R_{21}, T_{21} and A_{21} is stored in the raytracing process.

With this information, you can compute various reflection and transmission coefficients at the interface that has been declared as a raytrace BC. For example, assume that light is illuminated from Region 1 to Region 2. Within Region 2, there can be multiple reflections, and some rays may escape back into Region 1 through T_{21}.

Therefore, the power reflection coefficient for the case in is:

$$\tilde{R}_{12} = \frac{\sum R_{12} + \sum T_{21}}{\sum R_{12} + \sum T_{12} + \sum A_{12}} \tag{701}$$

The following syntax activates the feature for tracking and plotting interface fluxes:

```
Physics {...
  Optics (...
    OpticalSolver (...
      RayTracing (
        PlotInterfaceFlux
      )
    )
  )
}
```

This feature is limited to the unified raytracing interface. In the plot file, only the fluxes of the interfaces or contacts that have been declared as a raytrace BC are output. In addition, activating the `PlotInterfaceFlux` feature also enables the output of the absorbed photon density in every layer of the TMM BC. The output variables in the plot file are listed as follows:

```
RaytraceInterfaceFlux                    # directional
  R(region1/region3)
  T(region1/region3)
  A(region1/region3)
```

```
        R(region3/region1)
        T(region3/region1)
        A(region3/region1)

   RaytraceContactFlux                          # directional
        R(contactname1(region1/region3))        # the region is only a sample
        T(contactname1(region1/region3))
        A(contactname1(region1/region3))
        R(contactname1(region3/region1))
        T(contactname1(region3/region1))
        A(contactname1(region3/region1))

   RaytraceInterfaceTMMLayerFlux                # not directional
        A(region1/region3).layer1
        A(region1/region3).layer2
        A(region1/region3).layer3

   RaytraceContactTMMLayerFlux                  # not directional
        A(contactname1(region1/region3)).layer1
        A(contactname1(region1/region3)).layer2
        A(contactname1(region1/region3)).layer3
```

A contact-based BC can possibly intersect many region interfaces. In the plot file output, only a representative region interface is used to indicate the directional flow of photon flux for the entire contact BC.

When the `PlotInterfaceFlux` feature is activated, the `OpticalIntensity` computation will change such that the intensity within each region is scaled to the net photon flux gained in that region. Therefore, the `OpticalIntensity` values can be negative in some regions. Integration of the `OpticalIntensity` within the region recovers the net photon flux flowing into that region.

Far Field and Sensors for Raytracing

To collect information on the rays that exit a device, the concept of far field and sensors is introduced in the unified raytracer interface.

The far field is collected on a virtual circle for two dimensions and a virtual sphere for three dimensions. Ray collection does not destroy the rays. On the virtual far-field surface, the far-field intensity is computed based on a unit measure of radius, whereby the collected ray powers at each interval are divided by the radian angular arc (2D) or area (3D):

In 2D, far-field intensity $= \dfrac{\sum \text{raypowers}}{d\phi}$.

In 3D, far-field intensity $= \dfrac{\sum \text{raypowers}}{\{\cos((\theta_1) - \cos(\theta_2))\}d\phi}$.

On the other hand, a sensor sums the total power of all rays impinging the sensor. Two types of sensor can be defined:

- A line segment sensor in two dimensions or a flat rectangular sensor in three dimensions.

- An angular sensor that collects the power of the rays that radiate within the angular span of the sensor. In two dimensions, a range of ϕ defines the sensor; whereas in three dimensions, ranges of θ and ϕ are needed. These are defined according to the regular Cartesian coordinate system. In two dimensions, ϕ rotates from 0 at the positive x-axis in a counterclockwise direction towards the positive y-axis. In three dimensions, θ rotates from 0 at the positive z-axis towards the xy plane; whereas. ϕ is similarly defined as in two dimensions.

The `SensorSweep` option is also available for 3D simulations. It allows you to visualize the variation of ray power collected on a latitude or longitude ring band.

The syntax for activating the far field and sensors in the unified interface for optical generation computation is:

```
Physics {
   Optics (
      OpticalSolver (
         Raytracing(
            Farfield(
               Origin = auto | <vector>      # default is auto
               Discretization = <integer>    # default is 360 for 2D, 36 for 3D
               ObservationRadius = <float>    # default is 1e6 um (1 meter)
               Sensor(
                  Name = "sensorname1"
                  Rectangle (                # 3D only
                     Corner1 = <vector>
                     Corner2 = <vector>
                     Corner3 = <vector>
                     UseNormalFlux
                     AxisAligned             # 3D only
                  )
                  Line (                     # 2D only
                     Corner1 = <vector>
                     Corner2 = <vector>
                     UseNormalFlux
                  )
                  Angular (
                     Theta = (<float> <float>)
                     Phi = (<float> <float>)
                  )
               )
               Sensor(
                  Name = "sensorname2"
                  Rectangle ( ... )                    # 3D only
```

```
                    Line ( ... )                       # 2D only
                    Angular ( ... )
                )
                SensorSweep(                           # 3D only
                    Name = "sensorname3"
                    Ndivisions = <integer>
                    VaryPhi
                    Theta = (<float> <float>)          # Use with VaryPhi
                )
                SensorSweep(                           # 3D only
                    Name = "sensorname4"
                    Ndivisions = <integer>
                    VaryTheta
                    Phi = (<float> <float>)            # Use with VaryTheta
                )
            )
        )
    )
  )
}
```

Some comments about the syntax:

- Multiple far-field `Sensor` and `SensorSweep` sections can be defined. However, each `Sensor` and `SensorSweep` section must have a unique name for identification.

- When `Line` or `Rectangle` sensors are used, the option `UseNormalFlux` allows you to sum the normal-projected power from the ray that is impinging the sensor at an angle.

- In the case of a `Rectangle` sensor in three dimensions, if you specify `AxisAligned`, only opposing corners of the rectangle are required. Sentaurus Device automatically computes the other two corners of the rectangle.

- If an empty `Farfield()` section is specified, the far field is plotted with the default values of `Discretization`, `Origin`, and `ObservationRadius`.

- The far field takes values of intensity type. Therefore, to recover the total number of photons, you must integrate over the angle (in radian).

- The 3D far field is projected onto a staggered grid (see Staggered 3D Grid LED Radiation Pattern on page 947).

- The far field is plotted at every instance where the `Plot` statement in the `Solve` section is activated. The file names of the far field and sensor sweep are derived from the plot file name. For example, this syntax:

```
File {...
    Plot = "n99_des"
}
Solve {...
    Plot ( Range=(0,1) Intervals=5 )
}
```

produces the following far-field files:

```
n99_000000_des_farfield.tdr
n99_000001_des_farfield.tdr
...
n99_000000_des_sensorsweep.plt
n99_000001_des_sensorsweep.plt
...
```

- In the `SensorSweep` plot file, all the user-defined `SensorSweep` sections are defined in the following fields of the plot file:

```
sensorname3
    Phi
    Photons_DelTheta
sensorname4
    Theta
    Photons_DelPhi
```

- The values of the sensor are added to the general plot file of the simulation, and the field entries are:

```
RaytraceSensor
    sensorname1
    sensorname2
```

Dual-Grid Setup for Raytracing

Raytracing in Sentaurus Device is based on tracing the rays in each cell of the simulation mesh. For simulations in which the optical material properties do not vary on a short length scale, this may lead to the unnecessary deterioration of simulation performance. In such cases, a dual-grid setup can be used, which allows the use of a coarse mesh for raytracing, while the electronic equations are solved on a finer mesh (see Figure 36 on page 625).

The basic syntax for setting up a raytracing dual-grid simulation is:

```
File {
   Output  = "output"
   Current = "current"
}

Plot {
   OpticalIntensity
   OpticalGeneration
}

# Specify grid and material parameter file names for raytracing:
OpticalDevice OptGrid {
   File {
```

```
           Grid      = "raytrace.tdr"
           Doping    = "raytrace.tdr"
           Current   = "opto"
           Plot      = "opto"
           Parameter = "CIS.par"
       }
     Physics { HeteroInterface }
   }

   # Specify grid, material parameters, and physical models for electrical
   # simulation:
   Device CIS {
      Electrode {
         { Name="sub" Voltage = 0.0 }
         { Name="pd"  Voltage = 0.0 }
      }
      File {
         Grid      = "in_elec_pof.tdr"
         Doping    = "in_elec_pof.tdr"
         Parameter = "CIS.par"
         Current   = "current"
         Plot      = "plot"
      }
      Physics {
         AreaFactor = 1
         Optics(...
            ComplexRefractiveIndex(...
               WavelengthDep(real imag)
            )
            OpticalGeneration(...)
            Excitation(...)
            OpticalSolver(
               RayTracing (
                  RayDistribution(...)
                  DepthLimit = 1000
                  MinIntensity = 1e-3
               )
            )
         )
      }

   # Specify system connectivity:
   System {
      OptGrid opt ()
      CIS d1 (pd=vdd sub=0) { Physics{ OptSolver = "opt" } }
      Vsource_pset drive(vdd 0){ dc = 0.0 }
   }

   Solve { Poisson }
```

The dual-grid simulation setup also allows the unified raytracing interface to be used (see).
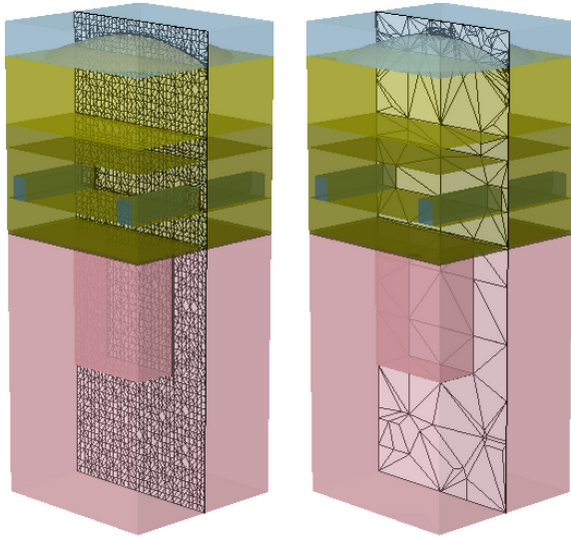
Figure 36   Comparison of two grids used in a 3D dual-grid CMOS image sensor simulation; the figures show cuts through the device center; (*left*) the electronic equations are solved on a fine grid and (*right*) a coarse grid is used for raytracing

Transfer Matrix Method

Sentaurus Device can calculate the propagation of plane waves through layered media by using a transfer matrix approach.

Physical Model

In the underlying model of the optical carrier generation rate, monochromatic plane waves with arbitrary angles of incidence and polarization states penetrating a number of planar, parallel layers are assumed. Each layer must be homogeneous, isotropic, and optically linear. In this case, the amplitudes of forward and backward running waves $A_j^\pm$ and $B_j^\pm$ in each layer in are calculated with help of transfer matrices.

These matrices are functions of the complex wave impedances Z_j given by $Z_j = n_j \cdot \cos\Theta_j$ in the case of E polarization (TE) and by $Z_j = n_j/(\cos\Theta_j)$ in the case of H polarization (TM). Here, n_j denotes the complex index of refraction and Θ_j is the complex counterpart of the angle of refraction ($n_0 \cdot \sin\Theta_0 = n_j \cdot \sin\Theta_j$).

The transfer matrix of the interface between layers j and $j + 1$ is defined by:

$$T_{j,j+1} = \frac{1}{2Z_j} \cdot \begin{bmatrix} Z_j + Z_{j+1} & Z_j - Z_{j+1} \\ Z_j - Z_{j+1} & Z_j + Z_{j+1} \end{bmatrix} \tag{702}$$

The propagation of the plane waves through layer j can be described by the transfer matrix:

$$T_j(d_j) = \begin{bmatrix} \exp\left(2\pi i \, n_j \cos\Theta_j \, \dfrac{d_j}{\lambda}\right) & 0 \\ 0 & \exp\left(-2\pi i \, n_j \cos\dfrac{\Theta_j d_j}{\lambda}\right) \end{bmatrix} \tag{703}$$

with the thickness d_j of layer j and the wavelength λ of the incident light.

The transfer matrices connect the amplitudes of Figure 37 as follows:

$$\begin{pmatrix} B_j^+ \\ A_j^+ \end{pmatrix} = T_{j,j+1} \cdot \begin{pmatrix} A_{j+1}^- \\ B_{j+1}^- \end{pmatrix}$$

$$\begin{pmatrix} A_j^- \\ B_j^- \end{pmatrix} = T_j(d_j) \cdot \begin{pmatrix} B_j^+ \\ A_j^+ \end{pmatrix} \tag{704}$$
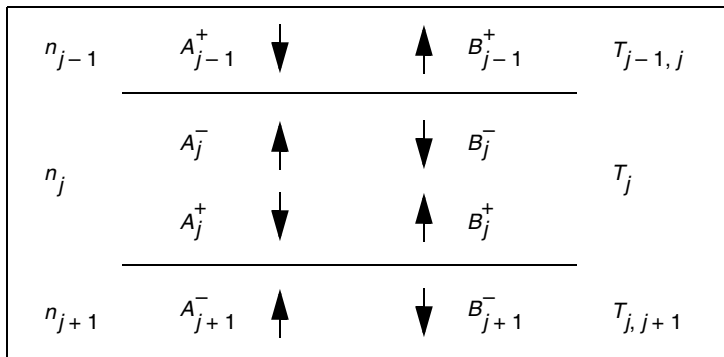
Figure 37   Wave amplitudes in a layered medium and transfer matrices connecting them

It is assumed that there is no backward-running wave behind the layered medium, and the intensity of the incident radiation is known. Therefore, the amplitudes $A_j^\pm$ and $B_j^\pm$ at each interface can be calculated with appropriate products of transfer matrices.

For both cases of polarization, the intensity in layer j at a distance d from the upper interface $(j, j+1)$ is given by:

$$I_{T(\text{TE, TM})}(d) = \frac{\Re(Z_j)}{\Re(Z_0)} \cdot \left\| T_j(d) \cdot \begin{pmatrix} A_j^- \\ B_j^- \end{pmatrix} \right\|^2 \tag{705}$$

with the proper wave impedances. If δ is the angle between the vector of the electric field and the plane of incidence, the intensities have to be added according to:

$$I(d) = I_{\text{TM}}(d) + I_{\text{TE}}(d) \tag{706}$$

where $I_{\text{TM}} = (1-a)I(d)$ and $I_{\text{TE}} = aI(d)$ with $a = \cos^2\delta$.

One of the layers must be the electrical active silicon layer where the optical charge carrier generation rate G^{opt} is calculated. The rate is proportional to the photon flux $\Phi(d) = I(d)/\hbar\omega$.

In the visible and ultraviolet region, the photon energy $\hbar\omega$ is greater than the band gap of silicon. In this region, the absorption of photons by excitation of electrons from the valence to the conduction band is the dominant absorption process for nondegenerate semiconductors. Far from the absorption threshold, the absorption is considered to be independent of the free carrier densities and doping. Therefore, the silicon layer is considered to be a homogeneous region.

The absorption coefficient α is the relative rate of decrease in light intensity along its path of propagation due to absorption. This decrease must be distinguished from variations caused by the superposition of waves. Therefore, the rate of generated electron–hole pairs is:

$$G_0^{\text{opt}} = \alpha\eta\frac{I(d)}{\hbar\omega} \tag{707}$$

where the absorption coefficient α is given by the imaginary part of $4\pi\, Z_{\text{Si}}/\lambda$. The quantum yield η is defined as the number of carrier pairs generated by one photon. More details about the available quantum yield models and their specification in the `OpticalGeneration` section of the command file are given in Quantum Yield Models on page 544.

Rough Surface Scattering

To model the effect of light trapping due to scattering of incident light at rough interfaces of a planar multilayer structure, the standard TMM approach describing the propagation of coherent light is extended. Part of the coherent light incident at a rough interface is scattered and spreads incoherently throughout the structure. Scalar scattering theory [4][5] allows to approximate the amount of scattered light at a rough interface. The so-called haze parameter defines the ratio of diffused (scattered) light to total (diffused + specular) light. The directional

dependency of the scattering process is modeled by angular distribution functions (ADFs). In this scenario, a rough interface is characterized by its haze function (haze parameter as a function of the wavelength of incident light) for reflection and transmission as well as the ADF for direct coherent light incident at the interface and the ADF for scattered light incident at the interface.

The implementation of rough surface scattering within the existing TMM framework follows the semi-coherent optical model outlined in [6]. It is based on the following assumptions:

- The haze factor determines the fraction of direct light, transferred to scattered light.

- Coherent and diffused light incident on a rough interface are scattered differently using different ADFs.

- Interfaces are nonabsorptive, meaning photon flux is conserved at interfaces.

- For scattered light incident at a rough interface, the mean value of TE and TM polarized light for reflectance and transmittance is used.

- For the scattered light, the total reflectance and transmittance for a rough interface are assumed to be equal to the ones for the corresponding flat interface.

- The phase change of the electric field traveling across a rough interface is the same as in the case of the corresponding flat interface.

- Scattered light incident at a rough interface is further split, according to its haze factor, into a specular part, which corresponds to light incident at a flat interface, and a diffused part leading to further spreading of the incident scattered light.

Given these assumptions, the specular and diffused components of light at each interface can be expressed in terms of the corresponding haze functions and ADFs. The description of coherent light incident at a rough interface differs from the approach taken in [6] in that a generalized interface matrix has been derived. It accounts for the reduced reflection and transmission according to the respective haze functions and allows to keep the common TMM computation approach for the electric field and intensity. The reduced interface matrix reads as follows:

$$
\tilde{T}_{j,j+1} = \frac{1}{h^t_{j+1,j}t} \begin{bmatrix} 1 & (h^r_{j+1,j}r_{j,j+1}) \\ (h^r_{j,j+1}r_{j,j+1}) & (h^t_{j,j+1}h^t_{j+1,j} + (h^r_{j+1,j}h^r_{j,j+1} - h^t_{j,j+1}h^t_{j+1,j})r^2_{j,j+1}) \end{bmatrix} \tag{708}
$$

where $r_{j,j+1}$ and $t_{j,j+1}$ denote the Fresnel reflection and transmission coefficients for normal incidence given by:

$$
r_{j,j+1} = \frac{n_j - n_{j+1}}{n_j + n_{j+1}} \tag{709}
$$

$$
t_{j,j+1} = \frac{2n_j}{n_j + n_{j+1}} \tag{710}
$$

and $h^r_{j,j+1}$ and $h^t_{j,j+1}$ are reduction factors determined by the haze functions for reflection and transmission:

$$h^r_{j,j+1} = \sqrt{1 - H^r_{j,j+1}} \tag{711}$$

$$h^t_{j,j+1} = \sqrt{1 - H^t_{j,j+1}} \tag{712}$$

The haze functions for reflection and transmission derived from the scalar scattering theory are:

$$H^r_{j,j+1}(\lambda, \varphi_j) = 1 - \exp\left[-\left(\frac{4\pi\sigma_{rms}c_r(\lambda, \sigma_{rms})n_j\cos\varphi_j}{\lambda} \right)^{a^r} \right] \tag{713}$$

$$H^t_{j,j+1}(\lambda, \varphi_j) = 1 - \exp\left[-\left(\frac{4\pi\sigma_{rms}c_t(\lambda, \sigma_{rms})|n_j\cos\varphi_j - n_{j+1}\cos\varphi_{j+1}|}{\lambda} \right)^{a^t} \right] \tag{714}$$

where σ_{rms} stands for the root-mean-square roughness of the interface and λ is the wavelength of the incident light. The exponent $a^{r/t}$ and the correction function $c_{r/t}$ are fitting parameters to better match experimental data.

NOTE The haze functions defined in Eq. 713 and Eq. 714 are given in their general form, which also covers light incident at the angle φ_j from the surface normal. This expression is needed in the description of scattered light incident at a rough interface.

For the propagation of the angular intensity components of scattered light through each layer, the effective path length is used to stay within the one-dimensional formalism:

$$I(\lambda, \varphi_j, d) = I(\lambda, \varphi_j)\exp\left(-\frac{\alpha(\lambda)d}{\cos\varphi_j} \right) \tag{715}$$

The scattering solver first propagates all forward-going components through the layer structure and completes a round trip by propagating all backward-going components. In each round trip, part of the light may be absorbed within the structure as well as transmitted through the front or back side, depending on the material properties at the given wavelength. This leads to a reduction of the light intensity components at the various interfaces with increasing number of iterations. When the ratio of the largest remaining intensity component in the system to the sum of all initial intensity components falls below the value of `Tolerance`, the solver terminates. As a consequence, the residual intensity of each component at all interfaces is not included in the extracted results.

The overall simulation flow consists of the following steps:

- Solving the coherent propagation problem following the default TMM solver algorithm, but using the generalized interface matrices for rough interfaces. In this step, the starting light intensity for scattered light is calculated at each interface as well.

- The scattered light is propagated through the structure following an iterative approach similar to raytracing as outlined in [6]. However, other than raytracing, instead of single rays, ray bundles with discrete angular distribution are propagated from layer to layer. The number of iterations needed to solve the scattering problem to the required accuracy mainly depends on how much light is absorbed within the structure and how much light is coupled out at the front and back ends during a single round trip.

- The scattered and coherent absorbed photon density profiles are summed and passed to the quantum yield model.

    NOTE   Support for rough surface scattering is limited to normal incident light.

For more information on how to apply the rough surface scattering model and its configuration options, see Using Scattering Solver on page 632.

Using Transfer Matrix Method

The transfer matrix method is only supported by the unified interface for optical generation computation (see Overview on page 533). The `OpticalGeneration` section activates the computation of the optical generation along with optional parameters such as the quantum yield. The `OpticalSolver` section determines the underlying optical solver together with solver-specific parameters as shown in the following example:

```
Physics {...
   Optics (...
      OpticalGeneration (...)
      ComplexRefractiveIndex (...)
      Excitation (...
         Window ("L1") (...)
      )
      OpticalSolver (
         TMM (
            PropagationDirection = Perpendicular # Default Refractive
            NodesPerWavelength = 20
            LayerStackExtraction (...
               WindowName = "L1"
               Medium (...)
            )
         )
      )
```

```
         Excitation (...
            Window ("L1") (...)
         )
      )
   }
```

The properties of the incident light such as `Wavelength`, `Intensity`, `Polarization`, and angle of incidence `Theta` are specified in the `Excitation` section (see Setting the Excitation Parameters on page 560) along with one or several illumination windows (see Illumination Window on page 562), which confine the incident light to a certain part of the device structure.

An illumination window determines how the 1D solution of the transfer matrix method is interpolated to the higher dimensional device grid. The minimum coordinate of the 1D profile is pinned to the illumination window, and the interpolation of the profile in propagation direction can be performed either perpendicular to it or according to Snell's law, which is the default. The corresponding keyword in the `TMM` section is `PropagationDirection`, which can take either `Perpendicular` or `Refractive` as its argument. The accuracy of the integrated absorbed photon density for 1D TMM solutions in a 2D or 3D device can be controlled by various parameters (see Accurate Absorbed Photon Density for 1D Optical Solvers on page 575).

The `LayerStackExtraction` section determines how a 1D complex refractive index profile is extracted automatically from the grid file (see Extracting the Layer Stack on page 570). Based on this profile, the polarization-dependent optical intensity is calculated and interpolated onto the grid according to the referenced illumination window and the value of `PropagationDirection`. The optical generation profile then is calculated from the window-specific intensities. For overlapping windows, the intensity are summed in the region of intersection.

By default, the surrounding media at the top and bottom of the extracted layer stack are assumed to have the material properties of vacuum. However, the default can be overwritten by specifying a separate `Medium` section in the `LayerStackExtraction` section for the top and bottom of the layer stack if necessary. In the `Medium` section, a `Location` must be specified and a `Material`, or, alternatively, the values of `RefractiveIndex` and `ExtinctionCoefficient`:

```
LayerStackExtraction(
   Medium (
      Location = top
      Material = "Silicon"
   )
   Medium (
      Location = bottom
      RefractiveIndex = 1.4
      ExtinctionCoefficient = 1e-3
```

```
      )
   )
```

If the optical generation profile is the sole quantity of interest, it is sufficient to specify the keyword `Optics` exclusively in the `Solve` section.

The TMM solver offers two options for computing the optical intensity from the complex field amplitudes of the forward-propagating and backward-propagating waves. Specifying `IntensityPattern=StandingWave` computes the optical intensity I as follows:

$$I = \text{Re}(A + B)^2 + \text{Im}(A + B)^2 \tag{716}$$

whereas using the syntax:

```
TMM (...
   IntensityPattern = Envelope
)
```

computes the optical intensity I using the following formula to prevent oscillations on the wavelength scale that may not be possible to resolve on the mixed-element simulation grid:

$$I = \text{Re}(A)^2 + \text{Im}(A)^2 + \text{Re}(B)^2 + \text{Im}(B)^2 \tag{717}$$

where A and B are the complex field amplitudes of the forward-propagating and backward-propagating waves, respectively. `IntensityPattern` can be specified globally, per region, or per material.

The keywords of `TMM` are summarized in .

Using Scattering Solver

To model the effect of scattering at rough interfaces, the scattering solver (see) must be configured in the command file, and the parameters characterizing each rough interface must be specified in the corresponding parameter file section.

Command File Specification

The scattering solver is activated by specifying a `Scattering` section within the `TMM` section. By default, all interfaces are treated as rough. However, whether part of the light incident on a specific interface is actually scattered depends on the corresponding haze functions for reflection and transmission defined in the parameter file. A haze function evaluating to zero is equivalent to the interface being treated as flat.

You can flag explicitly a specific region or material interface as not being rough as in the following example:

```
Physics {
   Optics (
      OpticalSolver (
         TMM (
             Scattering ( ... )
             RoughInterface      #Default
         )
      )
}

Physics (RegionInterface="<region1>/<region2>") {
   Optics (
      OpticalSolver (
         TMM (
             -RoughInterface
         )
      )
   )
}
```

Sometimes, it may be more practical to set all interfaces as flat by specifying -RoughInterface in the global Physics section and only to label specific interfaces as rough in a corresponding region or material interface Physics section.

The angular discretization of the interval $[-\pi/2, \pi/2]$ used for the ray bundles in the scattering solver can be set with the keyword AngularDiscretization in the Scattering section. The keywords Tolerance and MaxNumberOfIterations determine the termination condition of the iterative scattering solver (see Rough Surface Scattering on page 627):

```
Physics {
   Optics (
      OpticalSolver (
         TMM (
             Scattering (
                AngularDiscretization = 90
                MaxNumberOfIterations = 150
                Tolerance = 1e-3
             )
         )
      )
   )
}
```

For weakly absorbing structures, such as semiconductor layer stacks illuminated with light in the infrared part of the spectrum, many iterations may be necessary until the given `Tolerance` is reached. To detect such cases and to limit the total simulation time, it is advisable to adjust the value of `MaxNumberOfIterations`.

Parameter File Specification

All parameters characterizing a rough interface are defined in the `OpticalSurfaceRoughness` section of the respective region or material interface section in the parameter file. The parameters can be classified into two groups: One relates to the specification of the haze functions and one contains the selection of the various angular distribution functions (ADFs).

For specifying the haze function for reflection (`HazeFunction_R`) and transmission (`HazeFunction_T`), two options are available:

- `Constant`: For each of the two haze functions H_R and H_T, a constant value can be set using the keywords `H_R` and `H_T`. This option may be useful if a simulation is performed at a single wavelength and the surface roughness is not varied as the haze functions usually depend on both.

- `Analytic`: The analytic expressions given by [Eq. 713, p. 629](#) and [Eq. 714, p. 629](#) are evaluated. where the surface roughness σ_{rms}, the exponents a_R and a_T, and the correction functions c_R and c_T are supplied by the user. In the simplest approximation, c_R and c_T are assumed to be constants over the whole wavelength range. However, in general, the correction functions are used to fit the analytic haze functions against experimental data. For that purpose, tabulated values are supported by setting `CorrectionFunction_R` or `CorrectionFunction_T` equal to `Table`.

Besides the haze functions, the ADFs are used to characterize the behavior of light incident at rough interfaces. The model supports the specification of different ADFs for direct incident light at a rough interface as well as for scattered light incident at a rough interface. Some ADFs depend on an additional parameter apart from the angle of incidence, whose value must be supplied by the user.

The detailed syntax including all options for the definition of the haze functions and ADFs are given in the following tables (where applicable, the default value is given at the beginning of the description).

Table 120   Specification of haze functions

Symbol	Keyword	Value	Description
$H^r(\lambda, \varphi)$	`HazeFunction_R`	`=Constant | Analytic`	`Constant` Type of haze function for reflection.
$H^t(\lambda, \varphi)$	`HazeFunction_T`	`=Constant | Analytic`	`Constant` Type of haze function for transmission.

Table 120   Specification of haze functions (Continued)

Symbol	Keyword	Value	Description
H_R	H_R	=<float>	0 Constant value for haze function for reflection.
H_T	H_T	=<float>	0 Constant value for haze function for transmission.
σ_{rms}	Sigma	=<float>	0 Optical surface roughness in [nm] used in analytic haze functions for reflection and transmission.
a_R	a_R	=<float>	2 Exponent of analytic haze function for reflection.
a_T	a_T	=<float>	3 Exponent of analytic haze function for transmission.
	CorrectionFunction_R	=Constant | Table	Constant Type of correction function of analytic haze function for reflection.
	CorrectionFunction_T	=Constant | Table	Constant Type of correction function of analytic haze function for transmission.
c_R	c_R	=<float>	1 Constant value in interval [0 1] for correction function of analytic haze function for reflection.
c_T	c_T	=<float>	1 Constant value in interval [0 1] for correction function of analytic haze function for transmission.
$c_R(\lambda)$	c_R	(<table>)	Tabulated values for correction function of analytic haze function for reflection. First column contains wavelength in [μm] and second column contains value of correction function in interval [0 1].
$c_T(\lambda)$	c_T	(<table>)	Tabulated values for correction function of analytic haze function for transmission. First column contains wavelength in [μm] and second column contains value of correction function in interval [0 1].
	TableInterpolation_c_R	=Linear | Spline	Linear Type of interpolation used for tabulated values of correction function for analytic haze function for reflection.
	TableInterpolation_c_T	=Linear | Spline	Linear Type of interpolation used for tabulated values of correction function for analytic haze function for transmission.

Table 121   Specification of angular distribution functions (not normalized)

Symbol	Keyword	Value	Description
$f_1(\varphi)$	ADFDirect_R	=Constant | Triangle | Gauss | Lorentz | Cosine | Ellipse	Cosine Type of angular distribution function for direct incident light reflected at a rough interface.
C	CDirect_R	=<float>	2 Fitting parameter used in angular distribution function (where applicable) for direct incident light reflected at a rough interface.
$f_1(\varphi)$	ADFDirect_T	=Constant | Triangle | Gauss | Lorentz | Cosine | Ellipse	Cosine Type of angular distribution function for direct incident light transmitted through a rough interface.
C	CDirect_T	=<float>	2 Fitting parameter used in angular distribution function (where applicable) for direct incident light transmitted through a rough interface.
$f_2(\varphi)$	ADFScatter_R	=Constant | Triangle | Gauss | Lorentz | Cosine | Ellipse	Constant Type of angular distribution function for scattered light reflected at a rough interface.
C	CScatter_R	=<float>	1 Fitting parameter used in angular distribution function (where applicable) for scattered light reflected at a rough interface.
$f_2(\varphi)$	ADFScatter_T	=Constant | Triangle | Gauss | Lorentz | Cosine | Ellipse	Constant Type of angular distribution function for scattered light transmitted through a rough interface.
C	CScatter_T	=<float>	1 Fitting parameter used in angular distribution function (where applicable) for scattered light transmitted through a rough interface.

Table 122   Definition of different ADF types used in Table 121

Type	Formula
Constant	$f(\varphi) = 1$
Triangle	$f(\varphi) = 1 - 2|\varphi|/\pi$
Gauss	$f(\varphi) = e^{-\varphi^2/(2C)}$
Lorentz	$f(\varphi) = e^{1/(\varphi^2 + C^2)}$

Table 122 Definition of different ADF types used in Table 121 (Continued)

Type	Formula
Cosine	$f(\varphi) = \cos^{C}(\varphi)$
Ellipse	$f(\varphi) = \dfrac{\cos(\varphi)}{\cos^{2}(\varphi) + (2C)^{-2}\sin^{2}(\varphi)}$

The following figures illustrate the various ADFs specified in Table 121 on page 636.

Figure 38 ADF of type Constant and Triangle

Figure 39 ADF of type Gauss

Figure 40   ADF of type Lorentz

Figure 41   ADF of type Cosine

Figure 42   ADF of type Ellipse

The following `OpticalSurfaceRoughness` section is an example for the specification of analytic haze functions and the default angular distribution functions:

```
OpticalSurfaceRoughness {
   HazeFunction_R=Analytic
   HazeFunction_T=Analytic
   Sigma=20    #[nm]
   a_R=2
   a_T=3
   CorrectionFunction_R=Table
   TableInterpolation_c_R=Spline
   c_R(
      0.3 04
      0.4 0.65
      0.8 0.9
      1.3 0.95
   )
   CorrectionFunction_T=Constant
   c_T=0.7

   ADFDirect_R=Cosine
   CDirect_R=2
   ADFDirect_T=Cosine
   CDirect_T=2
   ADFScatter_R=Constant
   ADFScatter_T=Constant
}
```

Plot Quantities

When specifying `OpticalIntensity` and `AbsorbedPhotonDensity` in the `Plot` section of the command file, the following additional datasets are written to the plot file:

- `OpticalIntensityCoherent`: Specular part of optical intensity resulting from propagation of coherent light.

- `OpticalIntensityIncoherent`: Diffuse part of optical intensity resulting from propagation of incoherent light.

- `AbsorbedPhotonDensityCoherent`: Specular part of absorbed photon density resulting from propagation of coherent light.

- `AbsorbedPhotonDensityIncoherent`: Diffuse part of absorbed photon density resulting from propagation of incoherent light.

Loading Solution of Optical Problem From File

In solar-cell and CIS simulations, it is often necessary to load several optical generation profiles as a function of one or more parameters, for example, excitation wavelength or angle of incidence, in Sentaurus Device. These profiles then are used to compute the response to each of them separately or to compute the response to the spectrum as a whole. A typical example is the computation of white-light generation using several generation profiles previously computed by Sentaurus Device Electromagnetic Wave Solver (EMW) or different wavelengths of the visible spectrum.

The parameters corresponding to a specific absorbed photon density or optical generation profile are written to the respective output file as special TDR tags as well. For 1D profiles generated with external tools, such tags can be specified in the file header (see Importing 1D Profiles Into Higher-Dimensional Grids on page 642). This ensures that a profile can be identified later when loaded into a Sentaurus Device simulation. For example, if the optical problem is solved externally, it is not possible to determine the quantum yield, which is necessary to compute the optical generation based on the electronic properties of the underlying device structure. However, since the corresponding excitation wavelength is stored along with the optical solution, the quantum yield computation can be performed later in Sentaurus Device after loading the profile to compute the optical generation.

Absorbed photon density or optical generation profiles loaded into Sentaurus Device using the optical solver FromFile must meet one of the following requirements:

- Profiles must be saved in a TDR file.
- One-dimensional profiles that are to be imported into higher-dimensional grids must comply with the PLX file format described in Importing 1D Profiles Into Higher-Dimensional Grids on page 642.

If the grid on which the profile is saved is not the same as that used for the device simulation (different mixed-element grid or arbitrary tensor grid arising from EMW simulation), the profile is interpolated automatically onto the simulation grid upon loading. For more details on how to control the interpolation, including the truncation and shifting of the interpolation domain, see Controlling Interpolation When Loading Optical Generation Profiles on page 659.

The basic command file syntax for loading profiles from file is:

```
File {
   OpticalSolverInput = "<filename or filename pattern of profiles>"
}

Physics {
   Optics (
      OpticalGeneration (
         ComputeFromMonochromaticSource ()                    # or
```

```
         ComputeFromSpectrum ()
      )
   OpticalSolver (
      FromFile (
         DatasetName = AbsorbedPhotonDensity              # Default
         SpectralInterpolation = Linear                   # Default Off
         IdentifyingParameter = ("Wavelength" "Theta")
      )
   )
)
}
```

> **NOTE** The optical solver `FromFile` requires the specification of `ComputeFromMonochromaticSource` or `ComputeFromSpectrum` in the `OpticalGeneration` section. Otherwise, the computation of the optical generation based on the loaded profile is not activated.

The keyword `OpticalSolverInput` takes as its argument either the name of a single TDR or PLX file, or a UNIX-style file name pattern to select several such files whose names match the specified pattern. In both cases, a single file may contain more than one absorbed photon density or optical generation profile. In TDR files, the different profiles are saved in separate TDR states; whereas, in PLX files, they are simply listed sequentially, including their respective headers (see Importing 1D Profiles Into Higher-Dimensional Grids on page 642).

Each profile is characterized by its set of parameters, whose values must be unique among the profiles selected in the `File` section. As profiles may be characterized by different numbers of parameters, you must specify the ones to be considered for checking uniqueness by using the keyword `IdentifyingParameter`. Supported arguments are a simple parameter name such as `Wavelength` or, if ambiguous, a full parameter path such as `Optics/Excitation/Wavelength`. It is also possible to introduce new parameters, that is, parameters that do not exist in Sentaurus Device, by assigning them to a profile and referring to them in the list of `IdentifyingParameter`. Added parameters will appear under the path `Optics/OpticalSolver/FromFile/UserDefinedParameters/<Name of added parameter>`. User-defined parameters also are supported in the `IlluminationSpectrum` file in the `File` section (see Illumination Spectrum on page 536).

> **NOTE** Only profiles that carry intensity as a parameter tag are supported for loading from files. Other profiles are ignored with a warning message. However, intensity must not be listed as `IdentifyingParameter` unless you want to enforce explicitly that all profiles are also unique with respect to their intensity.

The intensity associated with each profile and saved as a parameter tag in the respective file plays a special role as it is needed to scale the loaded profile according to the requested

intensity. For `ComputeFromMonochromaticSource`, the loaded profile must be scaled to conform with the intensity specified in the `Excitation` section according to:

$$G = \frac{I_{\text{exc}}}{I_{\text{loaded}}} G_{\text{loaded}} \tag{718}$$

For `ComputeFromSpectrum`, the loaded profile for each spectral component is scaled to match the intensity given in the corresponding entry of the illumination spectrum file. The total optical generation is then computed as the sum over the scaled profiles given by:

$$G_{\text{tot}} = \sum_{n} \frac{I_{n,\text{spectrum}}}{I_{n,\text{loaded}}} G_{n,\text{loaded}} \tag{719}$$

When using the feature `ComputeFromSpectrum` (see Illumination Spectrum on page 536) or when ramping parameters, it is possible that, for a requested set of parameter values, no profile can be found that matches it. By default, the program will exit with an appropriate error message; however, you have two further options to deal with such situations. Using the keyword `SpectralInterpolation`, either `PiecewiseConstant` or `Linear` interpolation can be selected. Interpolation is based on the leading identifying parameter as opposed to complex multidimensional interpolation.

As mentioned earlier, two profile quantities are supported, absorbed photon density and optical generation, which can be selected using the keyword `DatasetName`. The choice determines whether a quantum yield model (see Quantum Yield Models on page 544) will be applied. If optical generation is specified, quantum yield is assumed to be 1. Otherwise, the corresponding quantum yield model specified in the `OpticalGeneration` section is used to compute the optical generation profile from the loaded absorbed photon density.

Importing 1D Profiles Into Higher-Dimensional Grids

Importing 1D profiles into higher-dimensional grids is supported for files in PLX format. The following example documents the syntax of PLX files for two 1D profiles characterized by three parameters in a single file:

```
# some comments
"<optional string for tagging a profile>"
Wavelength = 0.5 [um] Theta = 0 [deg] Intensity = 0.1 [W*cm^-2]
0.0 1e19
0.8 1e20
1.4 1e17
2.0 5e18

# some comments
"<optional string for tagging a profile>"
```

```
Wavelength = 0.6 [um] Theta = 30[deg] Intensity = 0.1 [W*cm^-2]
0.0 1e19
0.8 1e20
1.4 1e17
2.0 5e18
...
```

Each profile can be preceded by an optional comment starting with the hash sign (#), an optional tag given in double quotation marks, and a list of parameters with their corresponding value and unit as shown in the example above. If a tag is supplied, it will be used as a curve name when visualizing the file in Inspect, which also supports PLX files containing several profiles.

After the 1D profiles have been loaded into Sentaurus Device, they must be interpolated onto the 2D or 3D grid. Similar to the TMM solver (see Using Transfer Matrix Method on page 630), the concept of an illumination window is applied for this purpose and it requires the specification of at least one `Window` section in the `Excitation` section. See Illumination Window on page 562 for further details. The accuracy of the integrated APD for 1D profiles in a 2D or 3D device can be controlled by various parameters (see Accurate Absorbed Photon Density for 1D Optical Solvers on page 575).

> **NOTE** For the interpolation of the 1D profile onto the 2D or 3D grid, the first data point of a profile is always pinned to the illumination window plane, independent of its actual coordinate value.

Ramping Profile Index

The optical solver `FromFile` supports a keyword `ProfileIndex`, which can be used to address a certain profile directly by its index instead of its identifying parameters. The index is derived from all valid profiles sorted according to the value of the leading identifying parameter specified in the command file. This feature can be used to ramp through all available profiles in a `Quasistationary` statement without having to know the exact parameter values for each profile. The spectral interpolation options described in Loading Solution of Optical Problem From File on page 640 above also are supported for ramping the `ProfileIndex`. If an index value is requested in a `Quasistationary` statement that exceeds the number of valid profiles, the `Quasistationary` is finished and control is given to the following statement in the `Solve` section.

The following example shows the ramping of the `ProfileIndex`:

```
File {
   OpticalSolverInput = "absorbed_photon_density_input_*file.tdr"
}

Physics {
   OpticalGeneration (
      ComputeFromMonochromaticSource ()
   )
   OpticalSolver (
      FromFile (
         ProfileIndex = 0
         DatasetName = AbsorbedPhotonDensity
         SpectralInterpolation = Off
         IdentifyingParameter = ("Optics/Excitation/Wavelength" "Theta" "Phi")
      )
   )
}

Solve {
   Quasistationary (
      InitialStep=0.01 MaxStep=0.01 MinStep=0.01
      Plot { Range = ( 0., 1 ) Intervals = 5 }
      Goal { ModelParameter="ProfileIndex" value=100 }
   ) { Optics }
}
```

Note that the counting of profiles starts with index zero. For more information about ramping parameters, see .

Optical Beam Absorption Method

The optical beam absorption method in Sentaurus Device computes optical generation by simple photon absorption using Beer's law. Thereby, multiple optical beams can be defined to represent the incident light.

Physical Model

Figure 43 illustrates one optical beam and its optical intensity distribution in a 3D device.

Figure 43   Intensity distribution of an optical beam modeled by a rectangular illumination
window

J_0 denotes the optical beam intensity (number of photons that cross an area of 1 cm^2 per 1 s) incident on the semiconductor device. (x_{min}, y_{min}) and (x_{max}, y_{max}) define the rectangular illumination window. The space shape F_{xy} of the incident beam intensity is defined by the illumination window, where F_{xyv} is equal to 1 inside of it and zero otherwise.

The following equations describe useful relations for the photogeneration problem:

$$E_{\text{ph}} = \frac{hc}{\lambda}$$

$$J_0 = \frac{P_0}{E_{\text{ph}}}$$

(720)

where:

- P_0 is the incident wave power per area $[\text{W/cm}^2]$.
- λ is the wavelength $[\text{cm}]$.
- h is Planck's constant $[\text{J s}]$.
- c is the speed of light in a vacuum $[\text{cm/s}]$.
- E_{ph} is the photon energy that is approximately equal to $\frac{1.24}{\lambda[\mu\text{m}]}$ in eV.

The optical beam absorption model computes the optical generation rate along the z-axis taking into account that the absorption coefficient varies along the propagation direction of the beam according to:

$$G^{\text{opt}}(z, t) = J_0 F_t(t) F_{xy} \cdot \alpha(\lambda, z) \cdot \exp\left(-\left|\int_{z_0}^{z} \alpha(\lambda, z') dz'\right|\right) \qquad (721)$$

where:

- t is the time.

- $F_t(t)$ is the beam time behavior function. For a Gaussian pulse, it is equal to 1 for t in $[t_{\min}, t_{\max}]$ and shows a Gaussian distribution decay outside the interval with the standard deviation σ_t.

- z_0 is the coordinate of the semiconductor surface.

- $\alpha(\lambda, z)$ is the nonuniform absorption coefficient along the z-axis.

As described in the following section, the optical beam absorption method supports a wide range of window shapes (see Illumination Window on page 562) as well as arbitrary beam time behavior functions (see Specifying Time Dependency for Transient Simulations on page 547). It is also not limited to beams propagating along the z-axis. The example above has only been used for demonstration purposes.

Using Optical Beam Absorption Method

The optical beam absorption method is activated by the optical solver `OptBeam`. The profile of the absorption coefficient used in Eq. 721 is determined by the `LayerStackExtraction` section inside the `OptBeam` section; whereas, the shape of the beam is specified by the illumination window. The wavelength and intensity of the incident light are defined in the `Excitation` section.

The required syntax of the optical beam absorption method is summarized here:

```
Physics {
   ...
   Optics (
      ...
      Excitation (
         Wavelength = 0.5
         Intensity = 0.1
         Window("L1") (
            <window options>
         )
      )
```

```
OpticalSolver (
   OptBeam (
      LayerStackExtraction (
         WindowName = "L1"
         <layer stack extraction options>
      )
   )
)
}
```

Further details about the `Window` and `LayerStackExtraction` sections can be found in Illumination Window on page 562 and Extracting the Layer Stack on page 570, respectively. The accuracy of the integrated absorbed photon density for 1D profiles in a 2D or 3D device can be controlled by various parameters (see Accurate Absorbed Photon Density for 1D Optical Solvers on page 575).

> **NOTE** You can simulate several beams at the same time by specifying the corresponding number of `Window` and `LayerStackExtraction` sections. However, all beams are assigned the same wavelength and intensity, which is specified in the common `Excitation` section.

Beam Propagation Method

In Sentaurus Device, the beam propagation method (BPM) can be applied to find the light propagation and penetration into devices such as photodetectors. Despite being an approximate method, its efficiency and relative accuracy make it attractive for bridging the gap between the raytracer and the FDTD solver (EMW) featured in Sentaurus Device. The BPM solver is available for both 2D and 3D device geometries, where its computational efficiency compared with a full-wave approach becomes particularly apparent in three dimensions.

> **NOTE** The use of BPM for 3D CMOS image sensors is discouraged because the BPM cannot resolve the polarization transformation caused by the 3D lens.

Physical Model

The BPM implemented in Sentaurus Device is based on the fast Fourier transform (FFT) and is a variant of the FFT BPM, which was developed by Feit and Fleck [7].

The solution of the scalar Helmholtz equation:

$$\left[\nabla_t^2 + \frac{\partial^2}{\partial z^2} + k_0^2 n^2(x, y, z)\right]\phi(x, y, z) = 0 \tag{722}$$

at $z + \Delta z$ with $\nabla_t^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2$ and $n(x, y, z)$ being the complex refractive index can be written as:

$$\frac{\partial}{\partial z}\phi(x, y, z + \Delta z) = \mp i\sqrt{k_0^2 n^2 + \nabla_t^2}\,\phi(x, y, z) = \pm i\,\wp\,\phi(x, y, z) \tag{723}$$

In the paraxial approximation, the operator $\wp$ reduces to:

$$\wp \cong \sqrt{k_0^2 n_0^2 + \nabla_t^2} + k_0\delta n \tag{724}$$

where n_0 is taken as a constant reference refractive index in every transverse plane. By expressing the field ϕ at z as a spatial Fourier decomposition of plane waves, the solution to Eq. 722 for forward-propagating waves reads:

$$\phi(x, y, z + \Delta z) = \frac{1}{(2\pi)^2}\exp(ik_0\delta n\Delta z)\int_{-\infty}^{\infty}d\vec{k}_t\exp(i\vec{k}_t \cdot \vec{r})\exp(i\sqrt{k_0^2 n_0^2 - \vec{k}_t^2}\,\Delta z)\tilde{\phi}(\vec{k}_t, z) \tag{725}$$

where $\tilde{\phi}$ denotes the transverse spatial Fourier transform. As can be seen from Eq. 725, each Fourier component experiences a phase shift, which represents the propagation in a medium characterized by the reference refractive index n_0. The phase-shifted Fourier wave is then inverse-transformed and given an additional phase shift to account for the refractive index inhomogeneity at each $(x, y, z + \Delta z)$ position. In the numeric implementation of Eq. 725, an FFT algorithm is used to compute the forward and inverse Fourier transform.

Bidirectional BPM

The bidirectional algorithm is based on two operators as described by Kaczmarski and Lagasse [8]. The first operator defines a unidirectional propagation, which is outlined in the previous section. The second operator accounts for the reflections at interfaces of the refractive index along the propagation direction. In a first pass, the reflections at all interfaces are computed. The following pass in the opposite direction adds these contributions to the propagating field and calculates the reflections of the forward-propagating field. By iterating this procedure until convergence is reached, a self-consistent algorithm is established.

Boundary Conditions

Due to the finite size of the computational domain, appropriate boundary conditions must be chosen, which minimize any numeric errors in the propagation of the optical field related to

boundary effects. In the standard FFT BPM, any waves propagating through a boundary will reappear as a new perturbation at the opposite side of the computation window, effectively representing periodic boundary conditions. In situations where the optical field vanishes at the domain boundaries, this effect can be neglected. In other cases, an absorbing boundary condition is needed.

Perfectly matched layers (PMLs) boundary conditions have the advantage of absorbing the optical field when it reaches the domain boundaries. The BPM implemented in Sentaurus Device supports the PML boundary condition, which has been developed for continuum spectra.

The formulation is based on the introduction of a stretching operator:

$$\nabla_s \equiv \frac{1}{S_x}\hat{x}\frac{\partial}{\partial x} + \frac{1}{S_y}\hat{y}\frac{\partial}{\partial y} + \frac{1}{S_z}\hat{z}\frac{\partial}{\partial z} \tag{726}$$

from which an equivalent set of the Maxwell equations can be derived. In Eq. 726, S_x, S_y, and S_z are called stretching parameters, which are complex numbers defined in different PML regions. In non-PML regions, these stretching parameters are equal to one. The modified propagation equation then reads:

$$\phi(x, y, z + \Delta z) = \frac{1}{(2\pi)^2}\exp(\mathrm{i}S_z k_0 \delta n \Delta z)\iint_{-\infty}^{\infty} d\vec{k}_t \exp(\mathrm{i}\vec{k}_t \cdot \vec{r})\exp(\mathrm{i}S_z)\exp(\mathrm{i}\sqrt{k_0^2 n_0^2 - \hat{k}_t^2}\Delta z)\tilde{\phi}(\vec{k}_t, z) \tag{727}$$

where $\hat{k}_t^2 = (k_x/S_x)^2 + (k_y/S_y)^2$ is the square of the stretched transverse wave number. The stretching parameters can be fine-tuned to minimize spurious reflections.

Using Beam Propagation Method

General

The following code excerpt describes the general setup for using the scalar BPM solver to compute the optical generation. The computation of the optical generation is activated by an `OpticalGeneration` section, in which the `QuantumYield` model, as defined in Eq. 707, p. 627 and Eq. 708, p. 628, can be specified. Solver-specific parameters are listed in the `BPM` section. The excitation parameters are split into the general `Excitation` section for parameters common to all optical solvers and the `BPM Excitation` section. In the latter section, you can select either a `PlaneWave` or `Gaussian` excitation.

The `GridNodes` parameter determines the number of discretization points for each spatial dimension. In the next line, the reference refractive index is specified that is used in the operator expansion in Eq. 724, p. 648.

The parameters related to the excitation field and the boundary conditions for each spatial dimension are grouped in subsections as explained here:

```
Physics {
   ...
   Optics (
      OpticalGeneration (
         QuantumYield (
            ...
         )
      OpticalSolver (
         BPM (
            GridNodes = (256,256,1600)
            ReferenceRefractiveIndex = 2.2
            Excitation (
               ...
            )
            Boundary (
               ...
            )
         )
      )
      Excitation (
         Wavelength = 0.5
         Intensity = 0.1
         Theta = 0.0
      )
   )
}
```

As the reference refractive index can greatly influence the accuracy of the solution due its use in the expansion of the propagation operator, several options are available for its specification. The simplest option is to specify a globally constant value as shown above. For multilayer structures with large refractive index contrasts, better results can be achieved by using either the average or the maximum value of the refractive index in each propagation plane. In some cases, a reference refractive index that is computed as the field-weighted average of the refractive index in each propagation plane may be the best option. In addition to these options, a global offset can be specified to further optimize the results. For details about selecting the various options, see .

Bidirectional BPM

The bidirectional BPM solver is activated by specifying a `Bidirectional` section in the `BPM` section:

```
Optics (
   OpticalSolver (
      BPM (
         ...
         Bidirectional (
            Iterations = 3
            Error = 1e-3
         )
      )
   )
)
```

In the `Bidirectional` section, two break criteria can be set to control the total number of forward and backward passes that are performed in the beam propagation method. If the number of iterations exceeds the value of `Iterations` or if the relative error with respect to the previous iteration is smaller than the value of `Error`, it is assumed that the solution has been found. Note that a single iteration can be either a forward or backward pass. From a performance point of view, it is important to mention that consecutive iterations only require a fraction of CPU time compared with the initial pass.

For plotting the optical field after every iteration, the keyword `OpticalField` must be listed in the `Plot` section of the command file. If only the final optical intensity is of interest, it is sufficient to specify the keyword `OpticalIntensity` in the `Plot` section.

Excitation

In the beam propagation method, a given input field, which is referred to as excitation in the remainder of this section, is propagated through the device structure. Two types of excitation are supported: a `Gaussian` and a (truncated) `PlaneWave`. Both are characterized by a propagation direction, wavelength, and power as shown below. In two dimensions, the propagation direction is determined by the angle between the positive y-axis and the propagation vector. To specify the propagation direction in three dimensions, two angles, `Theta` and `Phi`, must be given. Their definition is illustrated in .

The incident light power in the plane wave is specified as the `Intensity` in [W/cm^2]. For a Gaussian excitation, the given value refers to its maximum. All of these parameters are listed in the global `Excitation` section.

Figure 44   Definition of angles for specification of propagation direction in three dimensions

The excitation parameters common to all types of excitation are:

```
Physics {
   ...
   Optics (
      Excitation (
         Theta = 10.0        # [degree]
         Phi = 60.0          # [degree], only in 3D
         Wavelength = 0.3    # [um]
         Intensity = 0.1     # [W/cm^2]
         ...
      )
      ...
   )
}
```

A Gaussian excitation along the propagation direction defined by k is determined by its half-width SigmaGauss [μm] and its center position CenterGauss [μm] as shown below for a 2D and 3D device geometry.

Gaussian excitation (2D):

```
Physics {
   ...
   Optics(
      OpticalSolver (
         BPM (
            Excitation (
               Type = "Gaussian"
               SigmaGauss = (2.0)     # [um]
               CenterGauss = (0.0)    # [um]
            )
         )
      )
```

```
         ...
      )
   }
```

Gaussian excitation (3D):

```
   Physics {
      ...
      Optics(
         OpticalSolver (
            BPM (
               Excitation (
                  Type = "Gaussian"
                  SigmaGauss = (2.0,4.0)    # [um]
                  CenterGauss = (0.0,1.0)   # [um]
               )
            )
         )
         ...
      )
   }
```

For a plane wave excitation, it is possible to specify the truncation positions for each coordinate axis as well as a parameter that determines the fall-off. For numeric reasons, a discrete truncation must be avoided. Instead, a Fermi function–like fall-off is available:

$$F_{xy} = \left[1 + \exp\left(\frac{|\tilde{x}| - x_0}{s_x}\right)\right]^{-1} \cdot \left[1 + \exp\left(\frac{|\tilde{y}| - y_0}{s_y}\right)\right]^{-1}$$

$$\phi(x, y, z = 0) = F_{xy} \cdot \phi_0$$

(728)

which can be tuned by adjusting the `TruncationSlope` and `TruncationPosition` parameters in the `Excitation` section. In Eq. 728, ϕ_0 is the amplitude of the incident light, $s_{x,y}$ denotes the `TruncationSlope`, $\tilde{x}, \tilde{y}$ is the position with respect to the symmetry point, and x_0, y_0 is the half width. Both $\tilde{x}, \tilde{y}$ and x_0, y_0 are deduced from the `TruncationPosition` parameters. In two dimensions, the second factor on the right-hand side in Eq. 728 is omitted.

Truncated plane wave excitation (2D):

```
   Physics {
      Optics (
         OpticalSolver (
            BPM (
               Excitation (
                  Type = "PlaneWave"
                  TruncationPositionX = (-1.0,1.0)
                  TruncationSlope = (0.3)
               )
```

```
            )
          )
          ...
        )
    }
```

Truncated plane wave excitation (3D):

```
Physics {
  Optics (
    OpticalSolver (
      BPM (
        Excitation (
          Type = "PlaneWave"
          TruncationPositionX = (-1.0,1.0)
          TruncationPositionY = (-2.0,3.0)
          TruncationSlope = (0.3,0.3)
        )
      )
    )
  )
}
```

Boundary

For every spatial dimension, a separate boundary condition and corresponding parameters can be defined. Periodic boundary conditions inherent to the FFT BPM solver are the default in the transverse dimensions. The specification of PML boundary conditions in the x-direction and y-direction is shown below. With the keyword `Order`, the spatial variation of the complex stretching parameter can be specified. In this example, a quadratic increase from the minimum value to the maximum value within the given number of `GridNodes` on either side has been chosen.

Optionally, several `VacuumGridNodes` can be inserted between the physical simulation domain and the PML boundary:

```
Physics {
  Optics(
    OpticalSolver (
      BPM (
        Boundary (
          Type = "PML"
          Side = "X"
          Order = 2
          StretchingParameterReal = (1.0,1,0)
          StretchingParameterImag = (1.0,5.0)
          GridNodes = (5,5)
```

```
            VacuumGridNodes = (4,4)
        )
        Boundary (
            Type = "PML"
            Side = "y"
            Order = 2
            StretchingParameterReal = (1.0,1,0)
            StretchingParameterImag = (1.0,4.0)
            GridNodes = (8,8)
        )
    )
)
...
)
}
```

Ramping Input Parameters

Several input parameters of the BPM solver such as the wavelength of the incident light can be ramped to obtain device characteristics as a function of the specified parameter. The general concept of ramping the values of physical parameters is described in . More detailed information about ramping `Optics` parameters can be found in .

Visualizing Results on Native Tensor Grid

For an accurate analysis of the BPM results, the complex refractive index, the complex optical field, and the optical intensity can be plotted on the native tensor grid. In general, the results from the BPM solver are interpolated from a tensor grid to a mixed-element grid on which the device simulation is performed.

For physical and numeric reasons, the mesh resolution of the optical grid needs to be much finer than that of the electrical grid in most regions of the device. This can lead to the introduction of interpolation errors, for example, by undersampling the respective dataset on the electrical grid. To obtain an estimate of the interpolation error, it can be beneficial to visualize the BPM results on its native tensor grid. As typical tensor grids in three dimensions tend to be very large, it is also possible to extract a limited domain for more efficient visualization. In two dimensions, a rectangular subregion or an axis-aligned straight line can be plotted; whereas in three dimensions, a subvolume, a plane perpendicular to the coordinate axes, and a straight line can be visualized directly on the tensor grid.

Tensor plots can be activated by specifying one or more `TensorPlot` sections and an optional base name for the tensor-plot file name in the `File` section.

The following syntax extracts a plane perpendicular to the z-axis at position $Z = 1.3 \, \mu m$, which extends from $-2 \, \mu m$ to $3 \, \mu m$, and from $-1 \, \mu m$ to $5 \, \mu m$ in the x- and y-direction, respectively:

```
File (
   ...
   TensorPlot = "tensor_plot"
)
...
TensorPlot (
   Name = "plane_z_const"
   Zconst = 1.3
   Xmin = -2
   Xmax = 3
   Ymin = -1
   Ymax = 5
){
   ComplexRefractiveIndex
   OpticalField
   OpticalIntensity
}
```

To extract a box in three dimensions that extends over the whole device horizontally but is bound in the vertical direction, the `TensorPlot` section looks like:

```
TensorPlot (
   Name = "bounded_box"
   Zmin = 3
   Zmax = 8
){
   ...
}
```

Composite Method

The composite method is an optical solver that composes an optical solution by summing the results of other optical solvers. Its flexibility targets applications with more complex optical setups that can be modeled as a linear superposition of individual solution components.

The unified interface for optical generation computation is limited in that the contribution from `ComputeFromMonochromaticSource` and `ComputeFromSpectrum` to the total optical generation rate is computed by the same optical solver. While some optical solvers allow the definition of different illumination windows, they still must share the same excitation parameters. It is also not possible to specify several `ComputeFromMonochromaticSource` and `ComputeFromSpectrum` sections at the same time to model, for example, different light sources illuminating a device. Sometimes you can work around these limitations by

precomputing the illumination by one light source and loading it in a subsequent simulation using `ReadFromFile`. However, it typically results in more complex simulation setups and tool flows.

With the composite method, these limitations can be overcome. Its implementation is based on the mixed-mode simulation framework that requires the creation of a separate optical device instance for each optical solver. An optical device instance is essentially a device instance limited to the computation of an optical problem. For details about mixed-mode in Sentaurus Device, see Chapter 3 on page 41.

Using the Composite Method

A typical simulation setup requires the definition of a named master `Device` or `OpticalDevice` (in the case of optics standalone simulations), and one or more additional definitions of `OpticalDevice`. In the master, the composite method is specified as the optical solver in the `Optics` section:

```
Device diode {
   File { ... }
   Electrode { ... }
   Plot { ... }
   Math { ... }
   Physics {
      ...
      Optics (
         ...
         OpticalDevice (Composite)
      )
   }
}

OpticalDevice optdevice {
   File { ... }
   Plot { ... }
   Math { ... }
   Physics {
      Optics (
         Excitation (
            Wavelength = 0.3
            Theta = 30
            Intensity = 0.1
         )
         OpticalDevice ( TMM (...) )
         ComplexRefractiveIndex ( ... )
         OpticalGeneration (
            ...
```

```
                   ComputeFromMonochromaticSource ( ... )
                   ComputeFromSpectrum ( ... )
                )
            )
        }
    }
```

> **NOTE**   Syntactically, there is no difference between a named `Device` and a
> named `OpticalDevice` section at the top level in the command file.
> However, instances created from these definitions fulfill different tasks.

Any of the other optical solvers listed in Specifying the Optical Solver on page 554 can be specified in the `OpticalDevice` definitions whose instances are accessed by the composite method. You can create more than one instance from a given `OpticalDevice` definition and overwrite specific parameters in the instantiation statement. This is particularly useful for modeling different illumination sources that share many common properties, for example:

```
System {
    diode d1 (
        "p-contact" = vdd "n-contact" = gnd
        OpticalDevice = [ "tmm1" "tmm2" "tmm3" ]
    ) { ... }
    optdevice tmm1 () { Physics { Optics ( Excitation (Wavelength = 0.4) ) } }
    optdevice tmm2 () { Physics { Optics ( Excitation (Theta = 50) ) } }
    optdevice tmm3 () { Physics { Optics ( Excitation (Intensity = 0.2) ) } }
}
```

In this example, the device instance `d1` is associated with the optical device instances `tmm1`, `tmm2`, and `tmm3` by the `OpticalDevice` statement. These are the optical device instances that the `Composite` solver defined in `Device diode` will consider when composing its solution.

In the `Solve` section, the different instances can be addressed separately by preceding the equation name with the instance name followed by a dot, or as a whole by specifying the equation only as shown in the optics standalone example:

```
Solve {
    tmm1.Optics
    Coupled (d1.Optics tmm2.Optics tmm3.Optics)
    Optics
}
```

In optoelectronic simulations, the `Optics` equation can be omitted and is solved implicitly (considering all device and optical device instances) if the corresponding optical generation models are activated:

```
Solve {
    Quasistationary (
        InitialStep = 1 MaxStep = 1 MinStep = 1
```

```
        Goal { OpticalDevice = "tmm1" ModelParameter = "Wavelength" = 0.8 }
        Goal { OpticalDevice = "tmm3" ModelParameter = "Wavelength" = 0.4 }
   ) {
        Coupled { Poisson Electron Hole }
   }
}
```

> **NOTE**   The `Coupled` command can contain either electrical transport
> equations such as `Poisson`, `Electron`, and `Hole`, or several instance-
> specific `Optics` equations, but not a combination of both. If you want
> to explicitly call `Optics` and electrical transport equations, you must
> use a `Plugin` statement.

Generally, simulation results such as spatial-dependent plots and current plots are produced for
each `Device` or `OpticalDevice` instance according to the respective `Plot` and
`CurrentPlot` sections. However, for ease of use, the most relevant spatial-dependent datasets
from `OpticalDevice` instances used by the `Composite` solver are written automatically to
corresponding TDR files.

Such datasets have their original dataset name appended with `FromInstance_<instance
name>`, for example, `OpticalGenerationFromInstance_tmm1`.

To access `CurrentPlot` quantities from one `Device` or `OpticalDevice` in another `Device`
or `OpticalDevice`, use either the `Device="<name>"` or `OpticalDevice="<name>"`
specification in the `CurrentPlot` section.

Controlling Interpolation When Loading Optical Generation Profiles

You can load optical generation and absorbed photon density profiles into Sentaurus Device
using either of two features:

- Loading and Saving Optical Generation From and to File on page 542
- Loading Solution of Optical Problem From File on page 640

If the optical generation or absorbed photon density profile to be loaded is defined on a grid
that is different from the one used in the device simulation, it is interpolated automatically onto
the simulation grid upon loading. The source grid can be either a mixed-element grid or a
tensor grid resulting from an EMW simulation. By default, vertex-based linear interpolation is
used.

For mixed-element to mixed-element interpolation, a conservative interpolation algorithm is
supported [9], which guarantees that the integral of the interpolation quantity on the source grid

is the same as on the destination grid. To select this option, set `GridInterpolation` to `Conservative` instead of `Simple`.

The result of the interpolation can be further controlled by specifying a relative shift between the source and the destination grid, as well as by restricting the source and destination domain used for the interpolation. This feature is useful when the optical solution has been computed on a smaller or larger domain than the electrical simulation grid and, therefore, must be aligned accordingly.

The `ShiftVector` is specified directly in the `ReadFromFile` or `FromFile` section; whereas, the source and destination domain is specified in a section called `ImportDomain`. A domain can be defined as either a list of regions or a box given by its lower-left and upper-right corners as shown in this example:

```
Physics {
  Optics (
    OpticalGeneration (
      ReadFromFile (
        GridInterpolation = Conservative
        ShiftVector = (0.5 1 2)
        ImportDomain (
          SourceRegions = ("substrate", "region_1")
          DestinationBoxCorner1 = (0.5 0.5 1)
          DestinationBoxCorner2 = (2 2 4)
        )
      )
    )
  )
}
```

Figure 45 on page 661 illustrates the concept of domain truncation using source and destination domains, as well as applying a relative shift between the optical and electrical grids. The interpolation algorithm always interpolates the values even if the material of the source and destination grid is different at a certain vertex. However, optical generation is always set to zero in nonsemiconductor regions irrespective of the source profile. For more details about specifying the source and destination domain in the `ImportDomain` section, see Table 243 on page 1442.

> **NOTE** `GridInterpolation`, `ShiftVector`, and `ImportDomain` are not supported for the importing of 1D profiles because the Illumination Window on page 562 already provides similar functionality.

> **NOTE** Region domains specified in the `ImportDomain` section are supported only for source grids that are mixed-element type or tensor type, containing region information (the `Extractor` section in EMW must contain `Region` in the `Quantity` list).

Figure 45   Illustration of domain truncation and shifting of source and destination grids used in interpolation

Optical AC Analysis

An optical AC analysis calculates the quantum efficiency as a function of the frequency of the optical signal intensity. The method is based on the AC analysis technique and provides real and imaginary parts of the quantum efficiency versus the frequency.

During an optical AC analysis, a small perturbation of the incident wave power δP_0 is applied. Therefore, the photogeneration rate is perturbated as $G^{\text{opt}} + \delta G^{\text{opt}} e^{i\omega t}$, where $\omega = 2\pi f$ (f is the frequency) and δG^{opt} is an amplitude of a local perturbation. The resulting small-signal

device current perturbation δI_{dev} is the sum of real and imaginary parts, and the expressions for the quantum efficiency are:

$$\eta = \frac{Re[\delta I_{dev}]/q}{\delta P^{tot}\lambda/hc}$$

$$C_{opt} = \frac{1}{\omega} \cdot \frac{Im[\delta I_{dev}]/q}{\delta P^{tot}\lambda/hc}$$ (729)

$$\delta P^{tot} = \int_S \delta P_0 ds$$

where the quantity $\delta P^{tot}\lambda/hc$ gives a perturbation of the total number of photons and $Re[\delta I_{dev}]/q$ is a perturbation of the total number of electrons at an electrode. As a result, for each electrode, Sentaurus Device places two values into the AC output file, `photo_a` and `photo_c`, that correspond to η and C_{opt}, respectively. To start the optical AC analysis, add the keyword `Optical` in the `ACCoupled` statement, for example:

```
ACCoupled ( StartFrequency=1.e4 EndFrequency=1.e9
   NumberOfPoints=31 Decade Node(a c) Optical )
   { poisson electron hole }
```

NOTE   If an element is excluded (`Exclude` statement) in optical AC (this is usually the case for voltage sources in regular AC simulation), it means that this element is not present in the simulated circuit and, correspondingly, it provides zero AC current for all branches that are connected to the element. Therefore, do *not* exclude voltage sources.

References

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CHAPTER 22 **Radiation Models**

This chapter presents the radiation models used in Sentaurus Device.

When high-energy particles penetrate a semiconductor device, they deposit their energy by the generation of electron–hole pairs. These charges can perturb the normal operation of the device. This chapter describes the models for carrier generation by gamma radiation, alpha particles, and heavy ions.

Generation by Gamma Radiation

Using Gamma Radiation Model

The radiation model is activated by specifying the keyword `Radiation(...)` (with optional parameters) in the `Physics` section:

```
Radiation{
    Dose = <float> | DoseRate = <float>
    DoseTime = (<float>,<float>)
    DoseTSigma = <float>
}
```

where `DoseRate` (in rad/s) represents D in Eq. 730. The optional `DoseTime` (in s) allows you to specify the time period during which exposure to the constant `DoseRate` occurs. `DoseTSigma` (in s) can be combined with DoseTime to specify the standard deviation of a Gaussian rise and fall of the radiation exposure. As an alternative to `DoseRate`, `Dose` (in rad) can be specified to represent the total radiation exposure over the `DoseTime` interval. In this case, `DoseTime` must be specified.

To plot the generation rate due to gamma radiation, specify `RadiationGeneration` in the `Plot` section.

Yield Function

Generation of electron–hole pairs due to radiation is an electric field–dependent process [1] and is modeled as follows:

$$G_r = g_0 D \cdot Y(F)$$

$$Y(F) = \left(\frac{F + E_0}{F + E_1}\right)^m \tag{730}$$

where D is the dose rate, g_0 is the generation rate of electron–hole pairs, and E_0, E_1, and m are constants.

All these constants can be specified in parameter file of Sentaurus Device as follows:

```
Radiation {
   g = 7.6000e+12   # [1/(rad*cm^3)]
   E0 = 0.1         # [V/cm]
   E1 = 1.3500e+06  # [V/cm]
   m = 0.9          # [1]
}
```

Alpha Particles

Using Alpha Particle Model

Specify the `AlphaParticle` in the `Physics` section:

```
Physics { ...
   AlphaParticle (<optional keywords>)
}
```

Table 276 on page 1463 lists the keyword options for alpha particles.

Table 123   Coefficients for carrier generation by alpha particles

Symbol	Parameter name	Default value	Unit
s	s	2×10^{-12}	s
w_t	wt	1×10^{-5}	cm
c_2	c2	1.4	1
a	alpha	90	cm^{-1}

Table 123   Coefficients for carrier generation by alpha particles (Continued)

Symbol	Parameter name	Default value	Unit
α_2 α_3	alpha2 alpha3	5.5×10^{-4} 2×10^{-4}	cm cm
E_p	Ep	3.6	eV
a_o a_1 a_2	a0 a1 a2	-1.033×10^{-4} 2.7×10^{-10} 4.33×10^{-17}	cm cm/eV cm/eV^2

To plot the instant generation rate $G(t)$ due to alpha particles, specify `AlphaGeneration` in the `Plot` section; to plot $\int_{-\infty}^{\infty} dt\, G$, specify `AlphaCharge`.

The generation by alpha particles cannot be used except in transient simulations. The amount of electron–hole pairs generated before the initial time of the transient is added to the carrier densities at the beginning of the simulation.

An option to improve the spatial integration of the charge generation is presented in References on page 673.

Alpha Particle Model

The generation rate caused by an alpha particle with energy E is computed by [2]:

$$G(u, v, w, t) = \frac{a}{\sqrt{2\pi} \cdot s} \exp\left[-\frac{1}{2}\left(\frac{t - t_m}{s}\right)^2 - \frac{1}{2}\left(\frac{v^2 + w^2}{w_t^2}\right)\right]\left[c_1 e^{\alpha u} + c_2 \exp\left(-\frac{1}{2}\left(\frac{u - \alpha_1}{\alpha_2}\right)^2\right)\right] \qquad (731)$$

if $u < \alpha_1 + \alpha_3$, and by:

$$G(u, v, w, t) = 0 \qquad (732)$$

if $u \geq \alpha_1 + \alpha_3$. In this case, u is the coordinate along the particle path and v and w are coordinates orthogonal to u. The direction and place of incidence are defined in the `Physics` section of the command file with the keywords `Direction` and `Location` (or `StartPoint`, see Note on page 671), respectively. Parameter t_m is the time of the generation peak defined by the keyword `Time`. A Gaussian time dependence can also be used to simulate the typical generation due to pulsed laser or electron beams.

The maximum of the Bragg peak, α_1, is fitted to data [3] by a polynomial function:

$$\alpha_1 = a_0 + a_1 E + a_2 E^2 \qquad (733)$$

The parameter c_1 is given by:

$$c_1 = \exp[\alpha(\alpha_1[10\text{MeV}] - \alpha_1[E])] \tag{734}$$

The scaling factor a is determined from:

$$\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty G(u, v, w, t)dtdwdvdu = \frac{E}{E_\text{p}} \tag{735}$$

where E_p is the average energy needed to create an electron–hole pair. The remaining parameters are listed in . They are available in the parameter set `AlphaParticle` and are valid for alpha particles with energies between $1\,\text{MeV}$ and $10\,\text{MeV}$.

Heavy Ions

When a heavy ion penetrates a device structure, it loses energy and creates a trail of electron–hole pairs. These additional electrons and holes may cause a large enough current to switch the logic state of a device, for example, a memory cell. Important factors are:

- The energy and type of the ion.
- The angle of penetration of the ion.
- The relation between the lost energy or linear energy transfer (LET) and the number of pairs created.

Using Heavy Ion Model

The simulation of an SEU caused by a heavy ion impact is activated by using the keyword `HeavyIon` in an appropriate `Physics` section:

```
# Default heavy ion
Physics {
   HeavyIon (<keyword_options>) }

# User-defined heavy ion.
Physics {
   HeavyIon (<IonName>) (<keyword_options>) }
# User-defined heavy ions do not have default parameters. Therefore,
# in the parameter file, a specification of the following form must appear:
# HeavyIon(<IonName>){ ... } (see Table 125 on page 671)
```

describes the options for `HeavyIon`. The generation rate by the heavy ion is generally used in transient simulations. The number of electron–hole pairs generated before the initial time of the transient is added to the carrier densities at the beginning of the

simulation. The total charge density and the instant generation rate are plotted using `HeavyIonCharge` and `HeavyIonGeneration` in the `Plot` section, respectively.

If the value of `Wt_hi` is 0, then uniform generation is selected. If the value of `LET_f` is 0, the keyword `LET_f` can be ignored.

An option to improve the spatial integration of the charge generation is presented in References on page 673.

Heavy Ion Model

Figure 46   A heavy ion penetrating a semiconductor; its track is defined by a length and the transverse spatial influence is assumed to be symmetric about the track axis

A simple model for the heavy ion impinging process is shown in Figure 46. The generation rate caused by the heavy ion is computed by:

$$G(l, w, t) = G_{\text{LET}}(l)R(w, l)T(t) \tag{736}$$

if $l < l_{\max}$ ($l_{\max}$ is the length of the track), and by:

$$G(l, w, t) = 0 \tag{737}$$

if $l \geq l_{\max}$. $R(w)$ and $T(t)$ are functions describing the spatial and temporal variations of the generation rate. $G_{\text{LET}}(l)$ is the linear energy transfer generation density and its unit is pairs/cm^3.

$T(t)$ is defined as a Gaussian function:

$$T(t) = \frac{2 \cdot \exp\left(-\left(\frac{t - t_0}{\sqrt{2} \cdot s_{\text{hi}}}\right)^2\right)}{\sqrt{2} \cdot s_{\text{hi}} \sqrt{\pi} \left(1 + \text{erf}\left(\frac{t_0}{\sqrt{2} \cdot s_{\text{hi}}}\right)\right)} \tag{738}$$

where t_0 is the moment of the heavy ion penetration (see the keyword Time in Table 277 on page 1463), and s_{hi} is the characteristic value of the Gaussian (see s_hi in Table 125 on page 671).

The spatial distribution, $R(w, l)$, can be defined as an exponential function (default):

$$R(w, l) = \exp\left(-\frac{w}{w_t(l)}\right) \tag{739}$$

or a Gaussian function:

$$R(w, l) = \exp\left(-\left(\frac{w}{w_t(l)}\right)^2\right) \tag{740}$$

where w is a radius defined as the perpendicular distance from the track. The characteristic distance w_t is defined as Wt_hi in the HeavyIon statement and can be a function of the length l (see Table 277 on page 1463).

In addition, the spatial distribution $R(w, l)$ can be defined as a PMI function (see Spatial Distribution Function on page 1257).

The linear energy transfer (LET) generation density, $G_{LET}(l)$, is given by:

$$G_{LET}(l) = a_1 + a_2 l + a_3 e^{a_4 l} + k'\left[c_1(c_2 + c_3 l)^{c_4} + LET\_f(l)\right] \tag{741}$$

where $LET\_f(l)$ (defined likewise by the keyword LET_f) is a function of the length l. Example 2 in Examples: Heavy Ions on page 671 shows how you can use an array of values to specify the length dependence of $LET\_f(l)$. A linear interpolation is used for values between the array entries of LET_f.

There are two options for the units of LET_f: pairs/cm^3 (default) or pC/μm (activated by the keyword PicoCoulomb). Depending on the units of LET_f chosen, k' takes on different values in order to make the above equation dimensionally consistent. The appropriate values of k' for different device dimensions are summarized in Table 124.

Table 124 Setting correct k' to make LET generation density equation dimensionally consistent

Condition	Two-dimensional device	Three-dimensional device
LET_f has units of pairs/cm^3 for $R(w, l)$ is exponential or Gaussian	$k' = k$	$k' = k$
LET_f has units of pC/μm and $R(w, l)$ is exponential	$k' = \dfrac{k}{2w_t d}$ $d = 1\mu m$	$k' = \dfrac{k}{2\pi w_t^2}$

Table 124   Setting correct k' to make LET generation density equation dimensionally consistent (Continued)

Condition	Two-dimensional device	Three-dimensional device
`LET_f` has units of $pC/\mu m$ and $R(w, l)$ is Gaussian	$k' = \dfrac{k}{\sqrt{\pi} w_t d}$ $d = 1\mu m$	$k' = \dfrac{k}{\pi w_t^2}$

Great care must also be exercised to choose the correct units for `Wt_hi` and `Length`. The default unit of `Wt_hi` and `Length` is centimeter. If the keyword `PicoCoulomb` is specified, the unit becomes μm. Examples illustrating the correct unit use are shown in Examples: Heavy Ions. The other coefficients used in Eq. 741 are listed in Table 125 with their default values, and they can be adjusted in the parameter file of Sentaurus Device.

Table 125   Coefficients for carrier generation by heavy ion (HeavyIon parameter set)

	s_{hi}	a_1	a_2	a_3	a_4	k	c_1	c_2	c_3	c_4
Keyword	s_hi	a_1	a_2	a_3	a_4	k_hi	c_1	c_2	c_3	c_4
Default value	2e-12	0	0	0	0	1	0	1	0	1
Default unit	s	pairs/cm^3	pairs/cm^3/cm	pairs/cm^3	cm^{-1}	1	pairs/cm^3	1	cm^{-1}	1
Unit if PicoCoulomb is chosen	s	pairs/cm^3	pairs/cm^3/μm	pairs/cm^3	μm^{-1}	1	pC/μm	1	μm^{-1}	1

> **NOTE**   The keyword `Location` defines a bidirectional track for which Sentaurus Device computes the generation rate in both directions from the place of incidence along the `Direction` vector. The keyword `StartPoint` defines a one-directional track. In this case, Sentaurus Device computes the generation rate only in the positive direction from the place of incidence.

Examples: Heavy Ions

Example 1

The track has a constant `LET_f` value of $0.2\,pC/\mu m$ across the track. The track length is $1\,\mu m$ ($l_{max} = 1\,\mu m$) and the heavy ion crosses the device at the time $0.1\,ps$. The unit of `LET_f` is $pC/\mu m$ and the spatial distribution is Gaussian. Since `PicoCoulomb` was chosen, the values of `Length` and `Wt_hi` are expressed in terms of μm.

The keyword `HeavyIonChargeDensity` in the `Plot` statement plots the charge density generated by the ion:

```
Physics { Recombination ( SRH(DopingDependence) )
   Mobility (DopingDependence Enormal HighFieldSaturation)
   HeavyIon (
      Direction=(0,1)
      Location=(1.5,0)
      Time=1.0e-13
      Length=1
      Wt_hi=3
      LET_f=0.2
      Gaussian
      PicoCoulomb )
}
Plot { eDensity hDensity ElectricField HeavyIonChargeDensity
}
```

Example 2

The `LET_f` and radius (`Wt_hi`) values are functions of the position along the track (in this case, $l_{max} = 1.7 \times 10^{-4}$ cm). Values in between the array entries are linearly interpolated. The unit of `LET_f` is $pairs/cm^3$ (because the keyword `PicoCoulomb` is not used), and the unit for `Length` and `Wt_hi` is centimeter. For each value of length, there is a corresponding value of `LET_f` and a value for the radius. The spatial distribution in the perpendicular direction from the track is exponential:

```
Physics { Recombination ( SRH(DopingDependence) )
   HeavyIon (
      Direction=(0,1)
      Location=(1.5,0)
      Time=1.0e-13
      Length = [1e-4 1.5e-4 1.6e-4 1.7e-4]
      LET_f = [1e6 2e6 3e6 4e6]
      Wt_hi = [0.3e-4 0.2e-4 0.25e-4 0.1e-4]
      Exponential )
}
```

Example 3

This example illustrates multiple ion strikes in the SEU model.

```
Physics { Recombination ( SRH(DopingDependence) )
   HeavyIon (
      Direction=(0,1)
      Location=(0,0)
      Time=1.0e-13
```

```
      Length = [1e-4 1.5e-4 1.6e-4 1.7e-4]
      LET_f = [1e6 2e6 3e6 4e6]
      Wt_hi = [0.3e-4 0.2e-4 0.25e-4 0.1e-4] )

   HeavyIon ("Ion1")(
   # User-defined heavy ions do not have default parameters. Therefore,
   # in the parameter file, a specification of the following form must appear:
   # HeavyIon("Ion1"){ ... } (see Table 125 on page 671)
      Direction=(0,1)
      Location=(1,0)
      Time=1.0e-13
      Length = [1e-4 1.5e-4 1.6e-4 1.7e-4]
      LET_f = [1e6 2e6 3e6 4e6]
      Wt_hi = [0.3e-4 0.2e-4 0.25e-4 0.1e-4] )
}
```

References

[1]   J.-L. Leray, "Total Dose Effects: Modeling for Present and Future," *IEEE Nuclear and Space Radiation Effects Conference (NSREC) Short Course*, 1999.

[2]   A. Erlebach, *Modellierung und Simulation strahlensensitiver Halbleiterbauelemente*, Aachen: Shaker, 1999.

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CHAPTER 23 Noise, Fluctuations, and Sensitivity

This chapter discusses noise analysis, fluctuation analysis, and sensitivity analysis in Sentaurus Device.

This chapter explains the Sentaurus Device features to model noise, statistical fluctuations of doping, trap concentration, workfunction, band edge, geometry, dielectric constant, metal conductivity, and sensitivity to variations of model parameters, doping, and geometry. All these topics deal with the response of the device characteristics to small, device-internal variations. For noise, these variations occur randomly over time within a single device; for statistical fluctuations, the variations are random device-to-device variations; and for sensitivity, the variations are user supplied. Despite the different nature of the variations, they all can be handled by the same linearization approach called the *impedance field method* and, therefore, Sentaurus Device treats them all in a common framework.

Using the Impedance Field Method explains how to perform noise, fluctuation, and sensitivity analysis. Noise Sources on page 680 discusses the noise and random fluctuation models that Sentaurus Device offers. Statistical Impedance Field Method on page 691 describes a modeling approach for random dopant fluctuations, trap concentration fluctuations, geometric variations, and workfunction variations based on statistical sampling. Deterministic Variations on page 703 discusses user-supplied variations of doping, geometry, and model parameters.

Impedance Field Method on page 709 discusses the background of the method [1], and Noise Output Data on page 710 summarizes the data available for visualization.

Using the Impedance Field Method

Sentaurus Device treats noise analysis, fluctuation analysis, and sensitivity analysis by the impedance field method, and as extensions of small-signal analysis (see Small-Signal AC Analysis on page 96).

> **NOTE** Currently, the impedance field method is not supported with the `HeteroInterface` option (see Abrupt and Graded Heterojunctions on page 10), the `Thermionic` option (see Thermionic Emission Current on page 763), or dipole layers (Dipole Layer on page 174).

For noise and random fluctuations, Sentaurus Device computes the variances and correlation coefficients for the voltages at selected circuit nodes, assuming the net current to these nodes is fixed. As the computation is performed in frequency space, the computed quantities are

called the noise voltage spectral densities. Sentaurus Device also computes the variances and correlation coefficients of the currents through the nodes, assuming fixed voltages; these quantities are the noise current spectral densities.

For the statistical impedance field method (sIFM) and for deterministic variations, Sentaurus Device computes responses of node voltages assuming fixed currents and responses of node currents assuming fixed voltages.

Specifying Variations

To use noise and random fluctuation analysis, specify the physical models for the microscopic origin of the deviations (called the local noise sources, LNS) as options to the keyword `Noise` in the `Physics` section of the command file of Sentaurus Device:

```
Physics {
   ...
   Noise <string> ( <Noisemodels> )
}
```

where `<Noisemodels>` is a list that specifies any number of noise models listed in Table 313 on page 1481. The name given by the string after `Noise` is optional. Using `Noise` specifications with different names allows you to investigate different specifications of noise in a single simulation run.

For the sIFM, specify `RandomizedVariation` in the global `Math` section and in a device-specific global `Physics` section:

```
Math {
   RandomizedVariation <string> ( <specification> )
   ...
}
Device <string> {
   Physics {
      RandomizedVariation <string> ( <specification> )
   }
}
```

where `<specification>` specifies the details for the randomization (see Statistical Impedance Field Method on page 691).

For deterministic variations, specify the variations as options to `DeterministicVariation` in the global `Physics` section:

```
Physics {
    DeterministicVariation( <variations> )
    ...
}
```

where `<variations>` is a list that specifies any number of deterministic variations (see Deterministic Variations on page 703 and Table 285 on page 1467).

Specifying the Solver

In any case, use the `ObservationNode` option to the `ACCoupled` statement to specify the device nodes for which the noise spectral densities or deviations are required, for example:

```
ACCoupled (
    StartFrequency = 1.e8 EndFrequency = 1.e11
    NumberOfPoints = 7 Decade
    Node (n_source n_drain n_gate)
    Exclude (v_drain v_gate)
    ObservationNode (n_drain n_gate)
    ACExtract = "mos"
    NoisePlot = "mos"
    ){
    poisson electron hole contact circuit
    }
}
```

The keyword `ObservationNode` enables noise and fluctuation analysis (in this case, for the nodes `n_drain` and `n_gate`). `NoisePlot` specifies a file name prefix for device-specific plots (see Noise Output Data on page 710). For more information on the `ACCoupled` statement, see Small-Signal AC Analysis on page 96.

> **NOTE** The observation nodes must be a subset of the nodes specified in `Node(...)`.

Analysis at Frequency Zero

You can perform variation analysis at frequency zero. If you specify in the `ACCoupled` statement the single frequency zero by:

```
StartFrequency = 0. EndFrequency = 0. NumberOfPoints = 1
```

this mode is enabled, which enhances both speed and memory consumption of the analysis, compared to the analysis at positive frequency. However, you must be aware of the following: First, capacitances of AC nodes cannot be extracted and are set to zero in the output files. Second, for general structures, only the current Green's functions (and their responses) are well defined and computed. The voltage Green's functions and their related responses cannot be computed. Therefore, their computation is disabled by default and corresponding output data is set to zero. However, if all parts of the structure are conductively (and not only capacitively) coupled, voltage responses are well defined and their computation can be enabled explicitly by specifying `VoltageGreenFunctions` as a parameter in the `ACCoupled` statement.

Output of Results

The results of the analysis are the noise voltage spectral densities, the noise current spectral densities, and voltage and current deviations. They appear in the `ACExtract` file (see Table 126) and, in the case of the sIFM, in a separate `.csv` file. The units are V^2s for the voltage spectral densities and A^2s for the current noise spectral densities. If the string specified after `Noise` is not empty, it is prefixed to the name of the spectral density in the `ACExtract` file.

Table 126   Noise and fluctuation data written into ACExtract file

Name	Description
S_V	Autocorrelation noise voltage spectral density (NVSD)
S_I	Autocorrelation noise current spectral density (NISD)
S_V_ee S_V_hh	Electron NVSD Hole NVSD
S_V_eeDiff S_V_hhDiff	Electron NVSD due to diffusion LNS Hole NVSD due to diffusion LNS
S_V_eeMonoGR S_V_hhMonoGR	Electron NVSD due to monopolar GR LNS Hole NVSD due to monopolar GR LNS
S_V_eeFlickerGR S_V_hhFlickerGR	Electron NVSD due to flicker GR LNS Hole NVSD due to flicker GR LNS
S_V_BandEdge S_I_BandEdge	NVSD and NISD due to band edge fluctuations
S_V_Conductivity S_I_Conductivity	NVSD and NISD due to metal conductivity fluctuations
S_V_Doping S_I_Doping	NVSD and NISD due to random dopant fluctuations
S_V_Epsilon S_I_Epsilon	NVSD and NISD due to dielectric constant variations

Table 126   Noise and fluctuation data written into ACExtract file (Continued)

Name	Description
`S_V_Geometric` `S_I_Geometric`	NVSD and NISD due to geometric fluctuations
`S_V_TrapConcentration` `S_I_TrapConcentration`	NVSD and NISD due to trap concentration fluctuations
`S_V_Trap` `S_I_Trap`	NVSD and NISD due to trapping noise
`S_V_Workfunction` `S_I_Workfunction`	NVSD and NISD due to workfunction fluctuations
`ReS_VXV` `ImS_VXV`	Real/imaginary parts of the cross correlation noise voltage spectral density (NVXVSD)
`ReS_IXI` `ImS_IXI`	Real/imaginary parts of the cross correlation noise current spectral density

`ReS_VXV_ee`
`ImS_VXV_ee`
`ReS_VXV_hh`
`ImS_VXV_hh`
	Real/imaginary parts of the electron/hole NVXVSD

`ReS_VXV_eeDiff`
`ImS_VXV_eeDiff`
`ReS_VXV_hhDiff`
`ImS_VXV_hhDiff`
	Real/imaginary parts of the electron/hole NVXVSD due to diffusion LNS

`ReS_VXV_eeMonoGR`
`ImS_VXV_eeMonoGR`
`ReS_VXV_hhMonoGR`
`ImS_VXV_hhMonoGR`
	Real/imaginary parts of the electron/hole NVXVSD due to monopolar GR LNS

`ReS_VXV_eeFlickerGR`
`ImS_VXV_eeFlickerGR`
`ReS_VXV_hhFlickerGR`
`ImS_VXV_hhFlickerGR`
	Real/imaginary parts of the electron/hole NVXVSD due to flicker GR LNS

`ReS_VXV_BandEdge` `ReS_IXI_BandEdge`	Real part of the NVXVSD and NIXISD due to band edge fluctuations
`ReS_VXV_Conductivity` `ReS_IXI_Conductivity`	Real part of the NVXVSD and NIXISD due to metal conductivity fluctuations
`ReS_VXV_Doping` `ReS_IXI_Doping`	Real part of the NVXVSD and NIXISD due to random dopant fluctuations
`ReS_VXV_Epsilon` `ReS_IXI_Epsilon`	Real part of the NVXVSD and NIXISD due to dielectric constant fluctuations
`ReS_VXV_Geometric` `ReS_IXI_Geometric`	Real part of the NVXVSD and NIXISD due to geometric fluctuations

Table 126   Noise and fluctuation data written into ACExtract file (Continued)

Name	Description
`ReS_VXV_TrapConcentration` `ReS_IXI_TrapConcentration`	Real part of the NVXVSD and NIXISD due to trap concentration fluctuations

`ReS_VXV_Trap`
`ImS_VXV_Trap`
`ReS_IXI_Trap`
`ImS_IXI_Trap`
	Real/imaginary parts of the NVXVSD and NIXISD due to trapping noise

`ReS_VXV_Workfunction` `ReS_IXI_Workfunction`	Real parts of the NVXVSD and NIXISD due to workfunction fluctuations
`dV<name>`	Voltage deviation due to deterministic variation `<name>`
`dI<name>`	Current deviation due to deterministic variation `<name>`

Noise Sources

> **NOTE**   Noise scales differently with the device width compared to currents or voltages. For all noise sources noted in this section, for 2D devices, the device width is assumed to be given by `AreaFactor`. Therefore, it is not necessary to perform a full 3D simulation to obtain the correct scaling behavior for an essentially 2D structure. For 3D structures, when simulating only half (or a quarter) of the structure, you can use `AreaFactor=2` (or `AreaFactor=4`) to obtain the correct scale for the full structure, provided that spatial correlations of the noise sources can be neglected.

Common Options

All noise sources discussed in this section can be specified with the parameters `SpaceMid`, `SpaceSig`, and `SpatialShape`. These parameters can restrict the noise source to a window. The possible values, the default values, and the modifier function specified by these keywords are described in Energetic and Spatial Distribution of Traps on page 450. The modifier function is applied to each of the two coordinates on which a noise source depends. For noise sources without spatial correlation, this means that the square of the modifier function is multiplied by the noise source.

For example, the following unnamed `Noise` section activates random dopant fluctuations globally:

```
Noise (Doping)
```

The following `Noise` section named `window` activates random dopant fluctuations in a cube of 20 nm side length, centered at the origin:

```
Noise "window" (
   Doping (
      SpaceMid = (0 0 0)
      SpaceSig = (0.01 0.01 0.01)
      SpatialShape = Uniform
   )
)
```

Diffusion Noise

The diffusion noise source (keyword `DiffusionNoise`) available in Sentaurus Device reads:

$$K_{n,n}^{\mathrm{Diff}}(\vec{r}_1, \vec{r}_2, \omega) = 4qn(\vec{r}_1)kT_{\mathrm{n}}(\vec{r}_1)\mu_n(\vec{r}_1)\delta(\vec{r}_1 - \vec{r}_2) \tag{742}$$

A corresponding expression is used for holes. $K_{n,n}^{\mathrm{Diff}}$ is a diagonal tensor.

T_{n} is either the lattice or carrier temperature, depending on the specification in the command file:

```
DiffusionNoise ( <temp_option> )
```

where `<temp_option>` is `LatticeTemperature`, `eTemperature`, `hTemperature`, or `e_h_Temperature`. The default is `LatticeTemperature`.

For example, if the following command is specified:

```
Physics {
   Noise ( DiffusionNoise ( eTemperature ) )
}
```

Sentaurus Device uses the electron temperature for the electron noise source and the lattice temperature for the hole noise source. The keyword `e_h_Temperature` forces the corresponding carrier temperature to be used for the diffusion noise source for each carrier type.

Equivalent Monopolar Generation–Recombination Noise

An equivalent monopolar generation–recombination (GR) noise source model (keyword `MonopolarGRNoise`) for a two-level, GR process can be expressed as a tensor [2]:

$$K_{n,n}^{\mathrm{GR}}(\vec{r}_1, \vec{r}_2, \omega) \;=\; \frac{\vec{J}_n(\vec{r}_1)\vec{J}_n(\vec{r}_1)}{n} \cdot \frac{4\alpha\tau_{\mathrm{eq}}}{1 + \omega^2\tau_{\mathrm{eq}}^2}\delta(\vec{r}_1 - \vec{r}_2) \tag{743}$$

where α is a fitting parameter and τ_{eq} an equivalent GR lifetime. The parameters τ_{eq} and α can be modified in the parameter file of Sentaurus Device. A similar expression is used for holes.

> **NOTE** This model does not use the actual generation–recombination models activated in the simulation. Therefore, it cannot be considered a physical model for recombination noise.

Bulk Flicker Noise

The flicker generation–recombination (GR) noise model (keyword `FlickerGRNoise`) for electrons (similar for holes) is:

$$K_{n,n}^{\mathrm{fGR}}(\vec{r}_1, \vec{r}_2, \omega) \;=\; \frac{\vec{J}_n(\vec{r}_1)\vec{J}_n(\vec{r}_1)}{n(\vec{r}_1)}\frac{2\alpha_{\mathrm{H}}}{\pi\nu\ln(\tau_1/\tau_0)}[\,\mathrm{atan}(\omega\tau_1) - \mathrm{atan}(\omega\tau_0)]\delta(\vec{r}_1 - \vec{r}_2) \tag{744}$$

where α_{H} is a fit parameter; $\omega = 2\pi\nu$, the angular frequency; and the time constants fulfill $\tau_0 < \tau_1$. The parameters α_{H}, τ_0, and τ_1 for electrons and holes are accessible in the parameter file. With increasing frequency, the noise source changes from constant to $1/\nu$ behavior close to the frequency $\nu_1 = 1/\tau_1$ and, ultimately, to $1/\nu^2$ behavior at $\nu_0 = 1/\tau_0$.

> **NOTE** This model does not use the actual generation–recombination and trap models activated in the simulation. Therefore, it cannot be considered a physical model for flicker noise.

Trapping Noise

The `Traps` option to `Noise` activates a trapping noise model that follows the microscopic model in [3]. The trapping noise sources are determined fully by the trap model and, therefore, do not require additional adjustable parameters. For example:

```
Physics { Noise(Traps) }
```

activates trapping noise for all traps is the device. It is not possible to activate trapping noise for selected traps only. All trap models apart from tunneling to electrodes are supported. For more details on traps, see Chapter 17 on page 449.

Consider a trap level k with concentration $N_{\text{t},k}$ and trap electron occupation f_k. Trapping noise is expressed by adding a Langevin source $s_{i,k}$ to the net electron capture rate for each process i:

$$R_{i,k} = N_{\text{t},k}(1-f_k)c_{i,k} - N_{\text{t},k}f_k e_{i,k} + s_{i,k} \tag{745}$$

where $c_{i,k}$ is the electron capture rate for a trap occupied by zero electrons, and $e_{i,k}$ is the electron emission rate for a trap occupied by one electron (see also Eq. 507, p. 455). Denoting the expectation value with $\langle\ \rangle$, the trapping noise source takes the form:

$$K^{\text{trap}}_{ij,k}(\omega) = 2q^2\int dt\,\langle s_{i,k}(0)s_{j,k}(t)\rangle\exp(-i\omega t) = 2q^2\delta_{ij}N_{\text{t},k}[(1-f_k)c_{i,k}+f_k e_{i,k}] \tag{746}$$

That is, different capture or emission processes are independent, and the noise source for a given process is twice the total trapping rate (the sum of the capture and emission rates). The model also assumes that different trap distributions are independent, so that their noise contributions add.

Random Dopant Fluctuations

The noise sources for random dopant fluctuations are activated by the `Doping` keyword. The noise source for acceptor fluctuations reads:

$$K^{\text{RDF}}_{\text{A}}(\vec{r}_1,\vec{r}_2,\omega) = N_{\text{A}}(\vec{r}_1)\frac{\Theta(0.5\,\text{Hz}-|\nu|)}{1\,\text{Hz}}\delta(\vec{r}_1-\vec{r}_2) \tag{747}$$

Here, $\nu = \omega/2\pi$ is the frequency. An analogous expression holds for the noise source for donors, $K^{\text{RDF}}_{\text{D}}$. Physically, the noise sources are static. However, to avoid a δ-function in frequency space, Sentaurus Device spreads the spectral density of the noise source over a 1 Hz frequency interval. Eq. 747 is based on the assumption that individual dopant atoms are completely uncorrelated.

Acceptors and donors are considered to be independent. Their contributions to the noise spectral densities add. By default, both acceptor and donor concentrations are assumed to fluctuate. Using either the option `Type=Acceptor` or `Type=Donor` of `Doping`, the fluctuation can be restricted to acceptors or donors, respectively. For example:

```
Physics {
   Noise "acceptor" ( Doping(Type=Acceptor) )
   Noise "donor" ( Doping(Type=Donor) )
}
```

declares two named `Noise` sections that allow you to examine the impact of the fluctuation of acceptors and donors separately.

By default, Sentaurus Device neglects the impact of the random dopant fluctuations on mobility and bandgap narrowing. To take their impact into account, specify the `Mobility` and `BandgapNarrowing` options to the `Doping` keyword. For example:

```
Physics { Noise( Doping(Mobility) ) }
```

activates the random dopant fluctuation noise source, taking into account the impact of the fluctuations on mobility.

> **NOTE**   It is strongly advisable to use either both the `BandgapNarrowing` and
> `Mobility` options or neither option. Otherwise, inconsistencies can
> arise when the mobility depends indirectly on bandgap narrowing. Even
> when this dependency is weak, the inconsistency can lead to large errors
> in IFM results.

Random Geometric Fluctuations

The geometric fluctuation model accounts for random displacements of electrodes on insulator, as well as metal–insulator, insulator–insulator, and semiconductor–insulator interfaces. The noise source reads:

$$K^{\text{geo}}(\vec{r}_1, \vec{r}_2, \omega) = \frac{\Theta(0.5\,\text{Hz} - |\nu|)}{1\,\text{Hz}} \langle \delta s(\vec{r}_1) \delta s(\vec{r}_2) \rangle \tag{748}$$

where $\nu = \omega/2\pi$ is the frequency, and the correlation of the displacements δs is given by:

$$\langle \delta s(\vec{r}_1)\delta s(\vec{r}_2) \rangle = \hat{n}(\vec{r}_1) \cdot \hat{n}(\vec{r}_2)[a_{\text{iso}}(\vec{r}_1) + |\vec{a}(\vec{r}_1) \cdot \hat{n}(\vec{r}_1)|][a_{\text{iso}}(\vec{r}_2) + |\vec{a}(\vec{r}_2) \cdot \hat{n}(\vec{r}_2)|]\exp\left[-\frac{(\vec{r}_1 - \vec{r}_2)^2}{\lambda^2}\right] \tag{749}$$

where:

- $\vec{r}_1$ and $\vec{r}_2$ are positions on the interface.
- $\hat{n}(\vec{r})$ is the local interface normal in point $\vec{r}$.
- a_{iso} (the isotropic correlation amplitude), $\vec{a}$ (the vectorial correlation amplitude), and λ (the correlation length) are adjustable parameters.

The correlation has the following noteworthy properties:

- Displacements of interface positions occur only in the interface normal direction.
- The displacement amplitude depends on the interface direction when $\vec{a}$ is nonzero.

■ Displacements are spatially correlated; the correlations decay with increasing distance.

■ Correlations depend on the relative normal direction. Perpendicular interfaces are uncorrelated; opposing interfaces are negatively correlated (so the actual shifts are positively correlated).

The impact of displacements is accounted for in the variation of the dielectric constant in the Poisson equation, in the variation of the space charge in the Poisson equation, and in the variation of the band-edge profile in the continuity and density gradient equations. The impact through other quantities, such as tunneling rates, is currently neglected.

To use geometric fluctuations, in the global `Math` section for a device, specify one or more surfaces. Each surface has a name and is the union of an arbitrary number of interfaces and electrodes. For example:

```
Device "MOS" {
   Math {
      Surface "S2" (
         RegionInterface="channel/gateoxide"
         MaterialInterface="PolySi/Oxide"
      )
   ...
   }
```

specifies a surface `S2` that consist of all poly–oxide interfaces in the device, as well as the `channel/gateoxide` region interface. The order in which regions or materials in the specification of interfaces are named determines the sense of interface displacements: The positive direction points from the region or material named first into the region or material named second.

The surfaces are then used to activate the noise sources. For example:

```
   Physics {
      Noise(
         GeometricFluctuations "S1"
         GeometricFluctuations "S2"
      ) ...
   } ...
} ...
```

activates geometric fluctuations for surfaces `S1` and `S2`. Points on the same surface are correlated according to Eq. 749. Points on different surfaces are uncorrelated. The contributions of different surfaces to the noise spectral densities add.

The parameters a_{iso}, $\vec{a}$, and λ are specified as the parameters `Amplitude_Iso`, `Amplitude` and `lambda` in a surface-specific `GeometricFluctuations` parameter set. All three parameters are given in micrometers, and default to zero. λ must be set to positive value. For example:

```
GeometricFluctuations "S1" {
   lambda = 5e-3
   Amplitude = (9e-4, 3e-4, 0)
   Amplitude_Iso = 1e-4
}
```

> **NOTE**   For 3D structures, the mesh spacing on the fluctuating interfaces must be small compared to the correlation length λ to be able to resolve the Gaussian in Eq. 749. For 2D structures, the mesh does not need to resolve the Gaussian.

The `GeometricFluctuations` keyword supports options, which are specified as follows:

```
GeometricFluctuations "S1" (
   Options = <0..1>                    * default 0
   WeightQuantumPotential = <float>   * default 0.5
   WeightDielectric = <float>         * default 0
)
```

When you specify geometric variations for a semiconductor–insulator interface, you can specify whether the variation should be applied to both sides of the interface (`Options=0`) or only to the semiconductor side (`Options=1`).

For example, in a MOSFET, if you want to change the thickness of the semiconductor body, but not the thickness of the gate insulator, you can use `Options=0` and include in the `Surface` specification both the (bottom) semiconductor–gate insulator interface and the (top) gate insulator–contact or poly interface, such that the movements of the top and bottom gate insulator interfaces leave the gate insulator thickness unaltered. Alternatively, you can use `Option=1` and include in the surface specification only the (bottom) semiconductor–gate insulator interface. Physically, both options are nearly equivalent; however, the latter can sometimes be numerically more accurate.

The values given with `WeightQuantumPotential` and `WeightDielectric` interpolate between two different approximations for the variation terms that arise from the density-gradient quantum correction and the dielectric constant. Calibrating these two parameters can improve the accuracy of geometric variation results. Doing so is usually only worthwhile when computing insulator position variations, while keeping the insulator thickness fixed.

Random Trap Concentration Fluctuations

Trap concentration variations are activated by the `TrapConcentration` option to `Noise`. For each trap level, Sentaurus Device uses a noise source of the form:

$$K_{ii}^{\text{trapconc}}(\vec{r}_1, \vec{r}_2, \omega) = N_i(\vec{r}_1)\frac{\Theta(0.5\,\text{Hz} - |\nu|)}{1\,\text{Hz}}\delta(\vec{r}_1 - \vec{r}_2) \qquad (750)$$

Here, N_i is the concentration for the trap level i.

All trap levels are assumed to be mutually independent. Their contributions to the noise spectral densities add.

The trap concentration fluctuation model accounts for the impact of the trap concentration on the space charge in the Poisson equation and on the trap-related generation–recombination rates in the continuity equations.

Random Workfunction Fluctuations

The random workfunction fluctuations describe the impact of the fluctuation of the workfunction at contacts on insulators and at metal–insulator interfaces. The noise source reads:

$$K^{\text{workfunction}}(\vec{r}_1, \vec{r}_1, \nu) = \frac{\Theta(0.5\,\text{Hz} - |\nu|)}{1\,\text{Hz}}a(\vec{r}_1)a(\vec{r}_2)\exp\left[-\frac{(\vec{r}_1 - \vec{r}_2)^2}{\lambda^2}\right] \qquad (751)$$

where:

- $\nu = \omega/2\pi$ is the frequency.
- a is the workfunction standard deviation.
- λ is the correlation length.

    NOTE   The spatial correlation in Eq. 751 differs from the one created by the randomization procedure used for the sIFM-based approach (see Workfunction Variations on page 697).

Workfunction fluctuations are activated by the `WorkfunctionFluctuations` option to `Noise`. This option must be followed by a string that denotes the name of a surface that consists exclusively of contacts on insulators and metal–insulator interfaces. For example:

```
Device "MOS" {
    Math {
        Surface "S3" (
            Electrode = "gate"
```

```
        MaterialInterface = "Nitride/Aluminum"
    )
  }
  Physics {
    Noise(WorkfunctionFluctuations "S3") ...
  } ...
} ...
```

The definition of surfaces is described in Random Geometric Fluctuations on page 684. Any number of WorkfunctionFluctuations (with different names) can be specified. They are considered to be uncorrelated, and their contributions to the noise spectral densities add.

The parameters a and λ are specified by Amplitude (in eV) and lambda (in μm) in a surface-specific WorkfunctionFluctuations parameter set, for example:

```
WorkfunctionFluctuations "S3" {
  lambda = 0.01
  Amplitude = 0.4
}
```

Random Band Edge Fluctuations

Random band edge fluctuations describe the effect of the variation of the electron affinity $\delta\chi$ and the band gap $\delta E_{g,tot} = \alpha\delta\chi + \delta E_g$, where α is a user-specified parameter, and $\delta\chi$ and δE_g are statistically independent ($\langle \delta\chi(\vec{r}_1)\delta E_g(\vec{r}_2)\rangle = 0$) fields with Gaussian correlations. Therefore, noise sources for conduction band and valence band variations are:

$$K^{E_C}(\vec{r}_1, \vec{r}_1, \nu) = \frac{\Theta(0.5\,\mathrm{Hz} - |\nu|)}{1\,\mathrm{Hz}}a_\chi^2 \exp\left[-\frac{(\vec{r}_1 - \vec{r}_2)^2}{\lambda^2}\right] \tag{752}$$

$$K^{E_V}(\vec{r}_1, \vec{r}_1, \nu) = \frac{\Theta(0.5\,\mathrm{Hz} - |\nu|)}{1\,\mathrm{Hz}}[(1 + \alpha)^2 a_\chi^2 + a_{E_g}^2]\exp\left[-\frac{(\vec{r}_1 - \vec{r}_2)^2}{\lambda^2}\right] \tag{753}$$

For $a_{E_g} = 0$, some interesting limiting cases exist:

- For $\alpha = 0$, the conduction band and valence band vary in the same direction with the same amplitude.

- For $\alpha = -1$, the valence band does not vary at all.

- For $\alpha = -2$, the conduction band and the valence band vary in opposite directions.

Band edge fluctuations are activated by the option `BandEdgeFluctuations` to `Noise`:

```
Physics {
   Noise(BandEdgeFluctuations <string>)
}
```

Here, the string identifies a volume specification that determines where, in the device, band edge fluctuations are active. Named volumes are specified in the device global `Math` section by providing lists of regions and materials that belong to the volume:

```
Math {
   Volume <string> (
      Regions = (<string>...)
      Materials = (<string>...)
   )
}
```

The dimensionless parameter α, the correlation length λ (μm), and the amplitudes a_χ and a_{E_g} are specified as `Chi2Eg`, `Lambda`, `Amplitude_Chi`, and `Amplitude_Eg` in a named global parameter set `BandEdgeFluctuations`:

```
BandEdgeFluctuations <string> {
   Amplitude_Chi = <float>   * in eV, default 0
   Amplitude_Eg = <float>    * in eV, default 0
   Chi2Eg = <float>          * dimensionless, default 0
   Lambda = <float>          * in µm, no default (required)
}
```

The string is the name with which the band edge fluctuations are activated as a `Noise` option in the device global `Physics` section.

Random Metal Conductivity Fluctuations

Metal conductivity fluctuations are activated by the option `ConductivityFluctuations` to `Noise`:

```
Physics {
   Noise(ConductivityFluctuations <string>)
}
```

Here, `<string>` identifies a named volume specification that determines where, in the device, metal conductivity fluctuations are active. For the specification of named volumes, see .

Metal conductivity fluctuations are assumed to have Gaussian spatial correlations. Parameters for metal conductivity fluctuations are specified in the named global `ConductivityFluctuations` parameter set in the parameter file:

```
ConductivityFluctuations <string> {
   Amplitude = <float>              * amplitude in A/cmV
   Lambda= <float>                  * correlation length in um
}
```

The string is the name with which the metal conductivity fluctuations are activated as a `Noise` option in the device global `Physics` section.

Random Dielectric Constant Fluctuations

Random dielectric constant fluctuations are activated by the option `EpsilonFluctuations` to `Noise`:

```
Physics {
   Noise(EpsilonFluctuations <string>)
}
```

Here, `<string>` identifies a named volume specification that determines where, in the device, dielectric constant fluctuations are active. For the specification of named volumes, see Random Band Edge Fluctuations on page 688. Random dielectric constant fluctuations are assumed to have Gaussian spatial correlations.

Parameters for random dielectric constant fluctuations are specified in the named global `EpsilonFluctuations` parameter set in the parameter file:

```
EpsilonFluctuations <string> {
   Amplitude = <float>              * amplitude, dimensionless
   Lambda= <float>                  * correlation length in um
}
```

The string is the name with which the dielectric constant fluctuations are activated as a `Noise` option in the device global `Physics` section.

Noise From SPICE Circuit Elements

To take into account the noise generated by SPICE circuit elements (see Compact Models User Guide, Chapter 1 on page 1), specify the `CircuitNoise` option to `ACCoupled`. The form of the noise source for a particular circuit element is defined by the respective compact model.

Due to a restriction of the SPICE noise models, SPICE circuit elements contribute only to the autocorrelation noise. For cross-correlation noise, Sentaurus Device considers SPICE circuit elements as noiseless. Non–SPICE compact circuit elements do not implement noise at all and, therefore, Sentaurus Device always treats them as noiseless.

Statistical Impedance Field Method

The statistical impedance field method (sIFM) can be applied to doping concentration, trap concentration, semiconductor–insulator and insulator–insulator interface positions, and the workfunction at contacts on insulators and metal–insulator interfaces. It creates a large number of randomized variations of the quantities under investigation (dopant concentrations, trap concentrations, or workfunction) and computes the modification of the device characteristics in linear response.

The sIFM is specified in the global `Math` section:

```
Math {
   RandomizedVariation <string> (
      NumberOfSamples = <int>
      Randomize = <int>
      ExtrudeTo3D
      RandomField(...)
   )
   ...
}
```

Any number of `RandomizedVariation` specifications can be present, each of which specifies the sample size and the random seed for one set of variations. The sets are distinguished by the optional string after the `RandomizedVariation` keyword.

`NumberOfSamples` determines the number of variations in a set. `Randomize` determines the seed for the random number generator. For a value of zero (the default), the seed value is selected automatically and differently in each simulation run. A negative value disables the sIFM, and a positive value is directly taken as the seed for the random number generator. The last possibility allows to reproduce results for different simulation runs of the same device, on the same platform, and the same release of Sentaurus Device.

For 2D structures, the keyword `ExtrudeTo3D` instructs Sentaurus Device to perform randomization for a 3D structure that is obtained by extruding the 2D structure to a width given by the `AreaFactor`. This is necessary to correctly model variations with spatial correlations, but it will increase runtime for these variations. By default, randomization is performed in two dimensions, which corresponds to variations that are perfectly correlated in the third spatial direction. `ExtrudeTo3D` has no effect on 3D structures.

`RandomField` allows you to specify the statistical properties of the spatial correlations for this `RandomizedVariation` specification (see Spatial Correlations and Random Fields on page 693).

The quantities to be randomized are specified in a device-global `Physics` section:

```
Device <string> {
   Physics {
      RandomizedVariation <string> (<specifications>)
   }
}
```

The string after `RandomizedVariation` in the `Physics` section is matched with the one after `RandomizedVariation` in the global `Math` section, and `<specifications>` is described along with the individual variations in the following sections.

For one `ACCoupled` statement, for each `RandomizedVariation` specification, the sIFM creates two files per `ObservationNode`: one for voltage and one for current variation at the node. The file names are derived from the base name given by `ACExtract`, the string after the `RandomizedVariation` keyword, the name of the type of variation (current or voltage), the node name, and the extension `.csv`. The file contains comma separated values (CSV), a very simple format that can be imported by many applications (for example, spreadsheet programs).

The first line contains the column headings, using double-quoted strings. Each subsequent line corresponds to one bias point and one frequency.

The first couple of columns contain the data specified in the `ACPlot` statement. They serve to connect each line to a bias point. The rest of the columns within each line correspond to the current or voltage shift for one particular randomized profile. For all lines, the same column always corresponds to the same profile. For frequencies larger than $0.5\,\mathrm{Hz}$, the shifts are zero.

Options Common to sIFM Variations

All variations supported by sIFM provide the keywords `SpatialShape`, `SpaceMid`, and `SpaceSig`. They allow you to multiply the variation by a space-dependent factor, and they work in the same way as for traps (see Energetic and Spatial Distribution of Traps on page 450). The shape functions must adequately be resolved by the mesh. For example:

```
Physics {
   RandomizedVariation "rnd" (
      Doping(
         SpatialShape = Gaussian
         SpaceMid = (0 0 0)
         SpaceSig = (0.01 0.01 0.01)
      )
```

```
      )
   }
```

activates random doping variations, which are damped with a Gaussian function on a length scale of 10 nm around the origin. Using `SpatialShape=Uniform` instead of `SpatialShape=Gaussian` would switch off the doping variation completely for points outside a cube of 20 nm side length centered at the origin.

By default, `SpatialShape` is `Uniform`, and `SpaceSig` is a vector with very large components. Therefore, by default, the space-dependent factor is one everywhere. If the mesh has dimension d, only the d first components of `SpaceMid` and `SpaceSig` are significant; additional components are ignored.

Spatial Correlations and Random Fields

Several variations supported by sIFM are spatially correlated. You can specify the statistical properties of the correlation either directly in the specification of the variation or by declaring `RandomField` in the `RandomizedVariation` section in the global `Math` section. If the statistical properties are specified directly in the specification of the variation, the variation is statistically independent from all other variations. In contrast, if `RandomField` is declared, all variations in the same `RandomizedVariation` section are correlated, and direct specifications are ignored.

Random fields are declared like this:

```
Math {
   RandomizedVariation <string> (
      RandomField(
         CorrelationFunction = Grain | Exponential | Gaussian
         AverageGrainSize = <vector>     * in µm
         Lambda = <vector>              * in µm
         Resolution = <vector>
         MaxInternalPoints = <int>
      )
      ...
   )
}
```

The spatial domain covered by a random field is obtained automatically from the spatial domains in which the variations that use it are active. A random field can have more than one component. The number of components in the random field is the largest number required by any of the variations that refer to the random field. Currently, only band edge variations require two components; the other variations require only one component. The components are numbered starting from zero. Variations with only one component always use the zero-th component of the random field.

`CorrelationFunction` determines the way in which spatial correlations are modeled.

If `CorrelationFunction = Grain` (default), first, grains are generated randomly. The creation of grains works as described in Metal Workfunction Randomization on page 243. If `AverageGrainSize` is the vector $(\lambda_x, \lambda_y, \lambda_z)$, the vertex at coordinate (x, y, z) belongs to the grain with the center (x_0, y_0, z_0) for which $(x - x_0)^2/\lambda_x^2 + (y - y_0)^2/\lambda_y^2 + (z - z_0)^2/\lambda_z^2$ becomes smallest.

For each grain and for each component of the random field, a random number g in the range from 0 to 1 is selected, with uniform probability and statistically independent from the random number for other grains or other components. For variations that use a list of discrete values for the variation, g is mapped into this list according to the variation-specific probability for the values in the list. If g is close to zero, the first value in the list will be taken. If g is close to 1, the last value in the list will be taken. For variations with continuous values, g will be mapped by a monotonically increasing function to the probability distribution for the variation.

If `CorrelationFunction` is `Exponential` or `Gaussian`, a Fourier approach is used to create fields $g(\vec{r})$ of exponentially correlated or Gaussian correlated, dimensionless random numbers. The fields for different components of the random field are uncorrelated.

The correlation length is given (in μm) by the components $(\lambda_x, \lambda_y, \lambda_z)$ of `Lambda`:

$$\langle g(x, y, z)g(x_0, y_0, z_0)\rangle = \exp\left(-\sqrt{(x - x_0)^2/\lambda_x^2 + (y - y_0)^2/\lambda_y^2 + (z - z_0)^2/\lambda_z^2}\right) \tag{754}$$

$$\langle g(x, y, z)g(x_0, y_0, z_0)\rangle = \exp\left(-(x - x_0)^2/\lambda_x^2 - (y - y_0)^2/\lambda_y^2 - (z - z_0)^2/\lambda_z^2\right) \tag{755}$$

The physical variation is obtained by multiplying $g(\vec{r})$ by a variation-specific amplitude.

For Gaussian and exponential correlations, `Resolution` (one to three dimensionless positive components; default `(0.25 0.25 0.25)`) can be used to specify how accurately spatial correlations should be resolved, for each spatial axis. The components specify this accuracy in units of `Lambda`. One possible application for `Resolution` is to use a large value for one axis to pretend that the domain is nearly flat along this direction, which reduces the dimension of the Fourier transform and can give a substantial speedup.

For Gaussian and exponential correlations, `MaxInternalPoints` specifies the maximum number of internal points used to compute the randomization. The default value is a very large integer. If the number of internal points used to compute the randomization exceeds the value set with `MaxInternalPoints`, Sentaurus Device aborts. The purpose of this is to avoid excessive computation time, which scales superlinearly with the number of internal points. To reduce the number of internal points, restrict the randomized domain, or increase `Lambda` or `Resolution`.

You can specify `Lambda` and `AverageGrainSize` as vectors with less than three components. In this case, the missing components are assumed equal to the last given component.

All options that are available in the `RandomField` section are also available as options to the specification of all variations with spatial correlation, with the same meaning of keywords.

The specification of variations with spatial correlation supports a string, which allows you to put several such variations into the same `RandomizedVariation` section. Their contribution is added. For example:

```
Physics {
   RandomizedVariation "rv" (
      Geometric "g1" ( ... )
      Geometric "g2" ( ... )
   )
}
```

Doping Variations

Doping variations are enabled using the `Doping` keyword:

```
Physics {
   RandomizedVariation <string> (
      Doping (
         Type = Doping | Acceptor | Donor
         SpatialShape = Uniform | Gaussian
         SpaceMid = <vector>
         SpaceSig = <vector>
         -Mobility
         -BandgapNarrowing
      )
   )
}
```

For `RandomizedVariation` specifications in the `Math` section for which no `RandomizedVariation` specification of the same name is present in the `Physics` section, dopant variations are enabled automatically.

`Type` determines which dopants to randomize. For `Acceptor`, only acceptors are randomized. For `Donor`, only donors are randomized. For `Doping` (default), both are randomized.

For the options of `Doping`, see Options Common to sIFM Variations on page 692.

Acceptor and donor concentrations are randomized independently, assuming dopants are spatially uncorrelated and using a Poisson distribution function. This means that for a vertex i

of the mesh with a box volume V_i and an average doping concentration N_i, the probability to find exactly k dopants in the box for vertex i is:

$$P_i(k) = \frac{(N_i V_i)^k}{k!} \exp(-N_i V_i) \tag{756}$$

The volume V_i is a 3D volume. If the simulated structure is 2D, the `AreaFactor` is taken into account to compute V_i. Eq. 756 is consistent with the assumptions that are used to obtain Eq. 747, p. 683.

The sIFM accounts for the impact of dopant concentration on space charge, mobility, and bandgap narrowing. The options `-Mobility` and `-BandgapNarrowing` disable the impact due to mobility and bandgap narrowing, respectively.

> **NOTE**   It is strongly advisable to use either both the `-BandgapNarrowing` and `-Mobility` options or neither option. Otherwise, inconsistencies can arise when the mobility depends indirectly on bandgap narrowing. Even when this dependency is weak, the inconsistency can lead to large errors in IFM results.

When the keyword `RandomizedDoping` appears in a device-specific `Plot` section, all randomized acceptor and donor profiles are written to the `Plot` file. The individual profiles are identified by a number in their name. This number is the same one that appears in the first line of the `.csv` files.

> **NOTE**   If the number of random samples is large, plotting randomized doping profiles can occupy a large amount of memory.

Trap Concentration Variations

For the sIFM, variations of the random trap concentration are activated with the keyword `TrapConcentration`:

```
Physics {
   RandomizedVariation <string> (
      TrapConcentration (
         SpatialShape = Uniform | Gaussian
         SpaceMid = <vector>
         SpaceSig = <vector>
      )
   )
}
```

All trap levels are randomized independently, assuming traps are spatially uncorrelated. The same expression as for doping concentration, Eq. 756, p. 696, is used. For the options of `TrapConcentration`, see Options Common to sIFM Variations on page 692.

The sIFM accounts for the impact of the trap concentration on the space charge in the Poisson equation and on the trap-related generation–recombination rates in the continuity equations.

Workfunction Variations

For the sIFM, workfunction variations are activated and controlled using the `Workfunction` keyword:

```
Physics {
  RandomizedVariation <string> (
    Workfunction <string> (
      Surface = <string>
      CorrelationFunction = Grain | Exponential | Gaussian
      AverageGrainSize = <vector>
      Lambda = <vector>
      Resolution = <vector>
      MaxInternalPoints = <int>
      GrainProbability = (<float>...)
      GrainWorkfunction = (<float>...)   * in eV
      Amplitude = <float>                * in eV
      SpatialShape = Uniform | Gaussian
      SpaceMid = <vector>
      SpaceSig = <vector>
    )
  )
}
```

`Surface` specifies the name of a surface that consists of contacts on insulators and metal–insulator interfaces only. The specification of surfaces is described in Random Geometric Fluctuations on page 684. The workfunction is randomized for interfaces and contacts that are part of the given `Surface`.

`GrainWorkfunction` is a list of workfunction values (in eV) that can occur for a metal grain. `GrainProbability` is a list that gives the probabilities with which these workfunctions occur. These two parameters are used for `Grain` correlations. `Amplitude` (in eV) is a multiplier to the dimensionless field $g(\vec{r})$ that is used for Gaussian and exponential correlations. For more details, see Spatial Correlations and Random Fields on page 693.

As the sIFM models the effect of deviations, the values of `GrainWorkfunction` are adjusted to have an average that agrees with the nominal workfunction specified for the electrode or metal. Therefore, adding the same value to all `GrainWorkfunction` values will not affect the results.

For the other options of `Workfunction`, see Options Common to sIFM Variations on page 692 and Spatial Correlations and Random Fields on page 693.

The sIFM accounts for the impact of the workfunction on the boundary condition for the electrostatic potential at metal–insulator interfaces and at contacts on insulators.

Geometric Variations

For the sIFM, geometric variations are activated and controlled using the `Geometric` keyword:

```
Physics {
   RandomizedVariation <string> (
      Geometric <string> (
         Surface = <string>
         CorrelationFunction = Grain | Exponential | Gaussian
         AverageGrainSize = <vector>
         Lambda = <vector>
         Resolution = <vector>
         MaxInternalPoints = <int>
         Amplitude = <vector>        * in micrometer
         Amplitude_Iso = <float>     * in micrometer
         SpatialShape = Uniform | Gaussian
         SpaceMid = <vector>
         SpaceSig = <vector>
         Options = <0..1>
         WeightQuantumPotential = <float>
         WeightDielectric = <float>
      )
   )
}
```

`Surface` specifies the name of a surface that consists of electrodes on insulator, metal–insulator, semiconductor–insulator, and insulator–insulator interfaces only. The specification of surfaces is described in Random Geometric Fluctuations on page 684. The interface position is randomized for interfaces that are part of the given `Surface`.

For `Grain` correlations, for each grain, a random number g is selected from a Gaussian distribution of average zero and variance one. For each surface point that is contained in the grain, the interface shift along the normal direction $\hat{n}$ is given by $g\hat{n} \cdot (a_{iso} + \vec{a} \cdot \hat{n})$. Here, a_{iso}

and $\vec{a}$ are the values specified (in μm) by `Amplitude_Iso` and `Amplitude`. For Gaussian and exponential variation, the field $g(\vec{r})$ of dimensionless correlated random numbers determines the interface shift along the normal direction $\hat{n}$ in a point $\vec{r}$ on the surface as $g(\vec{r})\hat{n} \cdot (a_{iso} + \vec{a} \cdot \hat{n})$. As above, a_{iso} and $\vec{a}$ are the values specified by `Amplitude_Iso` and `Amplitude`. For more details, see Spatial Correlations and Random Fields on page 693.

The keywords `Options`, `WeightQuantumPotential`, and `WeightDielectric` work as explained in Random Geometric Fluctuations on page 684.

For the other options of `Geometric`, see Options Common to sIFM Variations on page 692 and Spatial Correlations and Random Fields on page 693.

Band Edge Variations

For the sIFM, band edge variations are activated and controlled using the `BandEdge` keyword:

```
Physics {
   RandomizedVariation <string> (
      BandEdge <string> (
         Volume = <string>           * required
         CorrelationFunction = Grain | Exponential | Gaussian
         AverageGrainSize = <vector>
         Lambda = <vector>
         Resolution = <vector>
         MaxInternalPoints = <int>
         ChiComponent = <0..1>       * default 0, RandomField component to use
         EgComponent = <0..1>        * default 1, RandomField component to use
         GrainProbability = (<float>...) * dimensionless, nonnegative
         GrainChi = (<float>...)     * eV, same size as GrainProbability
         GrainEg = (<float>...)      * eV, default 0, same size as or smaller
                                     * than GrainProbability
         Chi2Eg = <float>            * dimensionless, default 0
         Amplitude_Chi = <float>     * eV
         Amplitude_Eg = <float>      * eV
         SpatialShape = Uniform | Gaussian
         SpaceMid = <vector>
         SpaceSig = <vector>
      )
   )
}
```

`Volume` specifies a named volume that determines where band edge variations are active. For the specification of named volumes, see Random Band Edge Fluctuations on page 688.

For `Grain` correlations, `GrainProbability` is a list that gives the probabilities with which these shifts occur. `GrainChi` is a list of affinity shifts $\delta\chi$ (in eV) with the same number of values as `GrainProbability`. Bandgap variations are computed as $\delta E_{g,\text{tot}} = \alpha\delta\chi + \delta E_g$, where α is given by the `Chi2Eg` keyword, and δE_g are values selected (statistically independently from the $\delta\chi$, but using the same `GrainProbability` list) from the list `GrainEg` (in eV). `GrainEg` has, at most, as many values as `GrainProbability`. Missing values is `GrainEg` are assumed to be zero.

The values in `GrainChi` and `GrainEg` automatically adjust to have zero average. Therefore, adding a constant to all components of these lists has no effect.

For exponential and Gaussian correlations, $\delta\chi$ and δE_g are obtained by multiplying `Amplitude_Chi` and `Amplitude_Eg` (in eV) by the zero-th and first component of the dimensionless field $g(\vec{r})$ that is used for Gaussian and exponential correlations.

For all correlations, if `RandomField` is used, `ChiComponent` and `EgComponent` allow you to specify the component of the random field used to determine $\delta\chi$ and δE_g.

For details about correlations, see . For the other remaining options, see .

Metal Conductivity Variations

For the sIFM, metal conductivity variations are activated and controlled using the `Conductivity` keyword:

```
Physics {
    RandomizedVariation <string> (
        Conductivity<string> (
            Volume = <string>                      * required
            CorrelationFunction = Grain | Exponential | Gaussian
            AverageGrainSize = <vector>
            Lambda = <vector>
            Resolution = <vector>
            MaxInternalPoints = <int>
            GrainProbability = (<float>...)     * dimensionless, nonnegative
            GrainConductivity = (<float>...)    * A/cmV, size as GrainProbability
            Amplitude = <float>                 * A/cmV
            SpatialShape = Uniform | Gaussian
            SpaceMid = <vector>
            SpaceSig = <vector>
        )
    )
}
```

`Volume` specifies a named volume that determines where metal conductivity variations are active. For the specification of named volumes, see Random Band Edge Fluctuations on page 688.

For `Grain` correlations, `GrainProbability` is a list that gives the probabilities with which these shifts occur. `GrainConductivity` is a list of a conductivity shifts (in A/cmV) with the same number of values as `GrainProbability`. The values in `GrainConductivity` are adjusted to have zero average. Therefore, adding a constant to all components of this list has no effect.

`Amplitude` (in A/cmV) is a multiplier to the dimensionless field $g(\overset{\rightharpoonup}{r})$ that is used for Gaussian and exponential correlations.

For details about correlations, see Spatial Correlations and Random Fields on page 693. For the other remaining options, see Options Common to sIFM Variations on page 692.

Dielectric Constant Variations

For the sIFM, relative dielectric constant variations are activated and controlled using the `Epsilon` keyword:

```
Physics {
    RandomizedVariation <string> (
        Epsilon <string> (
            Volume = <string>                * required
            CorrelationFunction = Grain | Exponential | Gaussian
            AverageGrainSize = <vector>
            Lambda = <vector>
            Resolution = <vector>
            MaxInternalPoints = <int>
            GrainProbability = (<float>...)   * dimensionless, nonnegative
            GrainEpsilon = (<float>...) * dimensionless, size as GrainProbability
            Amplitude = <float>          * dimensionless
            SpatialShape = Uniform | Gaussian
            SpaceMid = <vector>
            SpaceSig = <vector>
        )
    )
}
```

`Volume` specifies a named volume that determines where relative dielectric constant variations are active. For the specification of named volumes, see Random Band Edge Fluctuations on page 688.

For `Grain` correlations, `GrainProbability` is a list that gives the probabilities with which these shifts occur. `GrainEpsilon` is a list of a relative dielectric constant shifts with the same number of values as `GrainProbability`. The values in `GrainEpsilon` are adjusted to have zero average. Therefore, adding a constant to all components of this list has no effect.

`Amplitude` (dimensionless) is a multiplier to the dimensionless field $g(\vec{r})$ that is used for Gaussian and exponential correlations.

For details about correlations, see Spatial Correlations and Random Fields on page 693. For the other remaining options, see Options Common to sIFM Variations on page 692.

Doping Profile Variations

Doping profile variations are activated and controlled using the `DopingVariation` keyword:

```
Physics {
   RandomizedVariation <string> (
      DopingVariation <string> (
         CorrelationFunction = Grain | Exponential | Gaussian
         AverageGrainSize = <vector>
         Lambda = <vector>
         Resolution = <vector>
         MaxInternalPoints = <int>
         SFactor = <string>
         Amplitude = <vector>      * µm
         Amplitude_Iso = <float>   * µm
         Conc = <float>            * 1/ccm
         Type = Doping | Acceptor | Donor
         SpatialShape = Uniform | Gaussian
         SpaceMid = <vector>
         SpaceSig = <vector>
         -Mobility
         -BandgapNarrowing
      )
   )
}
```

The options `SFactor`, `Conc`, `Type`, `Amplitude`, and `Amplitude_Iso` are used to describe a doping profile shift based on the gradient of a dataset, as described in Deterministic Doping Variations on page 703. In addition to what is described there, for sIFM, the shift is multiplied by a spatially correlated, dimensionless, random field.

For grain correlations, the random number in each grain is Gaussian distributed, with zero average and variance of one. For exponential and Gaussian correlations, the dimensionless random field is the one obtained from the Fourier approach.

By default, the impact of doping concentration on space charge, mobility, and bandgap narrowing is accounted for. The options `-Mobility` and `-BandgapNarrowing` disable the impact due to mobility and bandgap narrowing, respectively.

> **NOTE** It is strongly advisable to use either both the `-BandgapNarrowing` and `-Mobility` options or neither option. Otherwise, inconsistencies can arise when the mobility depends indirectly on bandgap narrowing. Even when this dependency is weak, the inconsistency can lead to large errors in IFM results.

For the other options of `DopingVariation`, see Options Common to sIFM Variations on page 692 and Spatial Correlations and Random Fields on page 693.

Deterministic Variations

For deterministic variations, you specify the variations directly, by specifying the actual deviation in doping, geometry, or model parameters. Sentaurus Device computes the effect of the variations on the observation node voltages and currents in a linear response. As for random fluctuations, deterministic variations are assumed to be different from zero only for analysis frequencies up to $0.5\,\text{Hz}$.

Compared to random fluctuations, deterministic variations give you more control over the variation and are easier to understand, because no statistical interpretation is required and no second-order moments appear. In the case of geometric variations, the computational effort is smaller as well.

Deterministic Doping Variations

Deterministic doping variations are specified as an option to `DeterministicVariation` in the `Physics` section:

```
Physics {
   DeterministicVariation(
      DopingVariation <name> (
         SFactor = <string>
         Amplitude = <vector>
         Amplitude_Iso = <float>
         Amplitude_Abs = <float>
         Conc = <float>
         Factor = <float>
         Type = Doping | Acceptor | Donor
         SpatialShape = Gaussian | Uniform
         SpaceMid = <vector>
```

```
            SpaceSig = <vector>
            -Mobility
            -BandgapNarrowing
        ) ...
    ) ...
}
```

Here, `<name>` is a string that names the variation and will be used to identify output to the `ACExtract` file. If it coincides with the name of a geometric or a parameter variation, the contributions of the variations are added.

`SFactor` specifies a scalar dataset. Allowed datasets are doping concentrations and `PMIUserFields`. If you do not specify any dataset, a constant density of 1 cm^{-3} is assumed.

By specifying `Conc`, the concentration is normalized and then multiplied by the concentration specified with `Conc`. `Conc` is given in cm^{-3}. If `Conc` is not specified or is zero, the values from the dataset will be used unaltered.

If the `SFactor` dataset is a `PMIUserField` dataset or another dataset that is not a density, Sentaurus Device cannot properly determine the units of the dataset and, therefore, it interprets its value with a different scaling constant to the one you intended. Specifying `Conc` can be useful in this case, as the normalization of the `SFactor` eliminates the ambiguous units.

By default, the resulting concentration X determines the fluctuation δN directly, $\delta N = X$. If you use `Amplitude_Iso`, `Amplitude`, or `Amplitude_Abs` to specify nonzero isotropic or vectorial amplitudes a_{iso}, $\vec{a}$, and $\vec{a}_{\mathrm{abs}}$, the fluctuation is computed from X as $\delta N = -\vec{a} \cdot \nabla X - a_{\mathrm{iso}} |\nabla X| - \vec{a}_{\mathrm{abs}} \cdot \mathrm{abs}(\nabla X)$, where $\mathrm{abs}(\nabla X)$ is the vector obtained by taking the absolute value of ∇X component-wise. The vectorial amplitude models the small displacement of a profile, and the isotropic amplitude models a shift of a doping front (perpendicular to the equi-doping lines). For this to work properly, the mesh must accurately resolve the variations of X. Both amplitudes are specified in μm.

Optionally, a dimensionless value `Factor` can be specified, which is multiplied by the resulting δN. The factor defaults to one. Its purpose is to easily specify variations that are a certain percentage of a given doping data field.

Using the keywords `SpatialShape`, `SpaceMid`, and `SpaceSig`, you can multiply δN by either a Gaussian function or a window function. These keywords work in the same way as for traps (see Energetic and Spatial Distribution of Traps on page 450). The shape functions must adequately be resolved by the mesh.

`Type` selects whether the variation applies to the acceptor concentration ($\delta N_{\mathrm{A}} = \delta N$), the donor concentration ($\delta N_{\mathrm{D}} = \delta N$), or doping as a whole. In the latter case, a negative variation increases the acceptor concentration; a positive variation increases donor concentration.

By default, the impact of doping concentration on space charge, mobility, and bandgap narrowing is accounted for. The options `-Mobility` and `-BandgapNarrowing` disable the impact due to mobility and bandgap narrowing, respectively.

> **NOTE** It is strongly advisable to use either both the `-BandgapNarrowing` and `-Mobility` options or neither option. Otherwise, inconsistencies can arise when the mobility depends indirectly on bandgap narrowing. Even when this dependency is weak, the inconsistency can lead to large errors in IFM results.

For a summary of options to `DopingVariation`, see Table 288 on page 1468.

Deterministic Geometric Variations

Deterministic geometric variations are specified as an option to `DeterministicVariation` in the `Physics` section:

```
Physics {
   DeterministicVariation(
      GeometricVariation <name> (
         Surface = <string>
         Amplitude = <vector>
         Amplitude_Iso = <float>
         SpatialShape = Gaussian
         SpaceMid = <vector>
         SpaceSig = <vector>
         Options = <0..1>
         WeightQuantumPotential = <float>
         WeightDielectric = <float>
      ) ...
   ) ...
}
```

Here, `<name>` is a string that names the variation and will be used to identify output to the `ACExtract` file. If it coincides with the name of a doping or a parameter variation, the contributions of the variations are added.

`Surface` identifies the displaced interfaces. Its specification is described in Random Geometric Fluctuations on page 684. The amount of displacement along the positive normal in a point $\vec{r}$ on the surface is determined by `Amplitude_Iso` (a_{iso}) and `Amplitude` (a), both specified in μm, as $\delta s(\vec{r}) = a_{\mathrm{iso}}(\vec{r}) + \vec{a}(\vec{r}) \cdot \hat{n}(\vec{r})$.

Using the keywords `SpatialShape`, `SpaceMid`, and `SpaceSig`, you can multiply δs by a Gaussian function.

These keywords work in the same way as for traps (see Energetic and Spatial Distribution of Traps on page 450). The Gaussian must be resolved adequately by the mesh.

The keywords `Options`, `WeightQuantumPotential`, and `WeightDielectric` work as explained in Random Geometric Fluctuations on page 684.

For a summary of options of `GeometricVariation`, see Table 301 on page 1474.

Parameter Variations

Sentaurus Device allows to compute the linear response to the variation of any parameter that can be ramped. The parameter variations are specified as an option to `DeterministicVariation` in the `Physics` section:

```
Physics {
   DeterministicVariation (
      ParameterVariation <name> (
         (
            Material = <string>
            Region = <string>
            MaterialInterface = <string>
            RegionInterface = <string>
            Model = <string>
            Parameter = <string>
            Value    = <float>
            Factor   = <float>
            Summand  = <float>
         )...
      )...
   )...
}
```

Here, `<name>` is a string that names the variation and is used to identify output to the `ACExtract` file. If it coincides with the name of a doping or a geometry variation, the contributions of the variations are added.

The option of `ParameterVariation` is a list of an arbitrary number of individual parameter specifications, each of which is enclosed by a pair of parentheses. All these variations are performed together to compute their cumulative impact.

`Material`, `Region`, `MaterialInterface`, or `RegionInterface` specify the location of the parameter that is varied. At most, one of these keywords must be specified. `Model` specifies the name of the model to which the varied parameter belongs, and `Parameter` is the name of the parameter within this model. All these keywords specify a parameter in the same way as for parameter ramping (see Ramping Physical Parameter Values on page 78).

To specify the correct location for a parameter can be complicated. Combining Parameter Specifications on page 30 explains how the specifications in the parameter file determine the location from which the parameters used in the computation are taken.

Each varied parameter has an original value γ (the default value, or the value that was set in the parameter file). The modified value γ' can be given by one of two ways:

- Directly by specification of the modified value using `Value=`γ'

- By using the keywords `Factor` and `Summand`: $\gamma' = $ `Factor` $\cdot \gamma + $ `Summand`

Sentaurus Device assembles the right-hand side twice: once with the original parameters, and once with the modified parameters. Then, the difference in the right-hand sides is used to compute the variation of output characteristics in the linear response. However, as the right-hand sides are not linear in the parameters, the method is not perfectly linear, which becomes visible if the parameter variation $\gamma' - \gamma$ is not small. On the other hand, if the parameter variation becomes too small, numeric noise can obscure the results.

IFM Section

Instead of defining the noise and variation models in the `Math` and `Physics` sections, starting from Version N-2017.09, you can also define all these models in the `IFM` section as follows:

```
IFM {
   Noise (
      ...
   )
   RandomizedVariation (
      ...
   )
   DeterministicVariation (
      ...
   )
   ...
}
```

Parameters of the `Noise` model can be defined in the `IFM` section as well:

```
IFM {
   Noise (
      MonopolarGRNoise (
         e_alpha = 1...
      )...
   )...
}
```

Table 127 lists all the `Noise` model parameters.

Table 127   Noise model parameters

Model	Symbol	Default value	Unit
MonopolarGRNoise	e_alpha	1	1
	h_alpha	1	1
	e_tau	1e-7	s
	h_tau	1e-7	s
FlickerGRNoise	e_alpha_H	2e-3	1
	h_alpha_H	2e-3	1
	e_tau0	1e-6	s
	h_tau0	1e-6	s
	e_tau1	3e-4	s
	h_tau1	3e-4	s
GeometricFluctuations	lambda	0	µm
	Amplitude_Iso	-3e303	µm
	Amplitude	(-3e303,-3e303,-3e303)	µm
WorkfunctionFluctuations	lambda	0	µm
	Amplitude	-1	eV
BandEdgeFluctuations	lambda	0	µm
	Amplitude_chi	0	eV
	Amplitude_Eg	0	eV
	Chi2Eg	0	1
ConductivityFluctuations	lambda	0	µm
	Amplitude	-1	$A\,cm^{-1}V^{-1}$
EpsilonFluctuations	lambda	0	µm
	Amplitude	-1	1

Impedance Field Method

The impedance field method splits noise and fluctuation analysis into two tasks. The first task is to provide models for local microscopic fluctuations inside the devices. The selection of the appropriate models depends on the problem. You have to select the models according to the kind of fluctuation that interests you. The second task is to determine the impact of the local fluctuations on the terminal characteristics. To solve this task, the response of the contact voltage or contact current to local fluctuation is assumed to be linear. For each contact, Green's functions are computed that describe this linear relationship. In contrast to the first task, the second task is purely numeric, as the Green's functions are completely specified by the transport model.

A Green's function describes the response $G_\xi(x, \omega)$ of the current or voltage at node c due to a perturbation of quantity ξ at location x with angular frequency ω. Particularly important is the case where ξ is the right-hand side of the partial differential equation for a solution variable ϕ (see Eq. 37, p. 173), n or p (see Eq. 53, p. 181), T_n (see Eq. 73, p. 195), T_p (see Eq. 74, p. 196), or T.

Given the Green's function and a variation $\delta\xi$ of the quantity ξ, Sentaurus Device can compute the current response at node c as:

$$\delta I_c = \int G_\xi^c(x, \omega) \delta\xi(x, \omega) dx \tag{757}$$

Here, the integral runs over the entire device. For the sIFM (see Statistical Impedance Field Method on page 691), $\delta\xi$ is obtained by the randomization procedure specific to the type of variation and, for deterministic variations (see Deterministic Variations on page 703), $\delta\xi$ is given by users.

For noise (and noise-like descriptions of static variations; see Noise Sources on page 680), it is assumed that the expectation value $\langle \delta\xi \rangle$ of $\delta\xi$ vanishes, and the second-order statistic moment, the so-called noise source, is considered:

$$K(x, x', \omega) = \langle \delta\xi(x, \omega) \cdot \delta\xi^*(x', \omega) \rangle \tag{758}$$

From the noise source, the noise current spectral densities (or in the static case, the variances and covariances) are obtained as:

$$S_I^{c_1, c_2} = \iint G_\xi^{c_1}(x, \omega) K(x, x', \omega) G_\xi^{c_2*}(x', \omega) dx dx' \tag{759}$$

Similar relations are used for the noise voltage spectral densities S_V.

Some of the noise sources are local, $K(x, x', \omega) = \delta(x - x') K(x, \omega)$, which allows you to reduce the number of integrations in Eq. 759 to one. $K(x, \omega)$ is called the *local noise source*

(LNS), and the integrand of Eq. 759 in this case is called the *local noise current spectral density* (LNISD), and the corresponding integrand for S_V is called the *local noise voltage spectral density* (LNVSD).

Noise Output Data

Several variables can be plotted during noise analysis. For each device, a `NoisePlot` section can be specified similar to the `Plot` section, where the data to be plotted is listed. Besides the standard data, additional noise-specific data or groups of data can be specified, as listed in Table 128. In the tables, the abbreviations LNS (local noise source) and LNVSD (local noise voltage spectral density) are used.

Autocorrelation data refers to Eq. 759 when $c_1 = c_2$. Data selected in the `NoisePlot` section is plotted for each device and observation node at a given frequency into a separate file. File names with the following format are used:

```
<noise-plot>_<device-name>_<ob-node>_<number>_acgf_des.tdr
```

where `<noise-plot>` is the prefix specified by the `NoisePlot` option to `ACCoupled`.

> **NOTE** Only the noise data specified in a `Noise` section without a name, or with an empty string as a name, will be plotted.

In the case of $c_1 \neq c_2$ in Eq. 759, node cross-correlation spectra are computed and integrands become complex. Data specified in the `NoisePlot` section is plotted for each device and each pair of observation nodes at a given frequency into a separate file.

The file names have the format:

```
<noise-plot>_<device-name>_<ob-node-1>_<ob-node-2>_<number>_acgf_des.tdr
```

Table 128   Device noise data

Keyword	Description
`eeDiffusionLNS`	Electron diffusion LNS
`hhDiffusionLNS`	Hole diffusion LNS
`eeMonopolarGRLNS`	Trace of electron monopolar GR LNS
`hhMonopolarGRLNS`	Trace of hole monopolar GR LNS
`eeFlickerGRLNS`	Trace of electron flicker GR LNS
`hhFlickerGRLNS`	Trace of hole flicker GR LNS

Table 128   Device noise data (Continued)

Keyword	Description
`ReLNVXVSD` `ImLNVXVSD`	Real/imaginary parts of LNVSD
`ReLNISD` `ImLNISD`	Real/imaginary parts of local noise current spectral density
`ReeeLNVXVSD` `ImeeLNVXVSD`	Real/imaginary parts of LNVSD for electrons
`RehhLNVXVSD` `ImhhLNVXVSD`	Real/imaginary parts of LNVSD for holes
`ReeeDiffusionLNVXVSD` `ImeeDiffusionLNVXVSD`	Real/imaginary parts of diffusion LNVSD for electrons
`RehhDiffusionLNVXVSD` `ImhhDiffusionLNVXVSD`	Real/imaginary parts of diffusion LNVSD for holes
`ReeeMonopolarGRLNVXVSD` `ImeeMonopolarGRLNVXVSD`	Real/imaginary parts of electron monopolar LNVSD
`RehhMonopolarGRLNVXVSD` `ImhhMonopolarGRLNVXVSD`	Real/imaginary parts of hole monopolar LNVSD
`ReeeFlickerGRLNVXVSD` `ImeeFlickerGRLNVXVSD`	Real/imaginary parts of electron flicker GR LNVSD
`RehhFlickerGRLNVXVSD` `ImhhFlickerGRLNVXVSD`	Real/imaginary parts of hole flicker GR LNVSD
`ReTrapLNISD` `ImTrapLNISD`	Real/imaginary parts of local trapping noise current spectral density
`ReTrapLNVSD` `ImTrapLNVSD`	Real/imaginary parts of local trapping noise voltage spectral density

`PoECReACGreenFunction`
`PoECImACGreenFunction`
`CurECReACGreenFunction`
`CurECImACGreenFunction`
	Real/imaginary parts of G_n

`PoHCReACGreenFunction`
`PoHCImACGreenFunction`
`CurHCReACGreenFunction`
`CurHCImACGreenFunction`
	Real/imaginary parts of G_p

`PoETReACGreenFunction`
`PoETImACGreenFunction`
`CurETReACGreenFunction`
`CurETImACGreenFunction`
	Real/imaginary parts of G_{T_n}

Table 128   Device noise data (Continued)

Keyword	Description
PoHTReACGreenFunction PoHTImACGreenFunction CurHTReACGreenFunction CurHTImACGreenFunction	Real/imaginary parts of G_{T_p}
PoLTReACGreenFunction PoLTImACGreenFunction CurLTReACGreenFunction CurLTImACGreenFunction	Real/imaginary parts of G_T
PoPotReACGreenFunction PoPotImACGreenFunction CurPotReACGreenFunction CurPotImACGreenFunction	Real/imaginary parts of G_ϕ
PoGeoGreenFunction CurGeoGreenFunction	Real part of the Green's functions for geometric variations
GradPoECReACGreenFunction GradPoECImACGreenFunction GradPoHCReACGreenFunction GradPoHCImACGreenFunction GradPoETReACGreenFunction GradPoETImACGreenFunction GradPoHTReACGreenFunction GradPoHTImACGreenFunction	Real/imaginary parts of $\nabla \cdot G_n$, $\nabla \cdot G_p$, $\nabla \cdot G_{T_n}$, $\nabla \cdot G_{T_p}$ for voltage noise
Grad2PoECACGreenFunction Grad2PoHCACGreenFunction	$\left\lvert \underline{G}_n \right\rvert^2$ and $\left\lvert \underline{G}_p \right\rvert^2$ for voltage noise
AllLNS	All used LNS
AllLNVXVSD	All used LNVSD
GreenFunctions	Green's functions and their gradients

References

[1] F. Bonani *et al.*, "An Efficient Approach to Noise Analysis Through Multidimensional Physics-Based Models," *IEEE Transactions on Electron Devices*, vol. 45, no. 1, pp. 261–269, 1998.

[2] J.-P. Nougier, "Fluctuations and Noise of Hot Carriers in Semiconductor Materials and Devices," *IEEE Transactions on Electron Devices*, vol. 41, no. 11, pp. 2034–2049, 1994.

[3] F. Bonani and G. Ghione, "Generation–recombination noise modelling in semiconductor devices through population or approximate equivalent current density fluctuations," *Solid-State Electronics*, vol. 43, no 2, pp. 285–295, 1999.

Tunneling

This chapter presents the tunneling models available in Sentaurus Device.

In current microelectronic devices, tunneling has become a very important physical effect. In some devices, tunneling leads to undesired leakage currents (for gates in small MOSFETs). For other devices such as EEPROMs, tunneling is essential for the operation of the device.

The tunneling models discussed in this chapter refer to elastic charge-transport processes at interfaces or contacts. Tunneling also plays a role in some generation–recombination models (see Chapter 16 on page 391). These models do not deal with spatial transport of charge and, therefore, are not discussed here. In addition to tunneling, hot-carrier injection can also contribute to carrier transport across barriers. To model hot-carrier injection, see Chapter 25 on page 737. Tunneling to traps is discussed in Tunneling and Traps on page 463.

Tunneling Model Overview

Sentaurus Device offers three tunneling models. The most versatile tunneling model is the nonlocal tunneling model (see Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722). This model:

- Handles arbitrary barrier shapes.
- Includes carrier heating terms.
- Allows you to describe tunneling between the valence band and conduction band.
- Offers several different approximations for the tunneling probability.

Use this model to describe tunneling at Schottky contacts, tunneling in heterostructures, and gate leakage through thin, stacked insulators.

The second most powerful model is the direct tunneling model (see Direct Tunneling on page 718). This model:

- Assumes a trapezoidal barrier (this restricts the range of application to tunneling through insulators).
- Neglects heating of the tunneling carriers.
- Optionally, accounts for image charge effects (at the cost of reduced numeric robustness).

Use this model to describe leakage through thin gate insulators, provided those are of uniform or of uniformly graded composition.

The simplest tunneling model is the Fowler–Nordheim model (see Fowler–Nordheim Tunneling). Fowler–Nordheim tunneling is a special case of tunneling also covered by the nonlocal and direct tunneling models, where tunneling is to the conduction band of the oxide. The model is simple and efficient, and has proven useful to describe erase operations in EEPROMs, which is the application for which this model is recommended.

If the simulated device contains a floating gate, gate currents are used to update the charge on the floating gate after each time step in transient simulations. If EEPROM cells are simulated in 2D, it is generally necessary to include an additional coupling capacitance between the control and floating gates to account for the additional influence of the third dimension on the capacitance between these electrodes (see Floating Metal Contacts on page 223). The additional floating gate capacitance can be specified as `FGcap` in the `Electrode` statement (see Physical Models and the Hierarchy of Their Specification on page 18).

Fowler–Nordheim Tunneling

Using Fowler–Nordheim

To switch on the Fowler–Nordheim tunneling model, specify `Fowler` as an option to `GateCurrent` in an appropriate interface `Physics` section, as follows:

```
Physics(MaterialInterface="Silicon/Oxide"){ GateCurrent(Fowler) }
```

or:

```
Physics(MaterialInterface="Silicon/Oxide"){ GateCurrent(Fowler(EVB)) }
```

The second specification activates the tunneling of electrons from and to the valence band as discussed in Fowler–Nordheim Model on page 717.

If `GateCurrent` is specified as above, Sentaurus Device computes gate currents between all silicon–oxide interfaces and the electrodes. The computation can be restricted to selected interfaces using region-interface `Physics` sections.

For simple one-gate devices, the tunneling current can be monitored on a contact specified by the keyword `GateName` in the `GateCurrent` statement.

The Fowler–Nordheim tunneling model can be used with any of the hot-carrier injection models (see Chapter 25 on page 737), for example:

```
GateCurrent( Fowler Lucky )
```

switches on the Fowler–Nordheim tunneling model and the classical lucky electron injection model simultaneously.

Fowler–Nordheim Model

The Fowler–Nordheim model reads:

$$j_{FN} = A F_{ins}^2 \exp\left(-\frac{B}{F_{ins}}\right) \tag{760}$$

where j_{FN} is the tunnel current density, F_{ins} is the insulator electric field at the interface, and A and B are physical constants. The electric field at the interface shown by Sentaurus Visual is an interpolation of the fields in both regions, but Sentaurus Device uses the insulator field internally.

Due to the large energy difference between oxide and silicon conduction bands, tunneling electrons create electron–hole pairs in the erase operation when they enter the semiconductor. This additional carrier generation is included by an energy-independent multiplication factor $\gamma > 1$:

$$j_n = \gamma \cdot j_{FN} \tag{761}$$

$$j_p = (\gamma - 1) \cdot j_{FN} \tag{762}$$

If the electrons flow in an opposite direction, by default, $\gamma = 1$. The formulas above reflect the default behavior of Sentaurus Device, but sometimes the Fowler–Nordheim equation is used to emulate other tunneling effects, for example, the tunneling of electrons from the valence band into the gate. Such capability is activated by the additional keyword EVB in the command file. Sentaurus Device will continue to function even if $\gamma < 1$. For any electron tunneling direction, particularly a floating body SOI, this tunneling current is important because it strongly defines floating body potential. Different coefficients are needed for the write and erase operations because, in the first case, the electrons are emitted from monocrystalline silicon and, in the latter case, they are emitted from the polysilicon contact into the oxide.

The tunneling current is implemented as a current boundary condition at the interface where the current is produced. For transient simulations, if the Interface keyword is also present in the GateCurrent section, carrier tunneling with explicitly evaluated boundary conditions for continuity equations is activated (similar to carrier injection with explicitly evaluated

boundary conditions for continuity equations in).

Fowler–Nordheim Parameters

The parameters of the Fowler–Nordheim model can be modified in the `FowlerModel` parameter set. Sentaurus Device uses different parameters (denoted as `erase` and `write`) depending on the direction of the electric field between the contact and semiconductor in the oxide layer. For example, if the field points from the contact to the semiconductor (that is, electrons flow into the contact), the 'write' parameter set is used. Table 129 lists the parameters and their default values.

Table 129   Coefficients for Fowler–Nordheim tunneling (defaults for silicon–oxide interface)

Symbol	Parameter name	Default value	Unit	Remarks
A (erase)	Ae	1.87×10^{-7}	A/V^2	A for the erase cycle
B (erase)	Be	1.88×10^{8}	V/cm	B for the erase cycle
A (write)	Aw	1.23×10^{-6}	A/V^2	A for the write cycle
B (write)	Bw	2.37×10^{8}	V/cm	B for the write cycle
γ	Gm	1	1	

Direct Tunneling

Direct tunneling is the main gate leakage mechanism for oxides thinner than $3\,\mathrm{nm}$. It turns into Fowler–Nordheim tunneling at oxide fields higher than approximately $6\,\mathrm{MV/cm}$, independent of the oxide thickness. This section describes a fully quantum-mechanical tunneling model that is restricted to trapezoidal tunneling barriers and covers both direct tunneling and the Fowler–Nordheim regime. Optionally, the model considers the reduction of the tunneling barrier due to image forces.

A variant of this direct tunneling model is used to describe spin-selective tunneling through magnetic tunnel junctions (see).

Using Direct Tunneling

The direct tunneling model is specified as an option of the `GateCurrent` statement (see Using Fowler–Nordheim on page 716) in an appropriate interface `Physics` section:

```
Physics(MaterialInterface="Silicon/Oxide") {
   GateCurrent( DirectTunneling )
}
```

The keyword `GateName` and the compatibility with the hot-carrier injection models (see Chapter 25 on page 737) are as for the Fowler–Nordheim model, see Fowler–Nordheim Tunneling on page 716.

To switch on the image force effect, the parameters `E0`, `E1`, and `E2` must be specified (in eV) in the parameter file. If these values are all equal (the default), the image force is neglected. Recommended values for both electrons and holes are `E0=0`, `E1=0.3`, and `E2=0.7`. Including the image force effect degrades convergence. For most purposes, the effect can be approximated by reducing the overall barrier height. For more information on model parameters, see Direct Tunneling Parameters on page 721.

To plot the direct tunneling current, the keywords `eSchenkTunnel` or `hSchenkTunnel` must be included in the `Plot` section:

```
Plot { eSchenkTunnel hSchenkTunnel }
```

Direct Tunneling Model

This section summarizes the model described in the literature [1]. It presents the formulas for electrons only; the hole expressions are analogous. The electron tunneling current density is:

$$j_n = \frac{q m_{\mathrm{C}} k}{2\pi^2 \hbar^3} \int_0^\infty dE \Upsilon(E) \left\{ T(0) \ln\left(\exp\left[\frac{E_{\mathrm{F},n}(0) - E_{\mathrm{C}}(0) - E}{kT(0)} \right] + 1 \right) \right. \tag{763}$$
$$\left. - T(\mathrm{d}) \ln\left(\exp\left[\frac{E_{\mathrm{F},n}(\mathrm{d}) - E_{\mathrm{C}}(0) - E}{kT(\mathrm{d})} \right] + 1 \right) \right\}$$

where d is the effective thickness of the barrier, m_{C} is a mass prefactor, the argument 0 denotes one (the 'substrate') side of the barrier and d denotes the other ('gate') side, and E is the energy of the elastic tunnel process (relative to $E_{\mathrm{C}}(0)$).

$\Upsilon(E) = 2/(1 + g(E))$ is the transmission coefficient for a trapezoidal potential barrier, with:

$$g(E) = \frac{\pi^2}{2}\left\{ \sqrt{\frac{E_T}{E}}\sqrt{\frac{m_{Si}}{m_G}}(\text{Bi'}_d\text{Ai}_0 - \text{Ai'}_d\text{Bi}_0)^2 + \sqrt{\frac{E}{E_T}}\sqrt{\frac{m_G}{m_{Si}}}(\text{Bi}_d\text{Ai'}_0 - \text{Ai}_d\text{Bi'}_0)^2 + \right. \tag{764}$$

$$\left. \frac{\sqrt{m_G m_{Si}}}{m_{ox}}\frac{\hbar\Theta_{ox}}{\sqrt{EE_T}}(\text{Bi'}_d\text{Ai'}_0 - \text{Ai'}_d\text{Bi'}_0)^2 + \frac{m_{ox}}{\sqrt{m_G m_{Si}}}\frac{\sqrt{EE_T}}{\hbar\Theta_{ox}}(\text{Bi}_d\text{Ai}_0 - \text{Ai}_d\text{Bi}_0) \right\}$$

and:

$$\text{Ai}_0 = \text{Ai}\left(\frac{E_B(E) - E}{\hbar\Theta_{ox}}\right), \quad \text{Ai}_d = \text{Ai}\left(\frac{E_B(E) - qF_{ox}d - E}{\hbar\Theta_{ox}}\right) \tag{765}$$

and so on, where $\hbar\Theta_{ox} = (q^2\hbar^2 F_{ox}^2/2m_{ox})^{1/3}$ and $E_B(E)$ denotes the (substrate-side) barrier height for electrons of energy E. E_T is the tunneling energy with respect to the conduction band edge on the gate side, $E_T = E - E_C(d) - E_C(0)$.

For compatibility with an earlier implementation of the model, E_T is truncated to the value specified by the parameter E_F_M if it exceeds this value. $F_{ox} = V_{ox}/d$ is the electric field in the oxide (assumed to be uniform within the oxide, and including a band edge–related term when different barrier heights are specified at the two insulator interfaces). The quantities m_G, m_{ox}, and m_{Si} represent the electron masses in the three materials, respectively. Ai and Bi are Airy functions, and Ai' and Bi' are their derivatives.

Image Force Effect

Ultrathin oxide barriers are affected by the image force effect. If the latter is neglected, $E_B(E)$ is the bare barrier height E_B, which is an input parameter. The image force effect is included in the model by taking $E_B(E)$ as an energy-dependent pseudobarrier:

$$E_B(E) = E_B(E_0) + \frac{E_B(E_2) - E_B(E_0)}{(E_2 - E_0)(E_1 - E_2)}(E - E_0)(E_1 - E) - \frac{E_B(E_1) - E_B(E_0)}{(E_1 - E_0)(E_1 - E_2)}(E - E_0)(E_2 - E) \tag{766}$$

where E_0, E_1, and E_2 are chosen in the lower energy range of the barrier potential (between $0\,\text{eV}$ and $1.5\,\text{eV}$ in practical cases). If these values are chosen to be equal, the image force effect is automatically switched off. Otherwise, for each bias point:

$$S_{tra}(E) = S_{im}(E) \tag{767}$$

is solved for $E_j (j = 0, 1, 2)$, which results in three pseudobarrier heights $E_B(E_j)$ used in Eq. 766. In Eq. 767, $S_{tra}(E)$ is the action of the trapezoidal pseudobarrier:

$$S_{tra}(E) = \frac{2}{3}\left|\left[\frac{E_B(E) - qF_{ox}d - E}{\hbar\Theta_{ox}}\right]^{\frac{3}{2}}\Theta[E_B(E) - qF_{ox}d - E] - \left[\frac{E_B(E) - E}{\hbar\Theta_{ox}}\right]^{\frac{3}{2}}\right| \tag{768}$$

and $S_{im}(E)$ is the action of the respective image potential barrier:

$$S_{im}(E) = \sqrt{\frac{2m_{ox}}{\hbar^2}} \int_{x_l(E)}^{x_r(E)} d\xi \sqrt{E_B - qF_{ox}\xi + E_{im}(\xi) - E} \tag{769}$$

$x_{l,r}(E)$ denotes the classical turning points for a given carrier energy that follow from:

$$E_T - qF_{ox}x_{l,r} + E_{im}(x_{l,r}) = E \tag{770}$$

For the thickness of the pseudobarrier, $d = x_r(0) - x_l(0)$ is used, that is, the distance between the two turning points at the energy of the semiconductor conduction band edge of the interface. Therefore, d is smaller than the user-given oxide thickness, when the image force effect is considered. The image potential itself is given by:

$$E_{im}(x) = \frac{q^2}{16\pi\varepsilon_{ox}} \sum_{n=0}^{10} (k_1 k_2)^n \left[\frac{k_1}{nd+x} + \frac{k_2}{d(n+1)-x} + \frac{2k_1 k_2}{d(n+1)} \right] \tag{771}$$

with:

$$k_1 = \frac{\varepsilon_{ox} - \varepsilon_{Si}}{\varepsilon_{ox} + \varepsilon_{Si}}, \quad k_2 = \frac{\varepsilon_{ox} - \varepsilon_G}{\varepsilon_{ox} + \varepsilon_G} = -1 \tag{772}$$

In Eq. 772, ε_{ox}, ε_{Si}, and ε_G denote the dielectric constants for the oxide, substrate, and gate material, respectively.

Direct Tunneling Parameters

The parameters of the direct tunneling model are modified in the `DirectTunneling` parameter set. The appropriate default parameters for an oxide barrier on silicon are in Table 130. The parameters are specified according to the interface.

Table 130   Coefficients for direct tunneling (defaults for oxide barrier on silicon)

Symbol	Parameter name	Electrons	Holes	Unit	Description
ε_{ox}	eps_ins	2.13	2.13	1	Optical dielectric constant
$E_F(d)$	E_F_M	11.7	11.7	eV	Fermi energy for gate contact
m_G	m_M	1	1	m_0	Effective mass in gate contact
m_{ox}	m_ins	0.50	0.77	m_0	Effective mass in insulator
m_{Si}	m_s	0.19	0.16	m_0	Effective mass in substrate
m_C	m_dos	0.32	0	m_0	Semiconductor DOS effective mass

Table 130   Coefficients for direct tunneling (defaults for oxide barrier on silicon) (Continued)

Symbol	Parameter name	Electrons	Holes	Unit	Description
E_B	`E_barrier`	3.15	4.73	eV	Semiconductor/insulator barrier (no image force)
E_0 , E_1 , E_2	`E0, E1, E2`	0	0	eV	Energy nodes 0, 1, and 2 for pseudobarrier calculation

If tunneling occurs between two semiconductors, the coefficients for metal (`m_M` and `E_F_M`) are not used. The semiconductor parameters for the respective interface are used. It is not valid to have contradicting parameter sets for two interfaces of an insulator between which tunneling occurs. In particular, `eps_ins`, `m_ins`, `E0`, `E1`, and `E2` must agree in the parameter specifications for both interfaces.

Nonlocal Tunneling at Interfaces, Contacts, and Junctions

The tunneling current depends on the band edge profile along the entire path between the points connected by tunneling. This makes tunneling a nonlocal process. In general, the band edge profile has a complicated shape, and Sentaurus Device must compute it by solving the transport equations and the Poisson equation. The model described here takes this dependence fully into account.

To use the nonlocal tunneling model:

1. Construct a special purpose 'nonlocal' mesh (see Defining Nonlocal Meshes).

2. Specify the physical details of the tunneling model (see Specifying Nonlocal Tunneling Model on page 724).

3. Adjust the physical and numeric parameters (see Nonlocal Tunneling Parameters on page 726).

Defining Nonlocal Meshes

It is necessary to specify a special purpose 'nonlocal' mesh for each part of the device for which you want to use the nonlocal tunneling model. Nonlocal meshes consist of 'nonlocal' lines that represent the tunneling paths for the carriers.

To control the construction of the nonlocal mesh, use the options of the keyword `NonLocal` in the global `Math` section. Nonlocal meshes can be constructed using two different forms:

- In the simpler form, `NonLocal` specifies barrier regions. For example:

      Math { Nonlocal "NLM" (Barrier(Region="oxtop" Region="oxbottom")) }

constructs a nonlocal mesh for a tunneling barrier that consists of the regions `oxtop` and `oxbottom`. See Specification Using Barrier on page 149 for details.

- In the more general form, `NonLocal` specifies an interface or a contact where the mesh is constructed, and a distance `Length` (given in centimeters). Sentaurus Device then connects semiconductor vertices with a distance from the interface or contact no larger than `Length` to the interface or contact. These connections form the centerpiece of the nonlocal lines. For example, with:

  ```
  Math { Nonlocal "NLM" (Electrode="Gate" Length=5e-7) }
  ```

  Sentaurus Device constructs a nonlocal mesh called `"NLM"` that connects vertices up to a distance of 5 nm to the `Gate` electrode. See Specification Using a Reference Surface on page 150 for details.

Sentaurus Device introduces a coordinate along each nonlocal line. The interface or contact is at coordinate zero; the vertex for which the nonlocal line is constructed is at a positive coordinate. Below, the terms *upper* and *lower* refer to the orientation according to these nonlocal line–specific coordinates. This orientation is not related to the orientation of the mesh axes.

To form the nonlocal lines, Sentaurus Device extends the connection at the upper end, to fully cover the box for the vertex that is connected. Optionally, for nonlocal meshes at interfaces, the connection can be extended at the lower end (beyond the interface) by an amount specified by `Permeation` (in centimeters).

Sentaurus Device handles each nonlocal line separately. Therefore, two nonlocal lines connecting two vertices to the same interface do not allow the computing of tunneling between these vertices. To compute tunneling between vertices on the two sides of an interface, they must be covered by a single nonlocal line. This is where `Permeation` is needed.

For nonlocal meshes not used for trap tunneling, `Permeation` also affects the integration range for tunneling. With zero `Permeation`, the lower endpoint for tunneling is always at the interface; for positive `Permeation`, it can be anywhere on the nonlocal line. Therefore, for tunneling at smooth barriers (for example, band-to-band tunneling at a steep p-n junction), the nonlocal mesh used should not be reused for trap tunneling (see Tunneling and Traps on page 463), and `Permeation` should be positive.

When using the more general form of nonlocal mesh construction, specify a nonlocal mesh for only one side of a tunneling barrier. If on one side of the tunneling barrier there is a contact or a metal–nonmetal interface, specify the mesh there. In other cases, specify the nonlocal mesh for the interface from which the carriers will tunnel away. If this side can change during the simulation, specify a nonzero `Permeation` (approximately as much as `Length` exceeds the barrier thickness). For tunneling barriers with multiple layers, do not specify a nonlocal mesh for the interfaces internal to the barrier.

For more options to the keyword NonLocal, see Table 228 on page 1424. For details about the nonlocal mesh and its construction, see Constructing Nonlocal Meshes on page 149.

> **NOTE** The nonlocality of tunneling can increase dramatically the time that is needed to solve the linear systems in the Newton iteration. To limit the speed degradation, keep Length and Permeation as small as possible. Consider optimizing the nonlocal mesh using the advanced options of NonLocal (see Constructing Nonlocal Meshes on page 149).

Specifying Nonlocal Tunneling Model

The nonlocal tunneling model is activated and controlled in the global Physics section. Each tunneling event connects two points on a nonlocal line. Sentaurus Device distinguishes between tunneling to the conduction band and to the valence band at the lower of the two points.

To switch on these terms, use the options eBarrierTunneling and hBarrierTunneling. For example:

```
Physics {
    eBarrierTunneling "NLM" hBarrierTunneling "NLM"
}
```

switches on electron and hole tunneling for the nonlocal mesh called "NLM", and:

```
Physics {
    eBarrierTunneling "NLM" (PeltierHeat)
}
```

switches on tunneling to the conduction band only and activates the Peltier heating of the tunneling particles.

By default, all tunneling to the conduction band at the lower point on the line originates from the conduction band at the upper point, $j_C = j_{CC}$ ('electron tunneling'), see Eq. 783, p. 734. Likewise, by default, the tunneling to the valence band at the lower point originates from the valence band at the upper point, $j_V = j_{VV}$ (that is, 'hole tunneling').

In addition, Sentaurus Device supports nonlocal band-to-band tunneling. To include the contributions by tunneling to and from the valence band at the upper point in j_C, specify eBarrierTunneling with the Band2Band=Simple option. Then, $j_C = j_{CC} + j_{CV}$, see Eq. 783 and Eq. 785, p. 734. To include contributions by tunneling to and from the conduction band at the upper point to j_V, specify hBarrierTunneling with the Band2Band=Simple option. Then, $j_V = j_{VC} + j_{VV}$. With Band2Band=Full, the nonlocal band-to-band tunneling model uses Eq. 480, p. 437 instead of Eq. 784, p. 734 to calculate the band-to-band tunneling

contribution, which makes the model consistent with the Dynamic Nonlocal Path Band-to-Band Tunneling Model on page 436 provided that the dynamic nonlocal path band-to-band model uses the direct tunneling model with the Franz dispersion relation. With `Band2Band=UpsideDown` (or only `Band2Band`), an obsolete, physically flawed, band-to-band tunneling model is activated.

For backward compatibility, you can activate the nonlocal tunneling model in an interface-specific or contact-specific `Physics` section; in that case, specify `eBarrierTunneling` and `hBarrierTunneling` as options to `Recombination`, and omit the nonlocal mesh name. The specification applies to an unnamed nonlocal mesh that has been constructed for the same location (see Unnamed Meshes on page 152).

Figure 47 illustrates the four contributions to the total tunneling current.

Figure 47   Various nonlocal tunneling current contributions

By default, Sentaurus Device assumes a single-band parabolic band structure for the tunneling particles, uses a WKB-based model for the tunneling probability, and ignores band-to-band tunneling and Peltier heating. Options to `eBarrierTunneling` and `hBarrierTunneling` override the default behavior. For available options, see Table 238 on page 1439. For a detailed discussion of the physics of the nonlocal tunneling model, see Physics of Nonlocal Tunneling Model on page 729.

When specifying the `Multivalley` option, the tunneling model uses the multivalley band structure (see Multivalley Band Structure on page 267). This allows you to account for conduction and valence bands with multiple valleys, anisotropic masses, and possibly geometric confinement. See Multivalley Band Structure and Geometric Quantization on page 732 for more details.

When specifying the `BarrierLowering` option, the tunneling model accounts for position-dependent barrier lowering corrections in the conduction-band and valence-band edges. shifting them inwards, toward the midgap. See WKB Tunneling Probability on page 729 and Eq. 779, p. 731 for details.

Nonlocal Tunneling Parameters

The nonlocal tunneling model has several fit parameters. They are specified in the `BarrierTunneling` parameter set.

The parameter pair `g` determines the dimensionless prefactors g_C and g_V (see Eq. 782 and Eq. 784). For unnamed meshes, specify them in the parameter set that is specific to the contact or interface for which the nonlocal tunneling model is activated. For named meshes, specify them in the global parameter set.

The parameter pair `mt` determines the tunneling masses m_C and m_V (see Eq. 773 and Eq. 774). They are properties of the materials that form the tunneling barrier. Therefore, specify them (in units of m_0) in region-specific or material-specific parameter sets. For tunneling at contacts, also specify the masses for the contact parameter set when using `Transmission` or `Schroedinger` (see Eq. 778, p. 730 and Schrödinger Equation–Based Tunneling Probability on page 731).

Sentaurus Device treats effective tunneling masses of value zero as undefined. If an effective tunneling mass for a region is undefined, Sentaurus Device uses the effective tunneling mass for the interface or contact for which tunneling is activated (for unnamed meshes) or the tunneling mass from the global parameter set (for named meshes). By default, all effective tunneling masses are undefined. Finally, if the model is used with the `Multivalley` option (see Multivalley Band Structure and Geometric Quantization on page 732), masses extracted from the multivalley model override the tunneling masses wherever they are available.

The following example changes the prefactors g_C and g_V to 1 and 2, respectively:

```
BarrierTunneling {
    mt = 0.5, 0.5
    g = 1 , 2
}
Material = "Oxide" {
   BarrierTunneling {
      mt = 0.42 , 1.0
   }
}
```

The tunneling masses are set to $0.5m_0$. In oxide, it sets the tunneling masses m_C and m_V to 0.42 and 1, respectively; these values take precedence over the masses specified globally.

The parameters `eoffset` and `hoffset` are lists of nonnegative energy shifts (in eV) that are added to the conduction-band and valence-band edges, shifting them outwards, away from the midgap. Specify them in a region-specific or material-specific parameter set. By default, a single shift value of zero is assumed. Sentaurus Device computes the tunneling current as the sum of the currents for each shift. Shifts in different regions are combined according to the position where they appear in the list; if the lists in different regions have different lengths, the last value in the shorter lists are repeated to extend them to the length of the longest list.

The parameter pair `alpha` determines the fit factors α_n and α_p for the quantization corrections for tunneling from inversion layers through insulator barriers (see Density Gradient Quantization Correction on page 732). The default values are zero, disabling the corrections. To enable them, set the parameters to one (or another positive value) in the interface- or contact-specific parameter set (for unnamed meshes) or in the global parameter set (for named meshes).

The parameter pairs `QuantumPotentialFactor` and `QuantumPotentialPosFac` specify the prefactors for the electron and hole quantum potentials obtained from the density gradient model (see Density Gradient Quantization Model on page 294) that can be added to the band edges used for evaluating the tunneling rate. By default, the parameters are zero, such that the quantum potentials are neglected in the computation of tunneling. When they are nonzero, the quantum potentials multiplied by the corresponding prefactors are added to the conduction and valence band edges for the computation of tunneling current.

For `QuantumPotentialFactor`, an addition is performed irrespective of the sign of the quantum potential. For `QuantumPotentialPosFac`, an addition is performed only where the quantum potential is positive, that is, only where quantization causes an effective widening of the band gap.

The quantum corrections activated by giving `QuantumPotentialFactor` or `QuantumPotentialPosFac` a nonzero value are intended for situations where quantization is caused by confinement perpendicular to the tunneling direction. In contrast, `alpha` is intended for tunneling from an inversion layer, where quantization is due to confinement in the tunneling direction.

The regionwise barrier-lowering fitting factor A can be specified by the `A` parameter (default is 1):

```
Material = "Silicon" {
   BarrierTunneling {
      A = 1.02 , 1.0
   }
}
```

The barrier lowering parameter `BL_max` allows you to adjust the maximum of the barrier lowering (corresponding to the minimum-allowed distance to the contact or interface). Its default value is 0.3 eV.

`BarrierTunneling` can also be applied specifically to named nonlocal meshes. For example:

```
Material = "Oxide" {
   BarrierTunneling "NLM" {
      mt = 0.42 , 1.0
   }
}
```

changes the oxide tunneling mass for the nonlocal mesh `NLM` only. Specifications for named nonlocal meshes take precedence over the general specifications.

Specify numeric parameters for the model in the `Math` section, as an option of `NonLocal` for a given nonlocal mesh. The parameter `Digits` determines the relative accuracy (the number of valid decimal digits) to which Sentaurus Device computes the integrals in Eq. 783 and Eq. 785. The default value is 2. The parameter `EnergyResolution` (given in eV) is a lower limit for the energy step that Sentaurus Device uses to perform the integrations and it defaults to 0.005. The purpose of `EnergyResolution` is to limit the runtime for computing the tunneling currents in case the value of `Digits` is too large.

For example:

```
Math {
   NonLocal "NLM" (
      ...
      Digits=3
      EnergyResolution=0.001
   )
}
```

increases the energy resolution for tunneling on the nonlocal mesh `"NLM"` to $1\,\mathrm{meV}$ and the relative accuracy of the tunneling current computation to three digits.

Visualizing Nonlocal Tunneling

To visualize nonlocal tunneling, specify the keyword `eBarrierTunneling` or `hBarrierTunneling` in the `Plot` section (see Device Plots on page 122). The quantities plotted are in units of $\mathrm{cm^{-3}s^{-1}}$ and represent the rate at which electrons and holes are generated or disappear due to tunneling. To plot the Peltier heat generated in the conduction band and valence band due to nonlocal tunneling, specify `eNLLTunnelingPeltierHeat` and `hNLLTunnelingPeltierHeat`. The Peltier heat is plotted in units of $\mathrm{Wcm^{-3}}$ and is available regardless of whether it is accounted for in the temperature equation.

The rates are plotted vertexwise and are averaged over the semiconductor volume controlled by a vertex. Therefore, they depend on the mesh spacing. This dependence can become particularly strong at interfaces where the band edges change abruptly.

Physics of Nonlocal Tunneling Model

The nonlocal tunneling model in Sentaurus Device is based on the approach presented in the literature [2], but provides significant enhancements over the model presented there.

WKB Tunneling Probability

The computation of the tunneling probabilities $\Gamma_{C,\nu}$ (for carriers tunneling to the ν-th shifted conduction band at the interface or contact) and $\Gamma_{V,\nu}$ (for tunneling to the ν-th shifted valence band) is, by default, based on the WKB approximation.

The WKB approximation uses the local (imaginary) wave numbers of particles at position r and with energy ε:

$$\kappa_{C,\nu}(r,\varepsilon) = \sqrt{2m_C(r)\big|E_{C,\nu}(r)-\varepsilon\big|}\,\Theta[E_{C,\nu}(r)-\varepsilon]/\hbar \tag{773}$$

$$\kappa_{V,\nu}(r,\varepsilon) = \sqrt{2m_V(r)\big|\varepsilon-E_{V,\nu}(r)\big|}\,\Theta[\varepsilon-E_{V,\nu}(r)]/\hbar \tag{774}$$

Here, m_C is the conduction-band tunneling mass and m_V is the valence-band tunneling mass. Both tunneling masses are adjustable parameters (see Nonlocal Tunneling Parameters on page 726). $E_{C,\nu}$ and $E_{V,\nu}$ are the conduction and valence bands energies shifted by the ν-th value in eoffset and hoffset (see Nonlocal Tunneling Parameters on page 726).

Using the local wave numbers and the interface transmission coefficients $T_{CC,\nu}$ and $T_{VV,\nu}$, the tunneling probability between positions l and $u > l$ for a particle with energy ε can be written as:

$$\Gamma_{CC,\nu}(u,l,\varepsilon) = T_{CC,\nu}(l,\varepsilon)\exp\left(-2\int_l^u \kappa_{C,\nu}(r,\varepsilon)dr\right)T_{CC,\nu}(u,\varepsilon) \tag{775}$$

and:

$$\Gamma_{VV,\nu}(u,l,\varepsilon) = T_{VV,\nu}(l,\varepsilon)\exp\left(-2\int_l^u \kappa_{V,\nu}(r,\varepsilon)dr\right)T_{VV,\nu}(u,\varepsilon) \tag{776}$$

If the option `TwoBand` is specified to `eBarrierTunneling` (see Table 238 on page 1439), Sentaurus Device replaces $\kappa_{C,v}$ in Eq. 775 with the two-band dispersion relation:

$$\kappa_v = \frac{\kappa_{C,v}\kappa_{V,v}}{\sqrt{\kappa_{C,v}^2 + \kappa_{V,v}^2}} \tag{777}$$

If the option `TwoBand` is specified to `hBarrierTunneling`, Sentaurus Device replaces $\kappa_{V,v}$ in Eq. 776 with the two-band relation Eq. 777. Near the conduction and the valence band edge, the two-band dispersion relation approaches the single band dispersion relations Eq. 773 and Eq. 774, and provides a smooth interpolation in between. Figure 48 illustrates this.

The two-band dispersion relation does not distinguish between electrons and holes. In particular, for the two-band dispersion relation, $\Gamma_{CC,v} = \Gamma_{VV,v}$.

Figure 48   Comparison of two-band and single-band dispersion relations

The two-band dispersion relation is most useful when band-to-band tunneling is active (keyword `Band2Band`, see Table 238 on page 1439). However, the two-band dispersion relation can be used independently from band-to-band tunneling.

By default, the interface transmission coefficients $T_{CC,v}$ and $T_{VV,v}$ in Eq. 775 and Eq. 776 equal one. If the `Transmission` option is specified to `eBarrierTunneling` [3]:

$$T_{CC,v}(x,\varepsilon) = \frac{v_{-,v}(x,\varepsilon)\sqrt{v_{-,v}(x,\varepsilon)^2 + 16v_{+,v}(x,\varepsilon)^2}}{v_{+,v}(x,\varepsilon)^2 + v_{-,v}(x,\varepsilon)^2} \tag{778}$$

Here, $v_{-,v}(x,\varepsilon)$ denotes the velocity of a particle with energy ε on the side of the interface or contact at position x where the particle moves freely in the conduction band, and $v_{+,v}(x,\varepsilon)$ denotes the imaginary velocity on the side of the tunneling barrier (where the particle is in the gap). If the particle is free or in the barrier on both sides, $T_{CC,v}(x,\varepsilon) = 1$. Velocities are the derivatives of the particle energy with respect to the wave number, $v_v = |\partial\varepsilon/\partial\hbar\kappa_{C,v}|$. With the

TwoBand option, $v_{+,v} = |\partial \varepsilon / \partial \hbar \kappa_v|$ [4] (see Eq. 777). If the Transmission option is specified to hBarrierTunneling, analogous expressions hold for $T_{VV,v}$.

By default, the band-to-band tunneling probabilities $\Gamma_{CV,v}$ and $\Gamma_{VC,v}$ are also given by the expressions Eq. 775 and Eq. 776, respectively. When the TwoBand and Transmission options are specified for eBarrierTunneling to compute $\Gamma_{CV,v}$, $v_{-,v}$ in the expression for $T_{CC,v}(r, \varepsilon)$ (see Eq. 778) is the velocity of the particle in the valence band and is computed from valence-band parameters. The converse holds for $\Gamma_{VC,v}$ when those options are specified for hBarrierTunneling.

For metals and contacts, the band-edge energy to compute the interface transmission coefficients is obtained from the FermiEnergy parameter of the BandGap section for the metal or contact. The masses used to compute the velocities are the tunneling effective masses for the metal or contact.

For metals and contacts when the BarrierLowering option is specified for BarrierTunneling, the band edges are corrected by a position-dependent lowering potential given by:

$$\Delta \Phi_B(r) = \frac{Aq}{16\pi\varepsilon r} \tag{779}$$

where ε is the material dielectric constant, r is the distance from the interface or contact, and A is a dimensionless fitting parameter. Because Eq. 779 has a singularity for $r \to 0$, Sentaurus Device limits r by imposing a minimum value. You can set the minimum value for r by specifying a maximum value for $\Delta \Phi_B(r)$ using the parameter BL_max (see Nonlocal Tunneling Parameters on page 726).

Schrödinger Equation–Based Tunneling Probability

In addition to the WKB-based models discussed in WKB Tunneling Probability on page 729, Sentaurus Device can compute tunneling probabilities based on the Schrödinger equation. For the Schrödinger equation–based model, Sentaurus Device computes the tunneling probability $\Gamma_{CC,v}(E)$ (or $\Gamma_{VV,v}(E)$) by solving the 1D Schrödinger equation:

$$\left(-\frac{d}{dr}\frac{1}{m(r)}\frac{d}{dr} + E_{C,v}(r) \right)\Psi(r) = E(r)\Psi(r) \tag{780}$$

between the outermost classical turning points that belong to the tunneling energy E. For $m(r)$, Sentaurus Device uses the tunneling mass mt (see Nonlocal Tunneling Parameters on page 726). $E_{C,v}$ is the conduction-band energy shifted by the v-th value in eoffset (see Nonlocal Tunneling Parameters on page 726).

For boundary conditions, Sentaurus Device assumes incident and reflected plane waves outside the barrier on one side, and an evanescent plane wave on the other side. The energy for the

plane waves is the greater of kT_n and $E - E_{C,v}$, where T_n and $E_{C,v}$ c are taken at the point immediately outside the barrier on the respective side. The masses outside the barrier are the tunneling masses `mt` that are valid there.

Density Gradient Quantization Correction

Two different quantization corrections to tunneling are available with the density gradient model (see Density Gradient Quantization Model on page 294).

The first correction is intended for tunneling from an inversion layer through an insulator. The corrections are multipliers to $T_{CC,v}(r, \varepsilon)$ and read:

$$\exp\left(\alpha_n \frac{\Lambda_{\mathrm{fb},n}(r) - \Lambda_n(r)}{kT_n(r)}\right) \tag{781}$$

where α_n is an adjustable parameter (see Nonlocal Tunneling Parameters on page 726), and $\Lambda_{\mathrm{fb},n}$ is the solution of the 1D density gradient equations for flatband (that is, $\phi = \mathrm{const}$) conditions. A multiplier analogous to that in Eq. 781 exists for $T_{VV,v}$.

The second correction is intended for situations where quantization is due to confinement perpendicular to the tunneling direction, for example, for tunneling in the channel direction of a nanowire. For this correction, for the computation of tunneling, Λ_n and $-\Lambda_p$ are added to the conduction band edge and the valence band edge, with prefactors as described in Nonlocal Tunneling Parameters on page 726.

The motivation for doing this is: If confinement and tunneling are perpendicular, the problem can be separated into a 1D tunneling problem and 2D quantization problems. From the 2D quantization problems, a subband profile along the tunneling direction can be extracted. The lowest energy subbands for electrons and holes form the effective barrier for the 1D tunneling problem. The lowest subband energy profile is approximated by the sum of the band edge and the quantum potential. Note that the latter approximation interprets the quantum potential as an energy-like quantity, ignoring the fact that the quantum potential also describes the shape of the wavefunction.

Multivalley Band Structure and Geometric Quantization

When used with the `Multivalley` option, the tunneling model uses the multivalley band structure as described in Multivalley Band Structure on page 267. In particular, this means:

- Multiple tunneling processes are accounted for. For band-to-band tunneling, tunneling between all valleys of the conduction band to all valleys of the valence band is accounted for. For tunneling within the conduction band or within the valence band, tunneling within each valley is accounted for; while no tunneling between different valleys is taken into account.

■ The tunneling mass is the inverse of the reciprocal mass tensor specified by the multivalley parameters, projected in the tunneling direction. Where no multivalley parameters are available, the tunneling mass is determined from the tunneling parameters as described in Nonlocal Tunneling Parameters on page 726.

■ The conduction and valence band edges used to compute tunneling include the band offsets as described by the multivalley model parameters.

■ When the multivalley band structure is used with the `ThinLayer` model, the resulting quantum corrections due to geometric confinement are used in the tunneling model as well. The details of how this is performed are described next.

For the interplay of tunneling and quantization, two limiting cases can be distinguished:

■ When tunneling is perpendicular to the confinement, the quantization increases the tunneling barrier, as discussed in Density Gradient Quantization Correction on page 732.

■ When tunneling is in the confinement direction, quantization does not affect the tunneling barrier. However, quantization affects the density-of-states available to carriers in the bands to which they tunnel.

To connect the two limiting cases, Sentaurus Device uses the following heuristic approach: For each point along the tunneling path and for each valley, the angle β between the tunneling direction and the confinement direction is computed in a coordinate system where the mass tensor of the valley becomes diagonal. From β and the total quantization energy ε_1^i given by Eq. 205, p. 270, a "perpendicular" quantization energy is obtained, $\varepsilon_\perp^i = (1 + -\cos^2\beta)\varepsilon_1^i$. The latter is added to the band edges in computing the tunneling probability (see WKB Tunneling Probability on page 729 and Schrödinger Equation–Based Tunneling Probability on page 731).

The total energy is added to the bands in the expressions for the energy and position integrations (see Nonlocal Tunneling Current on page 733). None of these terms is added for the expressions for carrier heating (see Carrier Heating on page 735).

> **NOTE** It is recommended that the number of valleys and their names are the same on an entire tunneling path, even when the path runs in more than one region.

Nonlocal Tunneling Current

For a point at u, the expression for the net conduction band electron recombination rate due to tunneling to and from the ν-th shifted conduction band at point $l < u$ with energy ε is:

$$R_{CC,\nu}(u,l,\varepsilon) - G_{CC,\nu}(u,l,\varepsilon) = \frac{A_{CC}}{qk}\vartheta\left[\varepsilon - E_{C,\nu}(u), -\frac{dE_{C,\nu}}{du}(u)\right]\vartheta\left[\varepsilon - E_{C,\nu}(l), \frac{dE_{C,\nu}}{dl}(l)\right]\Gamma_{CC,\nu}(u,l,\varepsilon) \times \quad (782)$$

$$\left[T_n(u)\ln\left(1 + \exp\left[\frac{E_{F,n}(u)-\varepsilon}{kT_n(u)}\right]\right) - T_n(l)\ln\left(1 + \exp\left[\frac{E_{F,n}(l)-\varepsilon}{kT_n(l)}\right]\right)\right]$$

where $\vartheta(x, y) = \delta(x)|y|\Theta(y)$, $A_{CC} = g_C A_0$ is the effective Richardson constant (with $A_0 = 4\pi m_0 kq/h^3$ the Richardson constant for free electrons), and g_C is a fit parameter (see Nonlocal Tunneling Parameters on page 726). $R_{CC, v}$ relates to the first term and $G_{CC, v}$ to the second term in the second line of Eq. 782. $\Gamma_{CC, v}$ is the tunneling probability (see Eq. 775). For nonlocal lines with zero Permeation, the second ϑ-function is replaced with $\Theta[\varepsilon - E_{C, v}(l)]\delta(l - 0^-)$ (with 0^- infinitesimally smaller than 0). For contacts, metals, or in the presence of the option BandGap, the second ϑ-function is replaced with $\delta(l - 0^-)$.

The contribution to the electron tunneling current density by electrons that tunnel from the conduction band at points above l to the conduction band at point l is the integral over the recombination rate (Eq. 782):

$$\frac{dj_{CC}}{dl}(l) = -q\sum_v \int_l^\infty \int_{-\infty}^\infty [R_{CC, v}(u, l, \varepsilon) - G_{CC, v}(u, l, \varepsilon)]d\varepsilon\, du \tag{783}$$

The options for hBarrierTunneling and the expressions for the valence band to valence band tunneling current density j_{VV} are analogous.

Band-to-Band Contributions to Nonlocal Tunneling Current

When you specify the Band2Band option to eBarrierTunneling (see Table 238 on page 1439), the total current that flows to the conduction band at point l also contains electrons that originate from the valence band at position $u > l$.

For Band2Band=Simple, the recombination rate of the valence-band electrons with energy ε at point u (in other words, the generation rate of holes at u) due to tunneling to or from the v-th shifted conduction band at l is:

$$R_{CV, v}(u, l, \varepsilon) - G_{CV, v}(u, l, \varepsilon) = \frac{A_{CV}}{2qk}\vartheta\left[\varepsilon - E_{V, v}(u), \frac{dE_{V, v}}{du}(u)\right]\vartheta\left[\varepsilon - E_{C, v}(l), \frac{dE_{C, v}}{dl}(l)\right]\Gamma_{CV, v}(u, l, \varepsilon) \times \tag{784}$$
$$[T_p(u) + T_n(l)]\left[\left(1 + \exp\left[\frac{\varepsilon - E_{F, p}(u)}{kT_p(u)}\right]\right)^{-1} - \left(1 + \exp\left[\frac{\varepsilon - E_{F, n}(l)}{kT_n(l)}\right]\right)^{-1}\right]$$

where $A_{CV} = \sqrt{g_C g_V} A_0$. The prefactor g_V is a fit parameter, see Nonlocal Tunneling Parameters on page 726. $\Gamma_{CV, v}$ is the band-to-band tunneling probability discussed above. The modifications for zero Permeation, contacts, metals, and the BandGap option are as for Eq. 782.

The current density of electrons that tunnel from the valence band at points above l to the conduction band at point l is the integral over the recombination rate (Eq. 784):

$$\frac{dj_{CV}}{dl}(l) = -q\sum_v \int_l^\infty \int_{-\infty}^\infty [R_{CV, v}(r, l, \varepsilon) - G_{CV, v}(r, l, \varepsilon)]d\varepsilon\, dr \tag{785}$$

For band-to-band tunneling processes, the energy of the tunneling particles often lies deep in the gap of the barrier. The single-band dispersion relations that Sentaurus Device uses by default (see Eq. 773 and Eq. 774) are based on the band structure near the band edges, and may not be useful in this regime. The two-band dispersion relation according Eq. 777 is a better choice. To use the two-band dispersion relation, specify the option `TwoBand` to `eBarrierTunneling` (see Table 238 on page 1439).

The options for `hBarrierTunneling` and the expressions for the conduction band to valence band tunneling current density j_{VC} are analogous.

Carrier Heating

In hydrodynamic simulations, carrier transport leads to energy transport and, therefore, to heating or cooling of electrons and holes. The energy transport has a convective and a Peltier part. By default, Sentaurus Device ignores the Peltier part. To include the Peltier terms for the tunneling particles, specify the option `PeltierHeat` to `eBarrierTunneling` or `hBarrierTunneling` (see Table 238 on page 1439).

The convective part of the heat generation in the conduction and valence bands at position u due to tunneling of carriers with energy ε to and from the ν-th shifted conduction band at $l < u$ is approximated as:

$$H_{\mathrm{conv,CC},\nu}(u, l, \varepsilon) = \frac{\delta}{2}[G_{\mathrm{CC},\nu}(u)kT_n(l) - R_{\mathrm{CC},\nu}(u)kT_n(u)] \tag{786}$$

and:

$$H_{\mathrm{conv,CV},\nu}(u, l, \varepsilon) = \frac{\delta}{2}[R_{\mathrm{CV},\nu}(u)kT_p(u) - G_{\mathrm{CV},\nu}(u)kT_n(l)] \tag{787}$$

By default, Sentaurus Device neglects Peltier heating and uses $\delta = 3$, which corresponds to the three degrees of freedom of the carriers. If Peltier heating is included in a simulation, the convective contribution due to one degree of freedom is already contained in the Peltier heating term. Therefore, in this case, Sentaurus Device uses $\delta = 2$. The convective parts of the heat generation in the conduction band at l, due to tunneling of carriers of energy ε from the conduction band and the valence band at $u > l$, are $-H_{\mathrm{conv,CC},\nu}(u, l, \varepsilon)$ and $-H_{\mathrm{conv,CV},\nu}(u, l, \varepsilon)$. The expressions for the convective part of the heat generation in the valence band are analogous.

If the computation of Peltier heating is activated (see Table 238 on page 1439), Sentaurus Device computes additional heating terms. The Peltier part of the heat generation in the electron system at point u due to tunneling to and from the ν-th shifted conduction band at point $l < u$ is:

$$H_{\mathrm{Pelt,CC},\nu}(u, l, \varepsilon) = [E_C(u^+) - \varepsilon][R_{\mathrm{CC},\nu}(u, l, \varepsilon) - G_{\mathrm{CC},\nu}(u, l, \varepsilon)] \tag{788}$$

where u^+ is infinitesimally larger than u. Eq. 788 vanishes everywhere except at abrupt jumps of the band edge. The Peltier part of the heat generation in the electron system at point l due to tunneling from the conduction band at $u > l$ obeys an equation similar to Eq. 788, with $E_C(u^+) - \varepsilon$ replaced by $\varepsilon - E_C(l^-)$.

When the `Band2Band` option is used (see Table 238 on page 1439), Sentaurus Device also takes into account the band-to-band terms of the Peltier part of the heat generation at point u:

$$H_{\text{Pelt,CV},\nu}(u, l, \varepsilon) = [E_V(u^+) - \varepsilon][R_{\text{CV},\nu}(u, l, \varepsilon) - G_{\text{CV},\nu}(u, l, \varepsilon)] \tag{789}$$

and, similarly, for the Peltier heat generation at point l.

The expressions for $H_{\text{Pelt,VV},\nu}$ and $H_{\text{Pelt,VC},\nu}$ are analogous to those for conduction band tunneling.

References

[1] A. Schenk and G. Heiser, "Modeling and simulation of tunneling through ultra-thin gate dielectrics," *Journal of Applied Physics*, vol. 81, no. 12, pp. 7900–7908, 1997.

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[3] F. Li *et al.*, "Compact Model of MOSFET Electron Tunneling Current Through Ultra-thin SiO2 and High-k Gate Stacks," in *Device Research Conference*, Salt Lake City, UT, USA, pp. 47–48, June 2003.

[4] L. F. Register, E. Rosenbaum, and K. Yang, "Analytic model for direct tunneling current in polycrystalline silicon-gate metal–oxide–semiconductor devices," *Applied Physics Letters*, vol. 74, no. 3, pp. 457–459, 1999.

CHAPTER 25 Hot-Carrier Injection Models

This chapter discusses the hot-carrier injection models used in Sentaurus Device.

Hot-carrier injection is a mechanism for gate leakage. The effect is especially important for write operations in EEPROMs. Sentaurus Device provides different built-in hot-carrier injection models and a PMI for user-defined models:

- Classical lucky electron injection (Maxwellian energy distribution)
- Fiegna's hot-carrier injection (non-Maxwellian energy distribution)
- SHE distribution hot-carrier injection (non-Maxwellian energy distribution calculated from the spherical harmonics expansion (SHE) of the Boltzmann transport equation)
- Hot-carrier injection PMI (see Hot-Carrier Injection on page 1230)

Overview

To activate the hot-carrier injection models for electrons (or holes), use the `eLucky` (`hLucky`), `eFiegna` (`hFiegna`), `eSHEDistribution` (`hSHEDistribution`), or `PMIModel_name(electron)` (`PMIModel_name(hole)`) options to the `GateCurrent` statement in an interface-specific `Physics` section.

To activate the models for both carrier types, use the `Lucky`, `Fiegna`, `SHEDistribution`, or `PMIModel_name()` options. The hot-carrier injection models can be combined with all tunneling models (see Chapter 24 on page 715).

> **NOTE** The SHE distribution hot-carrier injection model calculates the tunneling component together with the thermionic emission term. Therefore, combining it with other tunneling models can result in double-counting of the tunneling component.

The meaning of a specification in the global `Physics` section is the same as for the Fowler–Nordheim model (see Fowler–Nordheim Tunneling on page 716).

Destination of Injected Current

The destination of the injection current depends on the user selection and the material properties of the hot interface (interface source for hot carriers).

When the hot interface is a semiconductor–insulator interface, the injection current is sent nonlocally across the insulator region to an associated closest vertex. For each vertex of a hot interface, Sentaurus Device searches for an associated closest vertex located on a contact or semiconductor–insulator interface. The contacts or semiconductor–insulator interfaces used in the searching algorithm must be connected through adjacent insulator regions to the hot interface. Then, each vertex of the hot interface is associated with the closest vertex on a valid contact or semiconductor–insulator interface. Each vertex of the hot interface has either an associated contact vertex or an associated semiconductor–insulator interface vertex (see Figure 49).

Figure 49   Mapping of hot interface vertices to associated contact or
             semiconductor–insulator interface vertices

When the hot interface is an interface between a semiconductor and a wide-bandgap semiconductor, you can select the destination. By default, the wide-bandgap semiconductor is treated as an insulator region, and the injection current is sent nonlocally across the region to the associated closest vertex as described for semiconductor–insulator interfaces. By using `Thermionic(HCI)` in the `Physics` section of the hot interface and specifying the injection region destination (the wide-bandgap semiconductor region) using the `InjectionRegion` option in the `GateCurrent` section, the points on the hot interface are made double-points and the injection current is injected locally in the same location where it was produced. The injected current on the wide-bandgap semiconductor side of the hot interface becomes the current boundary condition for the continuity equations solved in the region.

In the case where hot carriers are injected into semiconductor floating regions during transient simulations, the way the charge is added to the floating region is determined by the existence of a charge boundary condition (a region with a charge contact) associated with the region. If the charge boundary condition has been specified for a semiconductor floating region, the charge is added as a total charge update, using the integral boundary condition as defined by

Eq. 135, p. 224. If the charge boundary condition is not specified for the semiconductor floating region, the charge is added as an interface boundary condition for continuity equations (see Carrier Injection With Explicitly Evaluated Boundary Conditions for Continuity Equations on page 759). The total hot-carrier injection current added to semiconductor floating regions where the charge boundary condition is specified will be displayed on the electrode associated with the region (floating contact).

Floating semiconductor regions with a charge boundary condition inside a wide-bandgap semiconductor region are made possible by generalizing the concept of a semiconductor floating well.

Sentaurus Device defines a *semiconductor floating well* as a continuous zone of the same doping semiconductor regions in contact with each other and marked in the command file by a charge contact connected to one of regions in the zone. The concept is generalized by treating the inner semiconductor region (embedded floating region) as a separate well. Geometrically, the charge contact is defined on the interface between the inner and outer semiconductor regions. You must indicate in the `Electrode` section of the charge contact using either the `Region` or `Material` keyword which region is to be used as the floating region with a charge boundary condition.

Equilibrium boundary conditions are imposed on the surface of the special floating region previously described. The interface between the inner and outer semiconductor regions is treated as a heterointerface. You must specify the keyword `Heterointerface` in the `Physics` section of the interface between the inner and outer regions. If the inner region is the floating region, the boundary condition for continuity equations at the interface between the two regions, on the outer-region side, will be equilibrium for carrier concentrations. The charge update for the inner floating region is computed as the total current flowing through the floating region boundary (integral of current density over the floating region surface) multiplied by the time step.

Equilibrium carrier concentrations in a point on the double-point interface, on the outer-region side, are computed based on the carrier concentration on the inner-region side of the interface adjusted by $(N_{C,V}^{WB}/N_{C,V}^{FG})\exp(-\delta E_{C,V}/kT)$ where $\delta E_{C,V}$ is the jump in the conduction band for electrons or in the valence band for holes, and $N_{C,V}^{WB}/N_{C,V}^{FG}$ is the ratio between density-of-states in the two regions for electrons and holes, respectively. For example, to have a `PolySi` nanocrystal floating region with a charge boundary condition embedded in an outer `OxideAsSemiconductor` region, with the charge contact `"fg1"` geometrically somewhere on the interface between the two regions, you must specify:

```
Electrode {
    ...
    {Name "fg1" Charge= -1e-18 Material="PolySi"}
    ...
}
```

```
Physics(MaterialInterface="OxideAsSemiconductor/PolySi") {
   Heterointerface                                # required by GeneralizedFG
}
```

Metal floating gates inside a wide-bandgap semiconductor region are allowed as well. In this case, equilibrium boundary conditions are imposed for the carrier densities at the interface between the semiconductor and the metal floating gate (on metal floating contact). Electrostatic potential at the metal floating contact is determined by the charge on the metal floating gate according to Eq. 133, p. 223. The equilibrium quasi-Fermi potential on the metal floating contact is given by $\Phi = \Phi_n = \Phi_p = \phi + \phi_{MS}$, where ϕ_{MS} is the workfunction difference between the metal and the semiconductor. Carrier densities at the metal floating contact are determined then by ϕ_{MS}. The charge update for the metal floating gate is computed as the total current flowing through the metal floating region contact multiplied by the time step.

To activate this special case of the metal floating gate, you specify the `Metal` keyword in the `Electrode` section of the metal floating contact and give the value of the workfunction (which determines ϕ_{MS}):

```
Electrode {
   ...
   {Name "fg1" Charge=0 Metal Workfunction=4.1}
   ...
}
```

The workfunction can be used as a calibration parameter.

For simple one-gate devices where the sole purpose is to evaluate the hot-carrier current injected across the oxide layer into a semiconductor region, the keyword `GateName` must be specified in the `GateCurrent` statement. In this case, the hot-carrier current is displayed on the electrode specified by `GateName` for both quasistationary and transient simulations.

Injection Barrier and Image Potential

All hot-carrier injection models are implemented as a postprocessing computation after each Sentaurus Device simulation point. The lucky electron model and Fiegna model specify some properties of semiconductor–insulator interfaces. The most important parameter is the height of the Si–SiO$_2$ barrier (E_B).

The height is a function of the insulator field F_{ins} and, at any point along the interface, it can be written as:

$$E_B = \begin{cases} E_{B0} - \alpha q|F_{ins}|^{\frac{1}{2}} - \beta q|F_{ins}|^{\frac{2}{3}} - P_\perp V_{sem} & F_{ins} < 0 \\ \\ E_{B0} - \alpha q|F_{ins}|^{\frac{1}{2}} - \beta q|F_{ins}|^{\frac{2}{3}} - P_\perp V_{sem} + V_{ins} & F_{ins} > 0 \end{cases} \tag{790}$$

where E_{B0} is the zero field barrier height at the semiconductor–insulator interface. The second term in the equation represents barrier lowering due to the image potential. The third term of the barrier lowering is due to the tunneling processes. For the Si–SiO$_2$ interface, $\alpha = 2.59{\times}10^{-4} V^{1/2} cm^{1/2}$. There is a large deviation in the literature for the value of β, so it can be considered a fitting parameter. The fourth term $P_\perp V_{sem}$ appears only in the lucky electron model where $P_\perp$ is a model parameter ($P_\perp = 1$ by default), and V_{sem} represents the kinetic energy gain when carriers travel a distance y to the interface without losing any energy. In the Fiegna model, V_{sem} is zero.

The insulator field F_{ins} is defined as:

$$F_{ins} = \vec{F}_{ins} \cdot \hat{n} \left[1 - P_{total} + P_{total} \frac{|\vec{F}_{ins}|}{|\vec{F}_{ins} \cdot \hat{n}|} \right] \tag{791}$$

where $\hat{n}$ is a normal vector along the direction of hot-carrier injection, and P_{total} is a model parameter ($P_{total} = 0$ by default).

In addition, all hot-carrier models contain a probability P_{ins} of scattering in the image-force potential well:

$$P_{ins} = \begin{cases} \exp\left(-\dfrac{x_0}{\lambda_{ins}}\right) & F_{ins} < 0 \\ \\ \exp\left(-\dfrac{t_{ins} - x_0}{\lambda_{ins}}\right) P_{repel} & F_{ins} > 0 \end{cases} \tag{792}$$

where λ_{ins} is the scattering mean free path in the insulator, t_{ins} is the distance between the vertex at the hot interface and the closest associated vertex, P_{repel} is a model parameter ($P_{repel} = 1$ by default), and the distance x_0 is given as:

$$x_0 = \min\left(\sqrt{\frac{q}{16\pi\tilde{\varepsilon}_{ins}|F_{ins}|}}, \frac{t_{ins}}{2} \right) \tag{793}$$

In the above expression, $\tilde{\varepsilon}_{ins} = \varepsilon_{ins}(\varepsilon_{sem} + \varepsilon_{ins})/(\varepsilon_{sem} - \varepsilon_{ins})$ is the effective dielectric constant of the insulator where ε_{sem} and ε_{ins} are the high-frequency dielectric constant of the semiconductor and insulator, respectively. In the lucky electron model and Fiegna model, ε_{ins}

is directly accessible from the parameter file. In the SHE distribution model, ε_{sem} and ε_{ins} are separately set from the parameter file.

Effective Field

The lucky electron model and Fiegna model have an effective electric field F_{eff} as a parameter. In Sentaurus Device, there are three possibilities to calculate the effective field:

- With the electric field parallel to the carrier flow (switched on by the keyword `Eparallel`, which is default for hot carrier currents). See Driving Force on page 426.

- With recomputation of the carrier temperature of the hydrodynamic simulation (switched on by the keyword `CarrierTempDrive`). See Avalanche Generation With Hydrodynamic Transport on page 427.

- With a simplified approach (compared to the second method): The drift-diffusion model is used for the device simulation, and carrier temperature is estimated as the solution of the simplified and linearized energy balance equation. As this is a postprocessing calculation, the keyword `CarrierTempPost` activates this option.

These keywords are parameters of the model keywords. For example, the lucky electron model looks like `eLucky(CarrierTempDrive)`. However, you must remember that if the model includes the keyword `CarrierTempDrive`, `Hydro` and a carrier temperature calculation must be specified in the `Physics` section.

Classical Lucky Electron Injection

The classical total lucky electron current from an interface to a gate contact can be written as [1]:

$$I_{\text{g}} = \iint J_n(x, y) P_{\text{s}} P_{\text{ins}} \left(\int_{E_{\text{B}}}^{\infty} P_{\varepsilon} P_{\text{r}} d\varepsilon \right) dx dy \tag{794}$$

where P_{s} is the probability that the electron will travel a distance y to the interface without losing any energy, $P_{\varepsilon} d\varepsilon$ is the probability that the electron has energy between ε and $\varepsilon + d\varepsilon$, P_{ins} is the probability of scattering in the image force potential well (Eq. 792), and P_{r} is the probability that the electron will be redirected. These probabilities are given by the expressions:

$$P_{\text{r}}(\varepsilon) = \frac{1}{2\lambda_{\text{r}}} \left(1 - \sqrt{\frac{E_{\text{B}}}{\varepsilon}} \right) \tag{795}$$

$$P_s(y) = \exp\left(-\frac{y}{\lambda}\right) \tag{796}$$

$$P_\varepsilon(\varepsilon) = \frac{1}{\lambda F_{\text{eff}}} \exp\left(-\frac{\varepsilon}{\lambda F_{\text{eff}}}\right) \tag{797}$$

where λ is the scattering mean free path in the semiconductor, λ_r is redirection mean free path, F_{eff} is the effective electric field, see Effective Field on page 742. E_B is the height of the semiconductor–insulator barrier.

The model coefficients can be changed in the parameter file in the section:

```
LuckyModel { ... }
```

Table 131   Coefficients and their default values for the lucky electron model

Symbol	Parameter name (Electrons)	Default value (Electrons)	Parameter name (Holes)	Default value (Holes)	Unit
λ	eLsem	8.9×10^{-7}	hLsem	1.0×10^{-7}	cm
λ_{ins}	eLins	3.2×10^{-7}	hLins	3.2×10^{-7}	cm
λ_r	eLsemR	6.2×10^{-6}	hLsemR	6.2×10^{-6}	cm
E_{B0}	eBar0	3.1	hBar0	4.7	eV
α	eBL12	2.6×10^{-4}	hBL12	2.6×10^{-4}	$(\text{V} \cdot \text{cm})^{1/2}$
β	eBL23	3.0×10^{-5}	hBL23	3.0×10^{-5}	$(\text{V} \cdot \text{cm}^2)^{1/3}$
ε_{ins}	eps_ins	3.1	eps_ins	3.1	1
$P_\perp$	Pvertical	1	Pvertical	1	1
P_{repel}	Prepel	1	Prepel	1	1
P_{total}	Ptotal	0	Ptotal	0	1

Fiegna Hot-Carrier Injection

The total hot-carrier injection current according to the Fiegna model [2] can be written as:

$$I_g = q \int P_{\text{ins}}\left(\int_{E_{B0}}^{\infty} v_\perp(\varepsilon) f(\varepsilon) g(\varepsilon) d\varepsilon\right) ds \tag{798}$$

where ε is the electron energy, E_{B0} is the height of the semiconductor–insulator barrier, $v_\perp$ is the velocity normal to the interface, $f(\varepsilon)$ is the electron energy distribution, $g(\varepsilon)$ is the

density-of-states of the electrons, P_{ins} is the probability of scattering in the image force potential well as described by Eq. 792, and $\int ds$ is an integral along the semiconductor–insulator interface.

The following expression for the electron energy distribution was proposed for a parabolic and an isotropic band structure, and equilibrium between lattice and electrons:

$$f(\varepsilon) = A \exp\left(-\chi \frac{\varepsilon^3}{F_{\text{eff}}^{1.5}}\right) \tag{799}$$

Therefore, the gate current can be rewritten as:

$$I_{\text{g}} = q\frac{A}{3\chi}\int P_{\text{ins}} n \frac{F_{\text{eff}}^{3/2}}{\sqrt{E_{\text{B}}}} e^{-\frac{\chi E_{\text{B}}^3}{F_{\text{eff}}^{3/2}}} ds \tag{800}$$

where F_{eff} is an effective field (see Effective Field on page 742).

Table 132 Coefficients and their default values for the Fiegna model

Symbol	Parameter name (Electrons)	Default value (Electrons)	Parameter name (Holes)	Default value (Holes)	Unit
A	eA	4.87×10^4	hA	4.87×10^4	cm/s/eV$^{2.5}$
χ	eChi	1.3×10^8	hChi	1.3×10^8	(V/cm/eV)$^{1.5}$
λ_{ins}	eLins	3.2×10^{-7}	hLins	3.2×10^{-7}	cm
E_{B0}	eBar0	3.1	hBar0	4.7	eV
α	eBL12	2.6×10^{-4}	hBL12	2.6×10^{-4}	$(\text{V} \cdot \text{cm})^{1/2}$
β	eBL23	1.5×10^{-5}	hBL23	1.5×10^{-5}	$(\text{V} \cdot \text{cm}^2)^{1/3}$
ε_{ins}	eps_ins	3.1	eps_ins	3.1	1
P_{repel}	Prepel	1	Prepel	1	1
P_{total}	Ptotal	0	Ptotal	0	1

The above coefficients can be changed in the parameter file in the `FiegnaModel` section.

SHE Distribution Hot-Carrier Injection

To obtain the hot-carrier injection current, accurate knowledge of the nonequilibrium electron-energy distribution is required. The spherical harmonics expansion (SHE) distribution hot-carrier injection model calculates the hot-carrier injection current using the nonequilibrium

energy distribution f obtained from the lowest-order SHE of the semiclassical Boltzmann transport equation (BTE) (see Spherical Harmonics Expansion Method on page 746).

The total hot-carrier injection current is obtained from [3]:

$$I_{\mathrm{g}} = \frac{2qAg_{\mathrm{v}}}{4} \int P_{\mathrm{ins}} \left[\int_0^\infty g(\varepsilon)v(\varepsilon)f(\varepsilon) \left(\int_0^1 \Gamma \left[\varepsilon - \frac{h^3 g(\varepsilon)v(\varepsilon)x}{8\pi m_{\mathrm{ins}}} \right] dx \right) d\varepsilon \right] ds \tag{801}$$

where:

- A is a dimensionless prefactor ($A = 1$ by default).
- g_{v} is the valley degeneracy factor.
- P_{ins} is the probability of electrons moving from the interface to the barrier peak without scattering (see Eq. 792, p. 741).
- g is the density-of-states per valley and per spin.
- v is the magnitude of the electron velocity.
- Γ is the transmission coefficient obtained from the WKB approximation including the image-potential barrier-lowering.
- m_{ins} is the insulator effective mass.
- $\int ds$ is an integral along the semiconductor–insulator interface.

The transmission coefficient can be written as:

$$\Gamma(\varepsilon_\perp) = \exp\left(-\frac{2}{\hbar} \int_0^{t_{\mathrm{ins}}} \sqrt{2m_{\mathrm{ins}}[E_{\mathrm{B}}(r) - \varepsilon_\perp]} \Theta[E_{\mathrm{B}}(r) - \varepsilon_\perp] dr \right) \tag{802}$$

$$E_{\mathrm{B}}(r) = E_{\mathrm{B0}} + qF_{\mathrm{ins}}r + E_{\mathrm{im}}(r) \tag{803}$$

$$E_{\mathrm{im}}(r) = -\frac{q^2}{16\pi\varepsilon_{\mathrm{ins}}} \sum_{n=0}^\infty \left(\frac{\varepsilon_{\mathrm{sem}} - \varepsilon_{\mathrm{ins}}}{\varepsilon_{\mathrm{sem}} + \varepsilon_{\mathrm{ins}}} \right)^{2n+1} \left[\frac{1}{nt_{\mathrm{ins}} + r} + \frac{1}{(n+1)t_{\mathrm{ins}} - r} - \frac{2}{(n+1)t_{\mathrm{ins}}} \left(\frac{\varepsilon_{\mathrm{sem}} - \varepsilon_{\mathrm{ins}}}{\varepsilon_{\mathrm{sem}} + \varepsilon_{\mathrm{ins}}} \right) \right] \tag{804}$$

where E_{B0} is the barrier height.

To use the SHE distribution hot-carrier injection model, you must obtain the distribution function by solving the SHE method (see Spherical Harmonics Expansion Method on page 746).

Eq. 804 represents the image-potential barrier-lowering. You can switch off the image-potential barrier-lowering using:

```
Physics(MaterialInterface="Silicon/Oxide") { ...
   GateCurrent( eSHEDistribution( -ImagePotential ) )
}
```

Spherical Harmonics Expansion Method

The spherical harmonics expansion (SHE) method computes the microscopic carrier energy distribution function $f(\vec{r}, \varepsilon)$ by solving the lowest-order SHE of the Boltzmann transport equation (BTE) [4]:

$$-\nabla \cdot \left[\frac{v^2(\vec{r}, \varepsilon_t)}{3} \tau(\vec{r}, \varepsilon_t) g(\vec{r}, \varepsilon_t) \nabla f(\vec{r}, \varepsilon_t) \right] = g(\vec{r}, \varepsilon_t) s(\vec{r}, \varepsilon_t) \tag{805}$$

where:

- f is the occupation probability of electrons (f can be larger than one as nondegenerate statistics is assumed).
- ε_t is the total energy including the conduction band energy E_C and the kinetic energy ε.
- v is the magnitude of the electron velocity.
- $1/\tau$ is the total scattering rate.
- g is the density-of-states per valley and per spin.
- s is the net in-scattering rate due to inelastic scattering and generation–recombination processes.

In Eq. 805, $g(\varepsilon)$ and $v(\varepsilon)$ can be obtained from the energy–wavevector dispersion relation, $\varepsilon_b(\vec{k})$, of semiconductors:

$$g_v g(\varepsilon) = g_v \sum_{b=1}^{N_b} g_b(\varepsilon) = \sum_{b=1}^{N_b} \int_\varepsilon \frac{1}{4\pi^2 h v_b(\vec{k})} ds_{\vec{k}} \tag{806}$$

$$g_v g(\varepsilon) v^2(\varepsilon) = g_v \sum_{b=1}^{N_b} g_b(\varepsilon) v_b^2(\varepsilon) = \sum_{b=1}^{N_b} \int_\varepsilon \frac{v_b(\vec{k})}{4\pi^2 h} ds_{\vec{k}} \tag{807}$$

where:

- $\varepsilon = \varepsilon_t - E_C(\vec{r})$ is the kinetic energy.
- g_v is the valley degeneracy.

- b is the band index.

- N_b is the number of bands.

- $v_b(\vec{k})$ is the magnitude of wavevector-dependent group velocity.

- h is Planck's constant.

- The integration is over the equienergy surface of the first Brillouin zone.

In addition, the energy-dependent square wavevector is defined as:

$$g_v k^2(\varepsilon) = g_v \sum_{b=1}^{N_b} k_b^2(\varepsilon) = \sum_{b=1}^{N_b} \int_\varepsilon \frac{1}{4\pi} ds_{\vec{k}} \tag{808}$$

These energy-dependent, band structure–related quantities can be obtained either from the precalculated band-structure file or from the single band, analytic, nonparabolic, band-structure model. For more information on the band-structure file, see Using Spherical Harmonics Expansion Method on page 750.

The analytic nonparabolic band-structure model gives [5]:

$$\frac{v^2(\varepsilon)}{3} = \frac{2\varepsilon(1 + \alpha\varepsilon)}{3m_c(1 + 2\alpha\varepsilon)^2} \tag{809}$$

$$g(\varepsilon) = \frac{2\pi(2m_n)^{3/2}}{h^3}[\varepsilon(1 + \alpha\varepsilon)]^{1/2}(1 + 2\alpha\varepsilon) \tag{810}$$

$$k^2(\varepsilon) = \pi h g(\varepsilon) v(\varepsilon) \tag{811}$$

where α is the nonparabolicity factor, m_c is the conductivity effective mass, and m_n is the density-of-states effective mass.

The total scattering rate and the net in-scattering rate can be written as:

$$\frac{1}{\tau(\varepsilon)} = \frac{1}{\tau_c(\varepsilon)} + \frac{1}{\tau_{ii}(\varepsilon)} + \frac{1}{\tau_{ac}(\varepsilon)} + \frac{1}{\tau_{ope}(\varepsilon)} + \frac{1}{\tau_{opa}(\varepsilon)} \tag{812}$$

$$s(\varepsilon) = \frac{f_{loc}(\varepsilon) - f(\varepsilon)}{\tau_{ii}(\varepsilon)} + \frac{f(\varepsilon - \varepsilon_{op})\exp\left(-\frac{\varepsilon_{op}}{kT}\right) - f(\varepsilon)}{\tau_{ope}(\varepsilon)} + \frac{f(\varepsilon + \varepsilon_{op})\exp\left(\frac{\varepsilon_{op}}{kT}\right) - f(\varepsilon)}{\tau_{opa}(\varepsilon)} - \frac{R_{net} f_{loc}(\varepsilon)}{n} \tag{813}$$

where:

- $1/\tau_c$ is the Coulomb scattering rate.

- $1/\tau_{ii}$ is the impact ionization scattering rate.

- $1/\tau_{ac}$ is the acoustic phonon scattering rate.
- $1/\tau_{ope}$ is the scattering rate due to optical phonon emissions.
- $1/\tau_{opa}$ is the scattering rate due to optical phonon absorptions.
- ε_{op} is the optical phonon energy.
- R_{net} is the net recombination rate.
- n is the electron density.
- $f_{loc} = \exp[(E_{F,n} - E_C - \varepsilon)/kT]$ is the local equilibrium distribution function.

The Coulomb scattering rate can be written as [6]:

$$\frac{1}{\tau_c(\varepsilon)} = \frac{q^4 \pi^2 g(\varepsilon) N_{i,\mathrm{eff}}}{2h\varepsilon_{\mathrm{sem}}^2 [k^2(\varepsilon) + k_0^2]^2} \left[\ln(1+b) - \frac{b}{1+b} \right] \tag{814}$$

$$b(\varepsilon) = \frac{4[k^2(\varepsilon) + k_0^2]kT\varepsilon_{\mathrm{sem}}}{q^2(n+p)} \tag{815}$$

$$N_{i,\mathrm{eff}} = \begin{cases} (N_D + N_A)\zeta_{\mathrm{major}}(N_{\mathrm{major}}) & N_{\mathrm{major}} > N_{\mathrm{minor}} \\ (N_D + N_A)\zeta_{\mathrm{minor}}(N_{\mathrm{minor}}) & N_{\mathrm{major}} < N_{\mathrm{minor}} \end{cases} \tag{816}$$

where:

- $\varepsilon_{\mathrm{sem}}$ is the dielectric constant of a semiconductor material.
- k_0^2 is an adjustable parameter that controls the energy dependency of the impurity scattering.
- N_{major} is N_D for electrons and N_A for holes.
- N_{minor} is N_A for electrons and N_D for holes.
- ζ_{major} and ζ_{minor} are tabulated fitting functions introduced to match the experimental low-field mobility curve as a function of majority and minority doping concentrations, respectively.

Two different expressions for the impact ionization scattering rate are available. The first expression can be written as [6]:

$$\frac{1}{\tau_{ii}(\varepsilon)} = \begin{cases} \left(\dfrac{\varepsilon - \varepsilon_{ii,1}}{1\ \mathrm{eV}}\right)^{v_{ii,1}} s_{ii,1} & \varepsilon_{ii,1} < \varepsilon < \varepsilon_{ii,3} \\ \left(\dfrac{\varepsilon - \varepsilon_{ii,2}}{1\ \mathrm{eV}}\right)^{v_{ii,2}} s_{ii,2} & \varepsilon > \varepsilon_{ii,3} \end{cases} \tag{817}$$

where:

- $s_{\text{ii},1}$ and $s_{\text{ii},2}$ are the impact ionization coefficients.
- $\nu_{\text{ii},1}$ and $\nu_{\text{ii},2}$ are the exponents.
- $\varepsilon_{\text{ii},1}$, $\varepsilon_{\text{ii},2}$, and $\varepsilon_{\text{ii},3}$ are the reference energies.

The second expression can be written as [7]:

$$\frac{1}{\tau_{\text{ii}}(\varepsilon)} = \sum_{j=1}^{3} \left(\frac{\varepsilon - \varepsilon_{\text{ii},j}}{1\text{ eV}}\right)^{\nu_{\text{ii},j}} \Theta(\varepsilon - \varepsilon_{\text{ii},j}) s_{\text{ii},j} \tag{818}$$

Specifying `ii_formula=1` in the `SHEDistribution` parameter set activates the first expression; while `ii_formula=2` activates the second expression. The impact ionization model parameters for electrons and holes are obtained from [6] and [8], respectively.

The acoustic-phonon and optical-phonon scattering rates can be written as [5][6]:

$$\frac{g(\varepsilon)}{\tau_{\text{ac}}(\varepsilon)} = \sum_{i=1}^{N_{\text{b}}} \sum_{j=1}^{N_{\text{b}}} \frac{4\pi^2 kT D_{\text{ac},ij}^2}{h\rho c_{\text{L}}^2} g_i(\varepsilon) g_j(\varepsilon) \tag{819}$$

$$\frac{g(\varepsilon)}{\tau_{\text{ope}}(\varepsilon)} = \sum_{i=1}^{N_{\text{b}}} \sum_{j=1}^{N_{\text{b}}} \frac{h D_{\text{op},ij}^2}{2\rho\varepsilon_{\text{op}}} (N_{\text{op}} + 1) g_i(\varepsilon) g_j(\varepsilon - \varepsilon_{\text{op}}) \tag{820}$$

$$\frac{g(\varepsilon)}{\tau_{\text{opa}}(\varepsilon)} = \sum_{i=1}^{N_{\text{b}}} \sum_{j=1}^{N_{\text{b}}} \frac{h D_{\text{op},ij}^2}{2\rho\varepsilon_{\text{op}}} N_{\text{op}} g_i(\varepsilon) g_j(\varepsilon + \varepsilon_{\text{op}}) \tag{821}$$

where:

- i and j are the band indices.
- $D_{\text{ac},ij}$ and $D_{\text{op},ij}$ are the deformation potentials for acoustic and g-type optical phonons, respectively ($D_{\text{ac},ij} = D_{\text{ac},ji}$ and $D_{\text{op},ij} = D_{\text{op},ji}$).
- ρ is the mass density.
- c_{L} is the sound velocity.
- $N_{\text{op}} = [\exp(\varepsilon_{\text{op}}/kT) - 1]^{-1}$ is the phonon number.

If $D_{\text{ac},ij} = D_{\text{ac}}$ and $D_{\text{op},ij} = D_{\text{op}}$ regardless of the band indices, Eq. 819, Eq. 820, and Eq. 821 can be simplified to:

$$\frac{1}{\tau_{\text{ac}}(\varepsilon)} = \frac{4\pi^2 kT D_{\text{ac}}^2}{h\rho c_{\text{L}}^2} g(\varepsilon) \tag{822}$$

$$\frac{1}{\tau_{\text{ope}}(\varepsilon)} = \frac{hD_{\text{op}}^2}{2\rho\varepsilon_{\text{op}}}(N_{\text{op}} + 1)g(\varepsilon - \varepsilon_{\text{op}}) \tag{823}$$

$$\frac{1}{\tau_{\text{opa}}(\varepsilon)} = \frac{hD_{\text{op}}^2}{2\rho\varepsilon_{\text{op}}}N_{\text{op}}g(\varepsilon + \varepsilon_{\text{op}}) \tag{824}$$

Dirichlet boundary condition as $f(\varepsilon) = \exp[(E_{\text{F},n} - E_{\text{C}} - \varepsilon)/kT]$ is assumed for electrodes.

Boundary conditions for abrupt heterointerfaces are similar to the corresponding boundary conditions for the thermionic emission model. Assume that at the heterointerface between materials 1 and 2, the conduction band edge jump is positive ($\Delta E_{\text{C}} = E_{\text{C},2} - E_{\text{C},1} > 0$). If $J_{n,2}(\varepsilon)$ and $J_{n,1}(\varepsilon)$ are the energy-dependent electron current density per spin and per valley entering material 2 and leaving material 1, the interface condition can be written as:

$$J_{n,2}(\varepsilon) = J_{n,1}(\varepsilon) \tag{825}$$

$$J_{n,2}(\varepsilon) = \frac{q}{4}g_2(\varepsilon)v_2(\varepsilon)[f_2(\varepsilon) - f_1(\varepsilon)] \tag{826}$$

where $g_i(\varepsilon)$, $v_i(\varepsilon)$, and $f_i(\varepsilon)$ are the density-of-states, the group velocity, and the occupation probability of material i, respectively.

All other boundaries are treated with reflective boundary conditions.

Using Spherical Harmonics Expansion Method

The electron-energy distribution function is calculated from Eq. 805, p. 746 in the semiconductor regions specified by the global, region-specific, or material-specific `Physics` section:

```
Physics { eSHEDistribution( <arguments> ) ...}
```

By default, $g(\varepsilon)$, $v(\varepsilon)$, and $k^2(\varepsilon)$ are obtained from the analytic band model. These band structure–related quantities also can be obtained from the default electron-band file `eSHEBandSilicon.dat` in the directory `$STROOT/tcad/$STRELEASE/lib/sdevice/MaterialDB/she` by specifying the argument `FullBand`:

```
Physics { eSHEDistribution( FullBand ... ) ... }
```

The default electron-band file `eSHEBandSilicon.dat` contains the band-structure quantities obtained from the nonlocal empirical pseudopotential method for relaxed silicon.

Similarly, there is a default hole-band file `hSHEBandSilicon.dat` in the same directory.

NOTE   For silicon regions, it is recommended to use the `FullBand` option as the default model parameters are calibrated based on the full band structure. In addition, there is no performance penalty when using the `FullBand` option.

You also can specify your own band file as:

```
Physics { eSHEDistribution( FullBand = "filename" ... ) ... }
```

The band file is a plain text file composed of $1 + 3N_b$ columns of data where N_b is the number of bands ($1 \le N_b \le 4$). The first column represents the kinetic energy ε [eV]. The subsequent columns represent $g_v g_b(\varepsilon)$ [cm^{-3}eV^{-1}], $g_v g_b(\varepsilon) v_b^2(\varepsilon)$ [cm^{-1}s^{-2}eV^{-1}], and $g_v k_b^2(\varepsilon)$ [cm^{-2}] for band b ($1 \le b \le N_b$). The kinetic energy should start from zero, and the energy spacing between the neighbour rows should be uniform. Refer to `eSHEBandSilicon.dat` for more information.

When `FullBand` is specified for devices containing SiGe, the band-structure quantities for SiGe regions are taken from mole fraction–dependent files in the same directory where the silicon files are located. The band-structure data was obtained from the nonlocal empirical pseudopotential method for relaxed SiGe with mole-fraction values of 0.0, 0.1, 0.2, ..., 1.0:

- Electron files: `eSHEBandSiGeX0.0.dat, eSHEBandSiGeX0.1.dat, ...`
- Hole files: `hSHEBandSiGeX0.0.dat, hSHEBandSiGeX0.1.dat, ...`

Sentaurus Device automatically chooses the appropriate files based on the average x-mole fraction value in each SiGe region. Linear interpolation of band-structure quantities is used for intermediate x-mole fraction values.

NOTE   In the current release, the simulation of electrons in SiGe is deactivated.

NOTE   Model parameters in the `SHEDistribution` parameter set (see Table 133 on page 755) can be specified with mole-fraction dependency. As with data from the band-structure files, the average x-mole fraction value in each region is used to determine the parameter values.

Sentaurus Device provides a simplified SHE model based on the relaxation time approximation (RTA) for the hot-carrier injection current computation. Although the RTA is a poor approximation, the RTA can remove the energy coupling and reduce simulation time. You can activate the RTA mode as follows:

```
Physics { eSHEDistribution( RTA ... ) ... }
```

When the RTA mode is selected, the relaxation time is defined as:

$$\frac{1}{\tau_{\text{RTA}}(\varepsilon)} = \frac{v(\varepsilon)}{\lambda_{\text{sem}}} + \frac{1}{\tau_0} \tag{827}$$

where λ_{sem} and τ_0 are adjustable parameters representing a mean free path and relaxation time. In the RTA mode, Eq. 813 is replaced by:

$$s(\varepsilon) = \frac{f_{\text{loc}}(\varepsilon) - f(\varepsilon)}{\tau_{\text{RTA}}(\varepsilon)} \tag{828}$$

NOTE   In the RTA mode, you must specify `SHEIterations=1` together with `SHESOR` in the global `Math` section. The RTA mode should not be used for self-consistent computations as the carrier flux is not conserved.

In the SHE method, the low-field mobility is determined by the microscopic scattering rate:

$$\mu_{\text{low}} = \frac{q \int_0^\infty \tau(\varepsilon) g(\varepsilon) v^2(\varepsilon) \exp\left(-\frac{\varepsilon}{kT}\right) d\varepsilon}{3kT \int_0^\infty g(\varepsilon) \exp\left(-\frac{\varepsilon}{kT}\right) d\varepsilon} \tag{829}$$

The mobility obtained from Eq. 829 and that from the macroscopic mobility model specified in the `Physics` section generally differ. For example, Eq. 829 overestimates the low-field mobility in the inversion layer of MOSFETs as the scattering rate in Eq. 812, p. 747 does not account for the mobility degradation at interfaces. To resolve this inconsistency, the Coulomb scattering rate is adjusted locally to match the low-filed mobility obtained from the mobility model. This option is activated by default. To switch off this option, specify:

```
Physics { eSHEDistribution( -AdjustImpurityScattering ... ) ... }
```

Similarly, for the hole-energy distribution function, specify `hSHEDistribution` in the `Physics` section.

Eq. 805, p. 746 is a coupled energy-dependent conservation equation with diffusion and source terms. The number of unknown variables in the SHE method is much larger than that in the drift-diffusion model or hydrodynamic model because of the additional total energy coordinate.

By default, the blockwise successive over-relaxation (SOR) method is used to solve the equation iteratively where the SOR iteration is performed over different total energies. The linear solver for the block system, the number of SOR iterations, and the SOR parameter can be accessed by the keywords `SHEMethod`, `SHEIterations`, and `SHESORParameter` in the global `Math` section.

The default values are:

```
Math {
    SHEMethod=super
    SHEIterations=20
    SHESORParameter=1.1
}
```

Instead of using the blockwise SOR method, you also can solve Eq. 805, p. 746 for different energies simultaneously by switching off the keyword SHESOR in the global Math section. Although any matrix solver can be used, the iterative linear solver ILS is the only practical option to solve Eq. 805 because of the large matrix size.

The ILS default parameters in set=3 can be used for the SHE method. For example:

```
Math {
    -SHESOR
    SHEMethod=ILS(set = 3)
    ...
}
```

The ILS default parameters in set=3 are defined as:

```
set (3) {
    iterative (gmres(100), tolrel=1e-8, tolunprec=1e-4, tolabs=0, maxit=200);
    preconditioning (ilut(0.00011,-1));
    ordering ( symmetric=rcm, nonsymmetric=mpsilst );
    options ( compact=yes, verbose=0, refinebasis=0, refinescaling=none,
              refineresidual=0 );
};
```

The global Math section provides some parameters related to the energy grid specification. The minimum and the maximum of the total energy coordinate are defined as:

$$\varepsilon_{t,min} = \min[E_C(\vec{r})] \tag{830}$$

$$\varepsilon_{t,max} = \max[E_C(\vec{r})] + \varepsilon_{margin} \tag{831}$$

where ε_{margin} is an energy margin ($\varepsilon_{margin} = 1eV$ by default). The energy grid spacing is defined by the fraction of the phonon energy $\Delta\varepsilon_t = \varepsilon_{op}/N_{refine}$ where N_{refine} is a positive integer ($N_{refine} = 1$ by default).

The parameters ε_{margin} and N_{refine} can be set in the global Math section:

```
Math {
    SHETopMargin = 1.0  # e_margin [eV]
    SHERefinement = 1   # N_refine
```

```
   ...
}
```

While the total energy grid is used for the computation, a uniform kinetic energy grid is used for plotting. The maximum kinetic energy to be plotted can be specified by the keyword SHECutoff (5 eV by default) in the global Math section:

```
Math { SHECutoff = 5.0 ... }
```

By default, the carrier energy distribution is updated in the postprocessing computation after each Sentaurus Device simulation point. You can suppress or activate the postprocessing computation using the Set statement of the Solve section. For example:

```
Solve { ...
   Set ( eSHEDistribution (Frozen) )   # freeze the distribution function
   ...
   Set ( eSHEDistribution (-Frozen) )  # unfreeze the distribution function
   ...
}
```

As long as the distribution function is frozen, the distribution is unchanged during simulation.

Instead of the postprocessing computation, you also can obtain the self-consistent DC solution by using the Plugin statement. For example:

```
Solve { ...
   Plugin (iterations=100) { Poisson eSHEDistribution hole }
   ...
}
```

In the self-consistent mode, the carrier density and the terminal current are obtained directly from the SHE method. You also can include the quantum correction in the SHE method. For example:

```
Solve { ...
   Plugin { Coupled {Poisson eQuantumPotential} eSHEDistribution hole }
   ...
}
```

> **NOTE** In the self-consistent mode, you must specify the keyword DirectCurrent in the global Math section. In addition, you may need to increase SHERefinement to improve the resolution of the energy grid. The self-consistent mode does not support transient, AC, and noise analysis. In general, the lowest-order SHE method may not be sufficiently accurate to simulate nanoscale transistors as the contribution of higher-order terms increases with decreasing device length [9]. The convergence rate of the Plugin method can be very slow when large biases are applied.

For backward compatibility, the following pairs of keywords are recognized as synonyms in the command file:

- `SHEDistribution` and `TailDistribution`
- `eSHEDistribution` and `TaileDistribution`
- `hSHEDistribution` and `TailhDistribution`
- `SHEIterations` and `TailDistributionIterations`
- `SHEMethod` and `TailDistributionMethod`
- `SHESOR` and `TailDistributionSOR`
- `SHESORParameter` and `TailDistributionSORParameter`

In the PMI, you can read the distribution function, density-of-states, and group velocity obtained from the SHE method using the following read functions:

- `ReadeSHEDistribution`: Returns $f(\varepsilon)$ for electrons.
- `ReadeSHETotalDOS`: Returns $2g_{v}g(\varepsilon)$ for electrons.
- `ReadeSHETotalGSV`: Returns $2g_{v}g(\varepsilon)v^{2}(\varepsilon)$ for electrons.
- `ReadhSHEDistribution`: Returns $f(\varepsilon)$ for holes.
- `ReadhSHETotalDOS`: Returns $2g_{v}g(\varepsilon)$ for holes.
- `ReadhSHETotalGSV`: Returns $2g_{v}g(\varepsilon)v^{2}(\varepsilon)$ for holes.

For more information, see Chapter 38 on page 1043.

The parameters for the SHE method are available in the `SHEDistribution` parameter set. Table 133 lists the coefficients of models and their default values.

> **NOTE** The optical phonon energy ε_{op} is closely related to the energy grid spacing. Therefore, the same optical phonon energy must be used in the simulation domain.

Table 133   Default parameters for SHE distribution model

Symbol	Parameter name	Electrons	Holes	Unit
ρ	rho	2.329		g/cm^{3}
ε_{sem}	epsilon	11.7		ε_{0}
ε_{ins}	eps_ins	2.15		ε_{0}
m_{c}	m_s	0.26	0.26	m_{0}
m_{n}	m_dos	0.328	0.689	m_{0}
m_{ins}	m_ins	0.5	0.77	m_{0}
α	alpha	0.5	0.669	eV^{-1}

Table 133   Default parameters for SHE distribution model (Continued)

Symbol	Parameter name	Electrons	Holes	Unit
g_v	g	6	1	1
A	A	1	1	1
E_{B0}	E_barrier	3.1	4.73	eV
λ_{ins}	Lins	2.0×10^{-7}	2.0×10^{-7}	cm
λ_{sem}	Lsem	5.0×10^{-6}	1.0×10^{-6}	cm
τ_0	tau0	1.0×10^{-12}	1.0×10^{-12}	s
D_{ac}/c_L	Dac_cl	1.027×10^{-5}	6.29×10^{-6}	eVs/cm
D_{op}	Dop	1.25×10^{9}	8.7×10^{8}	eV/cm
ε_{op}	HbarOmega	0.06	0.0633	eV
k_0^2	swv0	0.0	0.0	cm^{-2}
	ii_formula1	1	1	
$s_{ii,1}$	ii_rate1	1.49×10^{11}	0.0	s^{-1}
$s_{ii,2}$	ii_rate2	1.13×10^{12}	1.14×10^{12}	s^{-1}
$s_{ii,3}$	ii_rate3	0.0	0.0	s^{-1}
$\varepsilon_{ii,1}$	ii_energy1	1.128	1.128	eV
$\varepsilon_{ii,2}$	ii_energy2	1.572	1.49	eV
$\varepsilon_{ii,3}$	ii_energy3	1.75	1.49	eV
$\nu_{ii,1}$	ii_exponent1	3.0	0.0	1
$\nu_{ii,2}$	ii_exponent2	2.0	3.4	1
$\nu_{ii,3}$	ii_exponent3	0.0	0.0	1

Table 134 on page 757 lists the coefficients and the default values of the tabulated doping-dependent fitting parameters ζ_{major} and ζ_{minor} for electrons and holes.

NOTE   By default, the fitting parameters ζ_{major} and ζ_{minor} are neglected as the impurity scattering rate is adjusted automatically according to the low-field mobility. You must switch off AdjustImpurityScattering to use these parameters.

Table 134   Default parameters for unitless doping-dependent functions ζ_{major} and ζ_{minor}

Doping	Parameter name (electrons)	ζ_{major} (electrons)	ζ_{minor} (electrons)	Parameter name (holes)	ζ_{major} (holes)	ζ_{minor} (holes)
$10^{15.00}/cm^3$	efit(0)	1.20698	2.63089	hfit(0)	2.36872	3.84998
$10^{15.25}/cm^3$	efit(1)	1.26585	2.61522	hfit(1)	2.47647	3.82989
$10^{15.50}/cm^3$	efit(2)	1.35031	2.62123	hfit(2)	2.65631	3.87730
$10^{15.75}/cm^3$	efit(3)	1.45972	2.64751	hfit(3)	2.91784	3.98847
$10^{16.00}/cm^3$	efit(4)	1.59727	2.68504	hfit(4)	3.28127	4.16424
$10^{16.25}/cm^3$	efit(5)	1.76810	2.73218	hfit(5)	3.77842	4.40187
$10^{16.50}/cm^3$	efit(6)	1.97625	2.77580	hfit(6)	4.44356	4.68485
$10^{16.75}/cm^3$	efit(7)	2.22278	2.80091	hfit(7)	5.29810	4.97515
$10^{17.00}/cm^3$	efit(8)	2.50474	2.79066	hfit(8)	6.33175	5.21189
$10^{17.25}/cm^3$	efit(9)	2.81348	2.72938	hfit(9)	7.48564	5.32107
$10^{17.50}/cm^3$	efit(10)	3.13088	2.60729	hfit(10)	8.64257	5.23752
$10^{17.75}/cm^3$	efit(11)	3.42620	2.42644	hfit(11)	9.62681	4.93200
$10^{18.00}/cm^3$	efit(12)	3.66329	2.20490	hfit(12)	10.2280	4.42987
$10^{18.25}/cm^3$	efit(13)	3.82090	1.97450	hfit(13)	10.2758	3.80695
$10^{18.50}/cm^3$	efit(14)	3.91451	1.77291	hfit(14)	9.74236	3.16136
$10^{18.75}/cm^3$	efit(15)	4.00744	1.63637	hfit(15)	8.78324	2.57856
$10^{19.00}/cm^3$	efit(16)	4.21180	1.59940	hfit(16)	7.66672	2.11166
$10^{19.25}/cm^3$	efit(17)	4.69302	1.70363	hfit(17)	6.65698	1.78292
$10^{19.50}/cm^3$	efit(18)	5.69842	2.01596	hfit(18)	5.94642	1.59808
$10^{19.75}/cm^3$	efit(19)	7.63117	2.65859	hfit(19)	5.66599	1.56334
$10^{20.00}/cm^3$	efit(20)	11.1923	3.85825	hfit(20)	5.94556	1.70207

Visualizing Spherical Harmonics Expansion Method

For plotting purposes, the SHE method provides several macroscopic variables that can be obtained from the energy distribution function:

$$n_{SHE} = 2g_v \int_0^\infty g(\varepsilon)f(\varepsilon)d\varepsilon \tag{832}$$

$$T_{n,\,\mathrm{SHE}} \;=\; \frac{2g_{\mathrm v}}{n_{\mathrm{SHE}}}\int_0^\infty \frac{2\varepsilon}{3k}g(\varepsilon)f(\varepsilon)d\varepsilon \tag{833}$$

$$G^{\mathrm{ii}}_{n,\,\mathrm{SHE}} \;=\; 2g_{\mathrm v}\int_0^\infty \frac{1}{\tau_{\mathrm{ii}}(\varepsilon)}g(\varepsilon)f(\varepsilon)d\varepsilon \tag{834}$$

$$\vec{J}_{n,\,\mathrm{SHE}} \;=\; \frac{2qg_{\mathrm v}}{3}\int_0^\infty g(\varepsilon)v^2(\varepsilon)\nabla f(\varepsilon)d\varepsilon \tag{835}$$

$$\vec{v}_{n,\,\mathrm{SHE}} \;=\; -\frac{\vec{J}_{n,\,\mathrm{SHE}}}{qn_{\mathrm{SHE}}} \tag{836}$$

where n_{SHE}, $T_{n,\,\mathrm{SHE}}$, $G^{\mathrm{ii}}_{n,\,\mathrm{SHE}}$, $\vec{J}_{n,\,\mathrm{SHE}}$, and $\vec{v}_{n,\,\mathrm{SHE}}$ are the electron density, the average energy, the avalanche generation rate, the current density, and the average velocity, respectively.

The corresponding keywords for plotting these macroscopic variables are:

```
Plot{
   eSHEDensity                 # electron density [/cm^3]
   eSHEEnergy                  # average electron energy [K]
   eSHEAvalancheGeneration     # electron avalanche generation rate [/cm^3s]
   eSHECurrentDensity/Vector   # electron current density [A/cm^2]
   eSHEVelocity/Vector         # electron average velocity [cm/s]
}
```

The corresponding keywords for holes are `hSHEDensity`, `hSHEEnergy`, `hSHEAvalancheGeneration`, `hSHECurrentDensity`, and `hSHEVelocity`.

To plot the position-dependent electron-energy distribution function f for each kinetic energy grid, specify `eSHEDistribution/SpecialVector` in the `Plot` section:

```
Plot{
   ...
   eSHEDistribution/SpecialVector
}
```

Similarly, for the hole-energy distribution function, specify `hSHEDistribution/SpecialVector`. The column i of the special vector represents the distribution function at $\varepsilon = (i+1)\Delta\varepsilon$. For example, `eSHEDistribution_C2` represents f at $\varepsilon = 3\Delta\varepsilon$.

In addition, Sentaurus Device allows you to plot the electron-energy distribution function versus kinetic energy at positions specified in the command file.

The plot file is a `.plt` file, and its name must be defined in the `File` section by the keyword `eSHEDistribution`:

```
File {
   ...
   eSHEDistribution = "edist"
}
```

Plotting is activated by including the `eSHEDistributionPlot` section (similar to the `CurrentPlot` section) in the command file with a set of coordinates of positions:

```
eSHEDistributionPlot {
   (-0.02 0) (0 0) (0.02 0)
   ...
}
```

For each position defined by its coordinates, Sentaurus Device determines the enclosing element and interpolates the distribution function using the data at the element vertices. Similarly, for the hole-energy distribution function, define `hSHEDistribution` in the `File` section and include the `hSHEDistributionPlot` section in the command file.

Carrier Injection With Explicitly Evaluated Boundary Conditions for Continuity Equations

Hot-carrier current can be added as an interface boundary condition for continuity equations in adjacent semiconductor regions. A typical structure (see Figure 50 on page 760) consists of sequences of semiconductor–insulator–semiconductor regions. Hot-carrier current produced at one semiconductor–insulator interface from the sequence is added to the second semiconductor–insulator interface, using the closest vertex algorithm described in Destination of Injected Current on page 738.

This feature is available only for transient simulations and is especially useful for writing and erasing memory cells.

At each time step after the solution is computed, the hot-carrier injection (HCI) currents are post-evaluated using the solution. For the next time step, the HCI currents are added using the current boundary condition for continuity equations in semiconductor regions, where carriers are injected, and then the whole carrier transport task is solved self-consistently.

The carriers leave the semiconductor region where they are produced and enter nonlocally into the semiconductor region where they are injected. To conserve current, injection current is subtracted from the former semiconductor region and added to the latter.

Figure 50   Injection of hot-carrier current in a MOSFET structure

By using this method, the solution is obtained self-consistently (with one time-step delay) even if there is no carrier transport through the insulator region.

The feature is activated automatically during a transient simulation when any of the hot-carrier injection models is activated in the `GateCurrent` section and the floating semiconductor region where the hot carriers are to be injected does not have a charge boundary condition specified. Specifying `GateName` in the `GateCurrent` section disables the feature.

In addition, hot-carrier injection and the currents of the Fowler–Nordheim tunneling model can be computed at semiconductor–oxide-as-semiconductor interfaces. This is an extension of the searching algorithm described in Destination of Injected Current on page 738. In this case, there is a semiconductor–semiconductor interface instead of semiconductor–insulator interface. To avoid ambiguity, one of the interface regions must be selected as an insulator using the keyword `InjectionRegion`:

```
Physics(RegionInterface="Region_sem12/Region_sem2") {
   GateCurrent(Fowler eLucky InjectionRegion="Region_sem2")
}
```

References

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[7]   E. Cartier *et al.*, "Impact ionization in silicon," *Applied Physics Letters*, vol. 62, no. 25, pp. 3339–3341, 1993.

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CHAPTER 26 Heterostructure Device Simulation

This chapter describes carrier transport boundary conditions for heterointerfaces.

Thermionic Emission Current

Conventional transport equations cease to be valid at a heterojunction interface, and currents and energy fluxes at the abrupt interface between two materials are better defined by the interface condition at the heterojunction. In defining thermionic current and thermionic energy flux, Sentaurus Device follows the literature [1].

Using Thermionic Emission Current

To activate the thermionic current model for electrons at a region-interface (material-interface) heterojunction, the keyword `eThermionic` must be specified in the appropriate region-interface (material-interface) `Physics` section, for example:

```
Physics(MaterialInterface="GaAs/AlGaAs") {
   eThermionic
}
```

Similarly, to activate thermionic current for holes, the keyword `hThermionic` must be specified. The keyword `Thermionic` activates the thermionic emission model for both electrons and holes. If any of these keywords is specified in the `Physics` section for a region `Region.0`, where `Region.0` is a semiconductor, the appropriate model will be applied to each `Region.0`–semiconductor interface.

For small particle and energy fluxes across the interface, the condition of continuous quasi-Fermi level and carrier temperature is sometimes used. This option is activated by the keyword `Heterointerface` in the appropriate `Physics` section. In realistic transistors, such an approach may lead to unsatisfactory results [2].

You can change the coefficients of the thermionic emission model in the `ThermionicEmission` parameter set in an interface-specific section in the parameter file:

```
RegionInterface = "regionA/regionB" {
   ThermionicEmission {
      A = 2, 2   # [1]
      B = 4, 4   # [1]
```

```
     C = 1, 1    # [1]
   }
 }
```

Thermionic Emission Model

Assume that at the heterointerface between materials 1 and 2, the conduction edge jump is positive, that is $\Delta E_C > 0$, where $\Delta E_C = E_{C,2} - E_{C,1}$ (that is, $\chi_1 > \chi_2$). If $J_{n,2}$ and $S_{n,2}$ are the electron current density and electron energy flux density entering material 2, and $J_{n,1}$ and $S_{n,1}$ are the electron current density and electron energy flux density leaving material 1, the interface condition can be written as:

$$J_{n,2} = J_{n,1} \tag{837}$$

$$J_{n,2} = a_n q \left[v_{n,2} n_2 - \frac{m_{n,2}}{m_{n,1}} v_{n,1} n_1 \exp\left(-\frac{\Delta E_C}{kT_{n,1}}\right) \right] \tag{838}$$

$$S_{n,2} = S_{n,1} + \frac{c_n}{q} J_{n,2} \Delta E_C \tag{839}$$

$$S_{n,2} = -b_n \left[v_{n,2} n_2 kT_{n,2} - \frac{m_{n,2}}{m_{n,1}} v_{n,1} n_1 kT_{n,1} \exp\left(-\frac{\Delta E_C}{kT_{n,1}}\right) \right] \tag{840}$$

where the 'emission velocities' are defined as:

$$v_{n,i} = \sqrt{\frac{kT_{n,i}}{2\pi m_{n,i}}} \tag{841}$$

and by default, the coefficients in the above equations are $a_n = 2$, $b_n = 4$, and $c_n = 1$, which corresponds to the literature [1]. Similar equations for the hole thermionic current and hole thermionic energy flux are presented below:

$$J_{p,2} = J_{p,1} \tag{842}$$

$$J_{p,2} = -a_p q \left[v_{p,2} p_2 - \frac{m_{p,2}}{m_{p,1}} v_{p,1} p_1 \exp\left(\frac{\Delta E_V}{kT_{p,1}}\right) \right] \tag{843}$$

$$S_{p,2} = S_{p,1} + \frac{c_p}{q} J_{p,2} \Delta E_V \tag{844}$$

$$S_{p,2} = -b_p \left[v_{p,2} p_2 kT_{p,2} - \frac{m_{p,2}}{m_{p,1}} v_{p,1} n_1 kT_{p,1} \exp\left(\frac{\Delta E_V}{kT_{p,1}}\right) \right] \tag{845}$$

$$v_{p,i} = \sqrt{\frac{kT_{p,i}}{2\pi m_{p,i}}} \tag{846}$$

An equivalent set of equations are used if Fermi carrier statistics is selected.

Thermionic Emission Model With Fermi Statistics

With Fermi statistics, the electron current density and the electron energy flux density are:

$$J_{n,2} = a_n q\left(v_{n,2} N_{C,2} \zeta_{n,2} - \frac{m_{n,2}}{m_{n,1}} v_{n,1} N_{C,1} \zeta_{n,1}\right) \tag{847}$$

$$S_{n,2} = -b_n\left(v_{n,2} k T_{n,2} N_{C,2} \zeta_{n,2} - \frac{m_{n,2}}{m_{n,1}} v_{n,1} k T_{n,1} N_{C,1} \zeta_{n,1}\right) \tag{848}$$

$$\zeta_{n,2} = \ln[1 + \exp(-\eta_{n,2})] + \eta_{n,2} \tag{849}$$

$$\zeta_{n,1} = \ln[1 + \exp(-\eta'_{n,1})] + \eta'_{n,1} \tag{850}$$

$$\eta'_{n,1} = \eta_{n,1} - \frac{\Delta E_C}{kT_{n,1}} \tag{851}$$

Here, η_n is given in Eq. 49, p. 177 and N_C is given in Eq. 182, p. 262. Similar equations apply to holes:

$$J_{p,2} = -a_p q\left(v_{p,2} N_{V,2} \zeta_{p,2} - \frac{m_{p,2}}{m_{p,1}} v_{p,1} N_{V,1} \zeta_{p,1}\right) \tag{852}$$

$$S_{p,2} = -b_p\left(v_{p,2} k T_{p,2} N_{V,2} \zeta_{p,2} - \frac{m_{p,2}}{m_{p,1}} v_{p,1} k T_{p,1} N_{V,1} \zeta_{p,1}\right) \tag{853}$$

$$\zeta_{p,2} = \ln[1 + \exp(-\eta_{p,2})] + \eta_{p,2} \tag{854}$$

$$\zeta_{p,1} = \ln[1 + \exp(-\eta'_{p,1})] + \eta'_{p,1} \tag{855}$$

$$\eta'_{p,1} = \eta_{p,1} + \frac{\Delta E_V}{kT_{p,1}} \tag{856}$$

Here, η_p is given in Eq. 50, p. 177 and N_V is given in Eq. 186, p. 263.

If Fermi statistics is used, this model can be activated by specifying `Formula=1` in the `ThermionicEmission` section of the parameter file:

```
ThermionicEmission {
    Formula=1
}
```

By default `Formula=0`, it activates the old model, where the Boltzmann-like thermionic emission equations similar to Eq. 837–Eq. 846 are used. This can lead to incorrect results in high carrier density. In this case, a warning message will be given.

> **NOTE** Always specify `Formula=1` when Fermi statistics is used. This option will become the default in later versions of Sentaurus Device. If Fermi statistics is not used, Eq. 837–Eq. 846 will be activated regardless of the `Formula` statement in the parameter file.

Gaussian Transport Across Organic Heterointerfaces

A thermionic-like current boundary condition has been introduced to correctly account for carrier transport across organic heterointerfaces. An organic heterointerface is defined in this context as an heterointerface with the Gaussian density-of-states (DOS) model (see Gaussian Density-of-States for Organic Semiconductors on page 264) activated in both regions that are adjacent to the heterointerface.

Using Gaussian Transport at Organic Heterointerfaces

The model is activated by switching to the Gaussian DOS model in both regions of the heterointerface that are meant to be organic:

```
Physics(Region="OrganicRegion_1") {
    EffectiveMass(GaussianDOS)
}
Physics(Region="OrganicRegion_2") {
    EffectiveMass(GaussianDOS)
}
```

and then specifying the keyword `Organic_Gaussian` as an option for the `Thermionic` model in the `Physics` section of the organic heterointerface:

```
Physics(RegionInterface="OrganicRegion_1/OrganicRegion_2") {
    Thermionic(Organic_Gaussian)
}
```

This syntax also automatically switches on the double points at the organic heterointerface.

The parameters $v_{n, \text{org}}$ and $v_{p, \text{org}}$ in Eq. 858 and Eq. 860, p. 767 can be adjusted in the `ThermionicEmission` section of the parameter file (their default values are 1×10^6 cm/s):

```
RegionInterface="OrganicRegion_1/OrganicRegion_2" {
   ThermionicEmission {
      vel_org = 1e7, 1e7   # [cm/s]
   }
}
```

Gaussian Transport at Organic Heterointerface Model

Assuming a positive conduction edge jump and a negative valence edge jump from material 1 to material 2, the boundary conditions at the organic heterointerface are given by:

$$J_{n, 2} = J_{n, 1} \tag{857}$$

$$J_{n, 2} = v_{n, \text{org}} q \left(n_2 - n_1 \exp \left(-\frac{\Delta E_C}{kT_{n, 1}} \right) \right) \tag{858}$$

$$J_{p, 2} = J_{p, 1} \tag{859}$$

$$J_{p, 2} = v_{p, \text{org}} q \left(p_2 - p_1 \exp \left(-\frac{\Delta E_V}{kT_{p, 1}} \right) \right) \tag{860}$$

where:

- $J_{n, 2}$ and $J_{n, 1}$ are the electron current densities entering material 2 and leaving material 1, respectively.

- $J_{p, 2}$ and $J_{p, 1}$ are the hole current densities leaving material 2 and entering material 1, respectively.

- $\Delta E_C = d_{C, 2} - d_{C, 1}$ where $d_{C, 2}$ and $d_{C, 1}$ are the distances of the Gaussian distribution peaks to the conduction band edges.

- $\Delta E_V = d_{V, 2} - d_{V, 1}$ where $d_{V, 2}$ and $d_{V, 1}$ are the distances of the Gaussian distribution peaks to the valence band edges.

References

[1]   D. Schroeder, *Modelling of Interface Carrier Transport for Device Simulation*, Wien: Springer, 1994.

[2]   K. Horio and H. Yanai, "Numerical Modeling of Heterojunctions Including the Thermionic Emission Mechanism at the Heterojunction Interface," *IEEE Transactions on Electron Devices*, vol. 37, no. 4, pp. 1093–1098, 1990.

CHAPTER 27 Energy-Dependent Parameters

This chapter describes extensions for the temperature-dependent models.

Overview

Sentaurus Device provides the possibility to specify some parameters as a ratio of two irrational polynomials. The general form of such ratio is written as:

$$G(w, s) = f \frac{\left(\left(\sum a_i w^{p_i}\right) + d_n s\right)^{g_n}}{\left(\left(\sum a_j w^{p_j}\right) + d_d s\right)^{g_d}} \tag{861}$$

where subscripts n and d corresponds to numerator and denominator, respectively; f is a factor, w is a primary variable, and s is an additional variable. It is possible to use Eq. 861 with different coefficients for different intervals k defined by the segment $[w_{k-1}^{\max}, w_k^{\max}]$. By default, it is assumed that only one interval $k = 0$ with the boundaries $[0, \infty]$ exists, and function G is constant, that is, $a_0 = 0$, $a_i = 0$, $p = d = 0$, $g = 1$. Factor f is defined accordingly for each model.

A simplified syntax is introduced to define the piecewise linear function G. The boundaries of the intervals and the value of factor must be specified, which means the value of G is at the right side of the interval. All other coefficients should not be specified to use this possibility. As there are some peculiarities in parameter specification and model activation, the specific models for which the approximation by Eq. 861 is supported are described here separately.

Energy-Dependent Energy Relaxation Time

For the specification of the energy relaxation time, the following modification of Eq. 861 is used:

$$\tau(w) = \tau_w^0 \frac{\left(\left(\sum a_i w^{p_i}\right)\right)^{g_n}}{\left(\left(\sum a_j w^{p_j}\right)\right)^{g_d}} \tag{862}$$

where $w = 1.5kT_n/q$ for electrons and $w = kT_p/q$ for holes. The factor f in Eq. 861 is defined by τ_w^0, which can be specified in the parameter file by the values `tau_w_ele` and `tau_w_hol`.

To activate the specification of the energy-dependent energy relaxation time, the parameter `Formula(tau_w_ele)` (or `Formula(tau_w_hol)` for holes) must be set to 2.

The following example shows the energy relaxation time section of the parameter file and provides a short description of the syntax:

```
EnergyRelaxationTime
{ *  Energy relaxation times in picoseconds
      tau_w_ele = 0.3   # [ps]
      tau_w_hol = 0.25  # [ps]
 * Below is the example of energy relaxation time approximation
 * by the ratio of two irrational polynomials.
 * If Wmax(interval-1) < Wc < Wmax(interval), then:
 * tau_w = (tau_w)*(Numerator^Gn)/(Denominator^Gd),
 * where (Numerator or Denominator)=SIGMA[A(i)(Wc^P(i))],
 * Wc=1.5(k*Tcar)/q (in eV).
 * By default: Wmin(0)=Wmax(-1)=0; Wmax(0)=infinity.
 * The option can be activated by specifying appropriate Formula equals 2
 *       Formula(tau_w_ele) = 2
 *       Formula(tau_w_hol) = 2
 *       Wmax(interval)_ele =
 *       tau_w_ele(interval) =
 *       Numerator(interval)_ele{
 *         A(0) =
 *         P(0) =
 *         A(1) =
 *         P(1) =
 *         D    =
 *         G    =
 *       }
 *       Denominator(interval)_ele{
 *         A(0) =
 *         P(0) =
 *         D    =
 *         G    =
 *       }
 *       Wmax(interval)_hol =
 *       tau_w_hol(interval) =
      tau_w_ele = 0.3   # [ps]
      tau_w_hol = 0.25  # [ps]

      Formula(tau_w_ele) = 2
      Numerator(0)_ele{
        A(0) = 0.048200
```

```
        P(0) = 0.00
        A(1) = 1.00
        P(1) = 3.500
        A(2) = 0.0500
        P(2) = 2.500
        A(3) = 0.0018100
        P(3) = 1.00
    }
    Denominator(0)_ele{
        A(0) = 0.048200
        P(0) = 0.00
        A(1) = 1.00
        P(1) = 3.500
        A(2) = 0.100
        P(2) = 2.500
    }
```

The following example shows a simplified syntax for piecewise linear specification of energy relaxation time:

```
EnergyRelaxationTime:
{ *  Energy relaxation times in picoseconds
     Formula(tau_w_ele) = 2
     tau_w_ele = 0.3        # [ps]

     Wmax(0)_ele = 0.5      # [eV]
     tau_w_ele(1) = 0.46    # [ps]

     Wmax(1)_ele = 1.0      # [eV]
     tau_w_ele(2) = 0.4     # [ps]

     Wmax(2)_ele = 2.0      # [eV]
     tau_w_ele(3) = 0.2     # [ps]

     tau_w_hol = 0.25       # [ps]
}
```

Spline Interpolation

Sentaurus Device also allows spline approximation of energy relaxation time over energy. In this case, the parameter `Formula(tau_w_ele)` for electron energy relaxation time (and similarly, parameter `Formula(tau_w_hol)` for hole energy relaxation time) must be equal to 3.

Inside the braces following the keyword `Spline(tau_w_ele)` (or `Spline(tau_w_hol)`), an energy [eV] and tau [ps] value pair must be specified in each line. For the values outside of the specified intervals, energy relaxation time is treated as a constant and equal to the closest boundary value.

The following example shows a spline approximation specification for energy-dependent energy relaxation time for electrons:

```
EnergyRelaxationTime {
   Formula(tau_w_ele) = 3
   Spline(tau_w_ele) {
      0.    0.3   # [eV] [ps]
      0.5   0.46  # [eV] [ps]
      1.    0.4   # [eV] [ps]
      2.    0.2   # [eV] [ps]
   }
}
```

NOTE   Energy relaxation times can be either energy-dependent or mole fraction–dependent (see Abrupt and Graded Heterojunctions on page 10), but not both.

Energy-Dependent Mobility

In addition to the existing energy-dependent mobility models (such as Caughey–Thomas, where the effective field is computed inside Sentaurus Device as a function of the carrier temperature), a more complex, user-supplied mobility model can be defined. For such specification of energy-dependent mobility, a modification to Eq. 861 is used:

$$\mu(\bar{w}, N_{\text{tot}}) = \mu_{\text{low}} \frac{\left(\left(\sum a_i \bar{w}^{p_i}\right) + d_n N_{\text{tot}}\right)^{g_n}}{\left(\left(\sum a_j \bar{w}^{p_j}\right) + d_d N_{\text{tot}}\right)^{g_d}} \tag{863}$$

where $\bar{w} = T_n/T$ for electrons or $\bar{w} = T_p/T$ for holes, and μ_{low} is the low field mobility.

To activate the model, `CarrierTemperatureDrivePolynomial`, the driving force keyword, must be specified as a parameter of the high-field saturation mobility model. Parameters of the polynomials must be defined in the `HydroHighFieldMobility` parameter set.

This example shows the output of the `HydroHighFieldMobility` section and the specification of coefficients:

```
HydroHighFieldDependence:
{ * Parameter specifications for the high field degradation in
  * some hydrodynamic models.
  * B) Approximation by the ratio of two irrational polynomials
  * (driving force 'CarrierTempDrivePolynomial'):
  * If Wmax(interval-1) < w < Wmax(interval), then:
  * mu_hf = mu*factor*(Numerator^Gn)/(Denominator^Gd),
  * where (Numerator or Denominator)={SIGMA[A(i)(w^P(i))]+D*Ni},
  * w=Tc/Tl; Ni(cm^-3) is total doping.
  * By default: Wmin(0)=Wmax(-1)=0; Wmax(0)=infinity.

  *      Wmax(interval)_ele =
  *      F(interval)_ele =
  *      Numerator(interval)_ele{
  *        A(0)   =
  *        P(0)   =
  *        A(1)   =
  *        P(1)   =
  *        D      =
  *        G      =
  *      }
  *      Denominator(interval)_ele{
  *        A(0)   =
  *        P(0)   =
  *        D      =
  *        G      =
  *      }
  *      F(interval)_hol =
  *      Wmax(interval)_hol =
       Denominator(0)_ele
{
         A(0)   = 0.3
         P(0)   = 0.0
         A(1)   = 1.0
         P(1)   = 2.
         A(2)   = 0.001
         P(2)   = 2.500
         D      = 3.00e-16
         G      = 0.2500
      }
}
```

Spline Interpolation

Instead of the rational polynomial in Eq. 863, a spline interpolation can be used as well. In this case, the option `CarrierTempDriveSpline` must be used for the high-field mobility model in the command file:

```
Physics {
   Mobility (
      HighFieldSaturation (CarrierTempDriveSpline)
   )
}
```

The energy-dependent mobility is computed as

$$\mu(\overline{w}) = \mu_{\text{low}} \cdot \text{spline}(\overline{w}) \tag{864}$$

where the function $\text{spline}(\overline{w})$ is defined by a sequence of value pairs in the parameter file:

```
HydroHighFieldDependence {
   Spline (electron) {
      0    1
      1    1
      2    2.5
      4    4
      10   5
   }

   Spline (hole) {
      0    1
      1    1
      2    0.75
      4    0.5
      10   0.2
   }
}
```

The given data points are interpolated by a cubic spline. Zero derivatives are imposed as boundary conditions at the end points. The spline function remains constant beyond the end points.

Energy-Dependent Peltier Coefficient

Sentaurus Device allows for the following modification of the expression of the energy flux equation:

$$\vec{S}_n = -\frac{5r_n}{2}\left(\frac{kT_n}{q}\vec{J}_n + f_n^{\text{hf}}\hat{\kappa}_n\frac{\partial(w_n\Pi_n)}{\partial w_n}\nabla T_n\right) \tag{865}$$

The standard expression corresponds to $\Pi_n = 1$. If $\Pi_n = 1 + P(\bar{w})$, then:

$$\frac{\partial(w_n\Pi_n)}{\partial w_n} = 1 + \bar{w}\frac{\partial P(\bar{w})C}{\partial\bar{w}} \tag{866}$$

Sentaurus Device allows you to specify the function Q:

$$Q(\bar{w}) = \bar{w}\frac{\partial P(\bar{w})}{\partial\bar{w}} \tag{867}$$

For the specification of Q, the following modification of Eq. 861 is used:

$$Q(\bar{w}) = f\frac{\left(\left(\sum a_i\bar{w}^{p_i}\right)\right)^{g_n}}{\left(\left(\sum a_j\bar{w}^{p_j}\right)\right)^{g_d}} \tag{868}$$

Coefficients must be specified in the `HeatFlux` parameter set, and the dependence can be activated by specifying a nonzero factor f.

For $\Pi_n = 1 + 1/(\sqrt{1 + \bar{w}^2})$, the result is $Q = 1/(\bar{w}^2 + 1)^{1.5}$. This is an example of the parameter file section for such a function Q_n:

```
HeatFlux
{ *  Heat flux factor (0 <= hf <= 1)
     hf_n = 1   # [1]
     hf_p = 1   # [1]
 * Coefficients can be defined also as:
 *      hf_new = hf*(1.+Delta(w))
 * where Delta(w) is the ratio of two irrational polynomials.
 * If Wmax(interval-1) < Wc < Wmax(interval), then:
 * Delta(w) = factor*(Numerator^Gn)/(Denominator^Gd),
 * where (Numerator or Denominator)=SIGMA[A(i)(w^P(i))], w=Tc/Tl
 * By default: Wmin(0)=Wmax(-1)=0; Wmax(0)=infinity.
 * Option can be activated by specifying nonzero 'factor'.
 *      Wmax(interval)_ele =
 *      F(interval)_ele = 1
 *      Numerator(interval)_ele{
```

```
*        A(0)   =
*        P(0)   =
*        A(1)   =
*        P(1)   =
*        G      =
*      }
*      Denominator(interval)_ele{
*        A(0)   =
*        P(0)   =
*        G      =
*      }
*      Wmax(interval)_hol =
*      F(interval)_hol = 1
     f(0)_ele = 1
     Denominator(0)_ele{
       A(0)   = 1.
       P(0)   = 0.
       A(1)   = 1.
       P(1)   = 2.
       G      = 1.5
     }
```

Spline Interpolation

Instead of the rational polynomial in Eq. 868, a spline interpolation can be used as well. The function $Q(\overline{w})$ is defined in the parameter file by a sequence of value pairs:

```
HeatFlux {
   hf_n = 1
   hf_p = 1

   Spline (electron) {
      0    1
      1    1
      2    2.5
      4    4
      10   5
   }

   Spline (hole) {
      0    1
      1    1
      2    0.75
      4    0.5
      10   0.2
   }
}
```

The given data points are interpolated by a cubic spline. Zero derivatives are imposed as boundary conditions at the end points. The spline function remains constant beyond the end points.

CHAPTER 28 Anisotropic Properties

This chapter discusses the anisotropic properties of semiconductor devices.

Overview

In general, all equations for semiconductor devices can be written in the following form:

$$-\nabla \cdot \vec{J} = R \tag{869}$$

Here, vector $\vec{J} = \hat{\mu}\vec{g}$ and the tensor coefficient $\hat{\mu} = \mu \cdot \hat{A}$, where μ is a scalar function, tensor $\hat{A}$ is a 3×3 (or 2×2, in two dimensions) symmetric matrix, and vector $\vec{g}$ is a first-order differential expression. In the isotropic case, tensor $\hat{A}$ is the unit matrix. In the common case, tensor $\hat{A}$ depends on the solution. Among the reasons why tensor $\hat{A}$ is a full matrix are the anisotropic properties of semiconductors (such as SiC) and the influence of mechanical stress (affects anisotropic mobility; see Chapter 31 on page 821).

Table 135 lists the anisotropic models for the tensor $\hat{\mu}$ that Sentaurus Device supports.

Table 135   Anisotropic models

Tensor coefficient	Equation or model
Mobility, $\hat{\mu}$	Continuity equation for electrons and holes
Electrical permittivity, $\hat{\varepsilon}$	Poisson equation
Thermal conductivity, $\hat{\kappa}$	Thermodynamics equation
Quantum potential parameter, $\hat{\alpha}$	Density gradient model

Sentaurus Device provides different anisotropic approximations for discretization for the Poisson, continuity, and thermodynamic equations, and for the density gradient model (see Anisotropic Approximations on page 780). Note that anisotropic properties may have not only factor $\hat{\mu}$, but also some generation–recombination models (see Anisotropic Avalanche Generation on page 791).

Anisotropic Approximations

Due to the difficulties of anisotropic simulation, Sentaurus Device offers different approximations:

- The accuracy of the default `AverageAniso` approximation depends on the Delaunay properties of the virtual mesh obtained after anisotropic transformation. If this mesh is Delaunay, the results are relatively accurate. Otherwise, the accuracy will degrade.

- `TensorGridAniso` is the most robust approximation but it has some accuracy issues for nonaxis-aligned meshes or if the anisotropy orientation does not coincide with the mesh orientation.

- The `AnisoSG` approximation gives the most accurate results and is independent of the mesh orientation. Convergence, however, may be worse than for `TensorGridAniso`, for example.

- The `StressSG` approximation gives the most accurate results and is independent of the mesh orientation. Convergence, however, may be worse than for `TensorGridAniso`.

AverageAniso

This is the default approximation and it uses a local (vertex-wise) linear transformation, which transforms an anisotropic problem to an isotropic one. After this, Sentaurus Device uses the `AverageBoxMethod` algorithm to compute control volumes and coefficients (see Chapter 37 on page 1011). The keyword `AverageAniso` in the `Math` section activates this algorithm. Due to the requirements of `AverageBoxMethod`, the `AverageAniso` option requires that either the input mesh consists of triangles only (tetrahedra in 3D) or the mesh is tensorial, with the main axes of this tensor mesh and the main axes of the anisotropy aligned to the simulation coordinate system.

TensorGridAniso

This approximation is simple and is correct only for tensor grids or grids close to tensor ones. The anisotropic effects are modeled using a tensor-grid approximation. The eigenvalues and eigenvectors of the tensor $\hat{A}$ are used as multiplication factors for the projections of the vector $\vec{g}$ on mesh edges. The following options in the `Math` section activate this algorithm:

```
Math {
    TensorGridAniso                # only for stress mobility
    TensorGridAniso(Piezo)         # stress task, same as above
    TensorGridAniso(Aniso)         # anisotropic models, see this chapter
    TensorGridAniso(Aniso Piezo)   # anisotropic models and stress mobility
}
```

AnisoSG

The anisotropic Scharfetter–Gummel (`AnisoSG`) approximation is available for the Poisson, continuity, and thermodynamics equations. If the anisotropic direction is inconsistent with the mesh, the `AverageAniso` and `TensorGridAniso` approximations may not be accurate enough (*mesh orientation effect*). The `AnisoSG` approximation has no dependency on mesh orientation. A description of this approximation for the continuity equation is provided here.

Traditionally, the Scharfetter–Gummel approximation is used for the continuity equation (see Chapter 37 on page 1011), where the argument of the Bernoulli function $x^* = (\vec{E^*}, \vec{l})$ is a projection of the effective field $\vec{E^*}$ on edge $\vec{l}$. If, for isotropic case, x^* depends on values at edge nodes only, for an anisotropic problem, it is necessary to compute vector $\vec{E^*}$ elementwise. This concept allowed to generalize the Scharfetter–Gummel approximation to the anisotropic case.

To activate the anisotropic Scharfetter–Gummel approximation, you must specify the keyword `AnisoSG` in the global `Math` section:

```
Math { AnisoSG }
```

The `AnisoSG` branch, if it converges, guarantees that concentrations remain positive. However, sometimes, there could be convergence problems. Switching off certain derivatives helps to mitigate this problem. These derivatives are switched off if the node concentration is below the `AnisoSG_DerivativeMinDen` value, which is $10\,[\mathrm{cm}^{-3}]$ by default. This value can be modified in the `Math` section:

```
Math {
   AnisoSG
   AnisoSG_DerivativeMinDen = 1e2  # [cm-3]
}
```

StressSG

The `StressSG` approximation is implemented for stress problems (it affects anisotropic mobility; see Chapter 31 on page 821). To activate this approximation, you must specify the `StressSG` keyword in the global `Math` section:

```
Math { StressSG }
```

Crystal and Simulation Coordinate Systems

Sentaurus Device uses two coordinate systems: the simulation system (mesh geometry) and the crystal system. Anisotropic material parameters are defined in the crystal system.

The x-axis and y-axis of the simulation coordinate system are defined in the parameter file:

```
LatticeParameters {
    X = (1, 0,  0)
    Y = (0, 0, -1)
}
```

The z-axis is computed as the outer vector product of the x-axis and y-axis. The simulation system is defined relative to the crystal system. If the keyword `CrystalAxis` is present, the crystal system is defined relative to the simulation system (see Using Stress and Strain on page 823).

In the above example, the x-axis of the simulation system coincides with the x-axis of the crystal system. The y-axis of the simulation system runs along the negative z-axis of the crystal system. This is a common definition for 2D simulations of `Piezoelectric_Polarization` (see Chapter 31 on page 821).

Instead of `LatticeParameters`, the keywords `Piezo` and `PiezoParameters` are recognized as well. By default, Sentaurus Device uses `X=(1,0,0)`, `Y=(0,1,0)`, and `Z=(0,0,1)`.

Cylindrical Symmetry

Sentaurus Device supports only anisotropy with cylindrical symmetry. This means matrix A can be written as:

$$A = Q \begin{bmatrix} e & & \\ & e & \\ & & e_a \end{bmatrix} Q^{\mathrm{T}} \text{ or } A = Q_{2:2} \begin{bmatrix} e & \\ & e_a \end{bmatrix} Q_{2:2}^{\mathrm{T}} \tag{870}$$

where e, e_a are eigenvalues of A, and Q is the 3×3 orthogonal matrix from eigenvectors of A:

$$Q = \begin{bmatrix} \vec{A}_x & \vec{A}_y & \vec{A}_z \end{bmatrix} \tag{871}$$

and the quantity $Q_{2:2}$ denotes the leading 2×2 submatrix of Q.

Anisotropic Direction

The vector $\vec{A}_z$ defines anisotropic direction. This direction may be defined in the `Aniso` section of the command file in crystal (default) or simulation system coordinates; the default value is the z-axis (the y-axis in the 2D case):

```
Physics {
   Aniso( direction = (1, 1, 0) ) # anisotropic direction in crystal system
   Aniso( direction(CrystalSystem) = (1, 1, 0) ) # same as above

   # anisotropic direction in simulation system coordinate
   Aniso(Mobility direction(SimulationSystem) = (0, 1, -1) )
}
```

The symbolic definition, such as `direction = zAxis` (`xAxis` or `yAxis`) is acceptable. This vector defines the anisotropic direction for all `Aniso` models (except for the density gradient model; see Anisotropic Directions for Density Gradient Model on page 784).

The next two examples are equivalent.

Example 1

```
Parameter file:
LatticeParameters {
     X = ( 0.8, 0.6, 0)
   Y = (-0.6, 0.8, 0)
}

Input command file:
Physics {
   Aniso(Poisson direction=(0.5, 0.5))
}
```

Example 2

```
Parameter file: default LatticeParameters, that is, X = (1, 0, 0) and Y = (0,
1, 0)

Input command file:
Physics {
   Aniso(Poisson direction=(0.7, 0.1))
}
```


Anisotropic Directions for Density Gradient Model

By default, the anisotropic direction of the density gradient model is the same as in all other models. However, the density gradient model can have other anisotropic directions; moreover, you can have three different axes of anisotropy.

Example 1

Global anisotropic models and density gradient model have different direction:

```
Physics {
   Aniso(
      # global anisotropic direction relative to crystal system
      Direction(CrystalSystem)=(0.6, 0.8) Poisson Temperature

      # aniso direction for DG model relative simulation system
      eQuantumPotential{ Direction(SimulationSystem)=(1,1,0) }
   )
}
```

Parameter file:

```
QuantumPotentialParameters {
   alpha[1] = 4 1  # aniso direction = (1, 1, 0) relative to simulation system
   alpha[2] = 1 1  # isotropic value
   alpha[3] = 1 1  # isotropic value, in 3D case alpha[3] = alpha[2]
}
```

Example 2

Anisotropic density gradient model has three anisotropic axes:

```
Aniso( eQuantumPotential(
   AnisoAxes(SimulationSystem) = {
      ( 0.6, 0.8, 0)
      (-0.8, 0.6, 0)
   }
))
```

Parameter file:

```
QuantumPotentialParameters {
   alpha[1] = 4 1  # aniso axis = ( 0.6, 0.8, 0)
   alpha[2] = 1 1  # aniso axis = (-0.8, 0.6, 0)
   alpha[3] = 2 1  # aniso axis = ( 0.0, 0.0, 1) this vector is computed
}
```

Orthogonal Matrix From Eigenvectors Q

If the anisotropic direction has the default value (z-axis in 3D or y-axis in 2D), then the matrix is:

$$Q = R^T, R = \left[\frac{\vec{X}}{\|\vec{X}\|} \quad \frac{\vec{Y}}{\|\vec{Y}\|} \quad \frac{\vec{Z}}{\|\vec{Z}\|} \right] \tag{872}$$

where $\vec{X}, \vec{Y}, \vec{Z}$ are defined in the `LatticeParameters` section.

If the anisotropic direction is a vector $\vec{A}_d = (x, y, z)$, then the matrix is:

$$Q = \left[\vec{A}_x \quad \vec{A}_y \quad \vec{A}_z \right], \vec{A}_z = R^T \cdot \vec{A}_d / \|\vec{A}_d\| \tag{873}$$

The vectors $\vec{A}_x, \vec{A}_y$ are computed by Sentaurus Device to ensure that the matrix Q is orthogonal.

Anisotropic Mobility

In some semiconductors, such as silicon carbide, the electrons and holes may exhibit different mobilities along different crystallographic axes.

Anisotropy Factor

In a 3D simulation, Sentaurus Device assumes that the electrons or holes exhibit a mobility μ along the x-axis and y-axis, and an anisotropic mobility μ_{aniso} along the z-axis. In a 2D simulation, the regular mobility μ is observed along the x-axis, and μ_{aniso} is observed along the y-axis. The anisotropy factor r is defined as the ratio:

$$r = \frac{\mu}{\mu_{aniso}} \tag{874}$$

Current Densities

In the isotropic case, the current densities can be expressed by:

$$\vec{J}_n = \mu_n \vec{g}_n \tag{875}$$

$$\vec{J}_p = \mu_p \vec{g}_p \tag{876}$$

where $\vec{g}_n$ and $\vec{g}_p$ are the *currents without mobilities*.

In the drift-diffusion model, you have:

$$\vec{g}_n = -nq\nabla\Phi_n \tag{877}$$

$$\vec{g}_p = -pq\nabla\Phi_p \tag{878}$$

as can be seen from Eq. 56 and Eq. 57, p. 183. For the thermodynamic model, Eq. 58 and Eq. 59, p. 183 imply that:

$$\vec{g}_n = -nq(\nabla\Phi_n + P_n\nabla T) \tag{879}$$

$$\vec{g}_p = -pq(\nabla\Phi_p + P_p\nabla T) \tag{880}$$

In the hydrodynamic case, you have:

$$\vec{g}_n = n\nabla E_C + kT_n\nabla n + f_n^{td}kn\nabla T_n - 1.5nkT_n\nabla\ln m_n \tag{881}$$

$$\vec{g}_p = p\nabla E_V - kT_p\nabla p - f_p^{td}kp\nabla T_p - 1.5pkT_p\nabla\ln m_p \tag{882}$$

according to Eq. 60 and Eq. 61, p. 184.

For anisotropic mobilities, Eq. 875 and Eq. 876 need to be rewritten as:

$$\vec{J}_n = \mu_n A_{r_n}\vec{g}_n \tag{883}$$

$$\vec{J}_p = \mu_p A_{r_p}\vec{g}_p \tag{884}$$

where r_n and r_p are the anisotropy factors for electrons and holes, respectively. If the crystal reference system coincides with the coordinate system of Sentaurus Device, the matrices A_r are given by:

$$A_r = \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1/r \end{bmatrix} \quad \text{or} \quad A_r = \begin{bmatrix} 1 & \\ & 1/r \end{bmatrix} \tag{885}$$

depending on the dimension of the problem.

In general, however, A_r needs to be written as:

$$A_r = Q\begin{bmatrix} 1 & & \\ & 1 & \\ & & 1/r \end{bmatrix}Q^T \quad \text{or} \quad A_r = Q_{2:2}\begin{bmatrix} 1 & \\ & 1/r \end{bmatrix}Q_{2:2}^T \tag{886}$$

where Q is defined in Eq. 870, p. 782 – Eq. 873, p. 785.

Driving Forces

In the isotropic case, the electric field parallel to the electron or hole current is given by (see Eq. 350, p. 370):

$$F_c = \frac{\vec{F}\cdot\vec{J}_c}{J_c} = \frac{\vec{F}\cdot\vec{g}_c}{g_c} \tag{887}$$

For anisotropic mobilities:

$$F_c = \frac{\vec{F} \cdot A\vec{g}_c}{|A\vec{g}_c|} \tag{888}$$

Similarly, the electric field perpendicular to the current, as given in Eq. 328, p. 355, needs to be rewritten as:

$$F_{c,\perp} = \sqrt{F^2 - \frac{(\vec{F} \cdot A\vec{g}_c)^2}{|A\vec{g}_c|^2}} \tag{889}$$

Eq. 352, p. 370 shows how the gradient of the Fermi potential Φ_c may be used as the driving force in high-field saturation models. Instead, for anisotropic mobilities, Sentaurus Device uses:

$$F_c = A\nabla\Phi_c \tag{890}$$

In the isotropic hydrodynamic Canali model, the driving force $\vec{F}_c$ satisfies:

$$\vec{F}_c \cdot \mu\vec{F}_c = \frac{w_c - w_0}{\tau_{ec}q} \tag{891}$$

as can be seen from Eq. 356, p. 372. To derive the appropriate expression in the anisotropic case, it is assumed that $\vec{F}_c$ operates parallel to the current, that is:

$$\vec{F}_c = F_c\hat{e}_c \tag{892}$$

where:

$$\hat{e}_c = \frac{A\vec{g}_c}{|A\vec{g}_c|} \tag{893}$$

is the direction of the electron or hole current.

Instead of Eq. 891, you now have:

$$\mu F_c^2(A\hat{e}_c) \cdot \hat{e}_c = \frac{w_c - w_0}{\tau_{ec}q} \tag{894}$$

or:

$$F_c = \sqrt{\frac{w_c - w_0}{\tau_{ec}q\mu A\hat{e}_c \cdot \hat{e}_c}} \tag{895}$$

Total Anisotropic Mobility

This is the simplest mode in Sentaurus Device. Only a total anisotropy factor r_e or r_h is specified in the command file:

```
Physics {
   Aniso(
      eMobilityFactor (Total) = re
      hMobilityFactor (Total) = rh
   )
}
```

Sentaurus Device computes the mobility μ for electrons or holes along the main crystallographic axis as usual. The mobility μ_{aniso} is then given by:

$$\mu_{aniso} = \frac{\mu}{r} \tag{896}$$

> **NOTE**　In this mode, Sentaurus Device does not update the driving forces as discussed in Driving Forces on page 787.

Self-Consistent Anisotropic Mobility

This is the most accurate, but also the most expensive, mode in Sentaurus Device. The electron and hole mobility models specified in the `Physics` section are evaluated separately for the major and minor crystallographic axes, but with different parameters for each axis. This option is activated in the `Physics` section for electron or hole mobilities as follows:

```
Physics {
   Aniso(
      eMobility
      hMobility
   )
}
```

To simplify matters, you can specify the following option to activate self-consistent, anisotropic, mobility calculations for both electrons and holes:

```
Physics {
   Aniso(
      Mobility
   )
}
```

Table 136 lists the mobility models that offer an anisotropic version.

Table 136   Anisotropic mobility models

Isotropic model	Anisotrophic model
ConstantMobility	ConstantMobility_aniso
DopingDependence	DopingDependence_aniso
EnormalDependence	EnormalDependence_aniso
HighFieldDependence	HighFieldDependence_aniso
UniBoDopingDependence	UniBoDopingDependence_aniso
UniBoEnormalDependence	UniBoEnormalDependence_aniso
UniBoHighFieldDependence	UniBoHighFieldDependence_aniso
HydroHighFieldDependence	HydroHighFieldDependence_aniso

The PMI also supports anisotropic mobility calculations. The constructors of the classes `PMI_DopingDepMobility`, `PMI_EnormalMobility`, and `PMI_HighFieldMobility` contain an additional flag to distinguish between the isotropic and anisotropic case (see Chapter 38 on page 1043).

For example, you can specify these parameters for the constant mobility model in the parameter file of Sentaurus Device:

```
ConstantMobility {
   mumax = 1.4170e+03, 4.7050e+02
   Exponent = 2.5, 2.2
}
```

The following parameters would then compute a reduced constant mobility along the anisotropic axis:

```
ConstantMobility_aniso {
   mumax = 1.0e+03, 4.0e+02
   Exponent = 2.5, 2.2
}
```

In each vertex, Sentaurus Device introduces the anisotropy factors r_e and r_h as two additional unknowns. For a given value of r, the driving forces F_c and $F_{c,\perp}$ are computed as discussed in Driving Forces on page 787, and the mobilities along the isotropic and anisotropic axes are obtained.

The equation for the unknown factor r is then given by:

$$r = \frac{\mu(r)}{\mu_{aniso}(r)} \tag{897}$$

This nonlinear equation is solved in each vertex for both electron and hole mobilities.

Plot Section

Table 137 lists the plot variables that may be useful for visualizing anisotropic mobility calculations.

Table 137   Plot variables for anisotropic mobility

Plot variable	Description
eMobility	Electron mobility along main axis
hMobility	Hole mobility along main axis
eMobilityAniso	Electron mobility along anisotropic axis
hMobilityAniso	Hole mobility along anisotropic axis
eMobilityAnisoFactor	Anisotropic factor for electrons
hMobilityAnisoFactor	Anisotropic factor for holes

Anisotropic Avalanche Generation

Sentaurus Device computes the avalanche generation according to Eq. 437, p. 413. In the isotropic case, the terms nv_n and pv_p can also be written, respectively, as:

$$nv_n = \mu_n \left| \vec{g}_n \right| \tag{898}$$

and:

$$pv_p = \mu_p \left| \vec{g}_p \right| \tag{899}$$

If anisotropic mobilities are switched on, Eq. 898 and Eq. 899 are replaced by:

$$nv_n = \mu_n \left| A_{r_n} \vec{g}_n \right| \tag{900}$$

and:

$$pv_p = \mu_p \left| A_{r_p} \vec{g}p \right| \tag{901}$$

NOTE Eq. 900 and Eq. 901 only apply to total direction–dependent and self-consistent mobility calculations. If the total anisotropic option (see Total Anisotropic Mobility on page 789) is selected, Eq. 898 and Eq. 899 are used.

Anisotropic avalanche calculations can be activated in the `Physics` section, independently for electrons and holes:

```
Physics {
   Aniso(
      eAvalanche
      hAvalanche
   )
}
```

The keyword `Avalanche` activates calculations of anisotropic avalanche for both electrons and holes:

```
Physics {
   Aniso(
      Avalanche
   )
}
```

In the anisotropic mode, different avalanche parameters can be specified along the isotropic and anisotropic axes. Table 138 shows the avalanche models that are supported.

Table 138   Anisotropic avalanche models

Isotropic model	Anisotrophic model
`vanOverstraetendeMan`	`vanOverstraetendeMan_aniso`
`Okuto`	`Okuto_aniso`

Sentaurus Device uses interpolation to compute avalanche parameters for an arbitrary direction of the current. Let $\hat{e}_c$ be the direction of the electron or hole current as defined in Eq. 893. In the crystal reference system, the current is given by:

$$\hat{e}'_c = Q^T \hat{e}_c = \begin{bmatrix} e'_x \\ e'_y \\ e'_z \end{bmatrix} \tag{902}$$

Sentaurus Device interpolates an avalanche parameter p depending on the direction of the current $\hat{e}_c$ according to:

$$p(\hat{e}'_c) = (e'^2_x + e'^2_y) \cdot p_{\text{isotropic}} + e'^2_z \cdot p_{\text{anisotropic}} \tag{903}$$

in a 3D simulation, and, in a 2D simulation:

$$p(\hat{e}'_c) = e'^2_x \cdot p_{\text{isotropic}} + e'^2_y \cdot p_{\text{anisotropic}} \tag{904}$$

The PMI also supports the calculation of anisotropic avalanche generation. The current without mobility $\vec{Ag}_c$ is passed as an input parameter, and it can be used by the PMI code to determine the model parameters depending on the direction of the current (see Avalanche Generation Model on page 1100).

> **NOTE**   The Hatakeyama avalanche model is another anisotropic avalanche model (see Hatakeyama Avalanche Model on page 423). However, it must not be used with an `Aniso(Avalanche)` specification.

Anisotropic Electrical Permittivity

The electrical permittivity ε in Eq. 37, p. 173 can have different values along different crystallographic axes. If the crystallographic axes coincide with the coordinate system of Sentaurus Device, the scalar ε is replaced by the matrix:

$$E = \begin{bmatrix} \varepsilon & & \\ & \varepsilon & \\ & & \varepsilon_{\text{aniso}} \end{bmatrix} \text{ or } E = \begin{bmatrix} \varepsilon & \\ & \varepsilon_{\text{aniso}} \end{bmatrix} \tag{905}$$

depending on the dimension of the problem. For general crystallographic axes, the matrix E is given by:

$$E = Q \begin{bmatrix} \varepsilon & & \\ & \varepsilon & \\ & & \varepsilon_{\text{aniso}} \end{bmatrix} Q^{\text{T}} \text{ or } E = Q_{2:2} \begin{bmatrix} \varepsilon & \\ & \varepsilon_{\text{aniso}} \end{bmatrix} Q^{\text{T}}_{2:2} \tag{906}$$

where Q is defined in Eq. 870, p. 782 – Eq. 873, p. 785.

Anisotropic electrical permittivity is switched on using the keyword `Poisson` in the `Physics` section of the command file (regionwise or materialwise specification is supported):

```
Physics (Material = "SiC"){
   Aniso (Poisson)
}
```

The model parameters for ε and ε_{aniso} can be specified in the parameter file. Table 139 lists the names of the corresponding models.

Table 139   Anisotropic electrical permittivity models

Isotropic model	Anisotrophic model
Epsilon	Epsilon_aniso

Different parameters can be specified for each region or each material. The following statement in the command file of Sentaurus Device can be used to plot the electrical permittivities:

```
Plot {
   DielectricConstant
   "DielectricConstantAniso"
}
```

Anisotropic Thermal Conductivity

The thermal conductivity κ in Eq. 68, p. 192 can have different values along different crystallographic axes. If the crystallographic axes coincide with the coordinate system of Sentaurus Device, the scalar κ is replaced by the matrix:

$$K = \begin{bmatrix} \kappa & & \\ & \kappa & \\ & & \kappa_{aniso} \end{bmatrix} \text{ or } K = \begin{bmatrix} \kappa & \\ & \kappa_{aniso} \end{bmatrix} \tag{907}$$

depending on the dimension of the problem.

For general crystallographic axes, the matrix K is given by:

$$K = Q \begin{bmatrix} \kappa & & \\ & \kappa & \\ & & \kappa_{aniso} \end{bmatrix} Q^{\mathrm{T}} \text{ or } K = Q_{2:2} \begin{bmatrix} \kappa & \\ & \kappa_{aniso} \end{bmatrix} Q_{2:2}^{\mathrm{T}} \tag{908}$$

where Q is defined in Eq. 870, p. 782 – Eq. 873, p. 785.

Anisotropic thermal conductivity is switched on using the keyword `Temperature` in the `Physics` section of the command file (regionwise or materialwise specification is supported):

```
Physics(Material = "SiC"){
   Aniso (Temperature)
}
```

The model parameters for κ and κ_{aniso} can be specified in the parameter file. Table 140 lists the names of the corresponding models.

Table 140   Anisotropic thermal conductivity models

Isotropic model	Anisotrophic model
Kappa	Kappa_aniso

Different parameters can be specified for each region or each material. The PMI can also be used to compute anisotropic thermal conductivities. The constructor of the class `PMI_ThermalConductivity` has an additional parameter to distinguish between the isotropic and anisotropic directions (see Thermal Conductivity on page 1167).

The following statement in the command file can be used to plot the thermal conductivities:

```
Plot {
   "ThermalConductivity"
   "ThermalConductivityAniso"
}
```

Anisotropic Density Gradient Model

The density gradient model provides support for anisotropic quantization. For more details, see Density Gradient Quantization Model on page 294 and Anisotropic Directions for Density Gradient Model on page 784.

CHAPTER 29 Ferroelectric Materials

This chapter explains how ferroelectric materials are treated in a simulation using Sentaurus Device.

In ferroelectric materials, the polarization $\vec{P}$ depends nonlinearly on the electric field $\vec{F}$. The polarization at a given time depends on the electric field at that time and the electric field at previous times. The history dependence leads to the well-known phenomenon of hysteresis, which is used in nonvolatile memory technology.

Using Ferroelectrics

Sentaurus Device implements a model for ferroelectrics that features minor loop nesting and memory wipeout. Figure 51 demonstrates these properties and Ferroelectrics Model on page 799 discusses them further.

Figure 51   Example polarization curve

To activate the model, specify the keyword `Polarization` in the `Physics` section of the command file. Use the optional parameter `Memory` to prescribe the maximum allowed nesting depth of minor loops. The smallest allowed value for `Memory` is 2; the default value is 10. If minor loop nesting becomes too deep, the nesting property of the minor loops can be lost. However, the polarization curve remains continuous.

The following example switches on the ferroelectric model in region `Region.17` and sets the size of the memory to 20 turning points for each element and each mesh axis:

```
Physics (region = "Region.17") {
   Polarization (Memory=20)
}
```

To obtain a plot of the polarization field, specify `Polarization/Vector` in the `Plot` section of the command file.

Sentaurus Device characterizes the static properties of a ferroelectric material by three parameters: the remanent polarization P_r, the saturation polarization P_s, and the coercive field F_c. The hysteresis curve in Figure 51 on page 797 illustrates these quantities. Furthermore, Sentaurus Device parameterizes the transient response of the ferroelectric material by the relaxation times τ_E and τ_P, and by a nonlinear coupling constant k_n (see Ferroelectrics Model on page 799).

Specify the values for these parameters in the `Polarization` parameter set, for example:

```
Polarization
{ * Remanent polarization P_r, saturation polarization P_s,
  * and coercive field F_c for x,y,z direction (crystal axes)
      P_r = (1.0000e-05, 1.0000e-05, 1.0000e-05) #[C/cm^2]
      P_s = (2.0000e-05, 2.0000e-05, 2.0000e-05) #[C/cm^2]
      F_c = (2.5000e+04, 2.5000e+04, 2.5000e+04) #[V/cm]
  * Relaxation time for the auxiliary field tau_E, relaxation
  * time for the polarization tau_P, nonlinear coupling kn.
      tau_E = (0.0000e+00, 0.0000e+00, 0.0000e+00) #[s]
      tau_P = (0.0000e+00, 0.0000e+00, 0.0000e+00) #[s]
      kn    = (0.0000e+00, 0.0000e+00, 0.0000e+00) #[cm*s/V]
}
```

The parameters in this example are the defaults for the material `InsulatorX`. For all other materials, all default values are zero. Each of the three numbers given for any of the parameters corresponds to the value for the respective coordinate axis of the mesh. If a `P_s` component is zero, the ferroelectric model is disabled along the corresponding direction. If a `P_s` component is nonzero, the respective `P_r` and `F_c` components must also be nonzero. Furthermore, the `P_r` component must be smaller than the `P_s` component. By default, the relaxation times are zero, which means that polarization follows the applied electric field instantaneously.

In devices with ferroelectric and semiconductor regions, it is sometimes difficult to obtain an initial solution of the Poisson equation. In many cases, the `LineSearchDamping` option can solve these problems. To use this option, start the simulation like:

```
coupled (LineSearchDamping=0.01) { Poisson }
```

See Damped Newton Iterations on page 139 for details about this parameter.

Ferroelectrics Model

The vector quantity $\vec{P}$ is split into its components along the main axes of the mesh coordinate system. This results in one to three scalar problems. Sentaurus Device handles each problem separately using the model from [1] with extensions for transient behavior [2].

First, Sentaurus Device computes an auxiliary field F_{aux} from the electric field F:

$$\frac{d}{dt}F_{\text{aux}}(t) = \frac{F(t) - F_{\text{aux}}(t)}{\tau_E} \tag{909}$$

Here, τ_E is a material-specific time constant. For $\tau_E = 0$ or for quasistationary simulations, $F_{\text{aux}} = F$.

From the auxiliary field, Sentaurus Device computes the auxiliary polarization P_{aux}. The auxiliary polarization P_{aux} is an algebraic function of the auxiliary field F_{aux}:

$$P_{\text{aux}} = c \cdot P_{\text{s}} \cdot \tanh(w \cdot (F_{\text{aux}} \pm F_{\text{c}})) + P_{\text{off}} \tag{910}$$

where P_{s} is the saturation polarization, F_{c} is the coercive field, and:

$$w = \frac{1}{2F_{\text{c}}}\ln\frac{P_{\text{s}} + P_{\text{r}}}{P_{\text{s}} - P_{\text{r}}} \tag{911}$$

where P_r is the remanent polarization. In Eq. 910, the plus sign applies to the decreasing auxiliary field and the minus sign applies to the increasing auxiliary field. The different signs reflect the hysteretic behavior of the material. P_{off} and c in Eq. 910 result from the polarization history of the material, see below.

Finally, from the auxiliary polarization and auxiliary field, Sentaurus Device computes the actual polarization P:

$$\frac{d}{dt}P(t) = \frac{P_{\text{aux}}[F_{\text{aux}}(t)] - P(t)}{\tau_P}\left(1 + k_{\text{n}}\left|\frac{d}{dt}F_{\text{aux}}(t)\right|\right) \tag{912}$$

Here, τ_P and k_{n} are material-specific constants. For $\tau_P = 0$ or for quasistationary simulations, $P = P_{\text{aux}}$.

Upper and lower turning points are points in the P_{aux}-F_{aux} diagram where the sweep direction of the auxiliary field F_{aux} changes from increasing to decreasing, and from decreasing to increasing, respectively. At each bias point, the most recent upper and lower turning points, (F_u, P_u) and (F_l, P_l), must both be on each of the two curves defined by Eq. 910; this requirement determines P_{off} and c.

Sentaurus Device 'memorizes' turning points as they are encountered during a simulation. The memory always contains (∞, P_s) as the oldest and $(-\infty, -P_s)$ as the second oldest turning point. By using Eq. 910, these two points define a pair of curves with $c = 1$ and $P_{off} = 0$; together, the two curves form the saturation loop. All other pairs of turning points result in $c < 1$ and define a pair of curves forming minor loops.

When the auxiliary field leaves the interval defined by F_l and F_u of the two newest turning points, these two turning points are removed from the memory; this reflects the memory wipeout observed in experiments. The pair of turning points that are newest in the memory, after this removal, determines the further $P_{aux}(F_{aux})$ relationship.

As the older of the dropped turning points was originally reached by walking on the curve defined by the turning points that now (after dropping) again determine $P_{aux}(F_{aux})$, the polarization curve remains continuous. For example, see points e, f, and i in Figure 51 on page 797. Furthermore, the minor loop defined by the two dropped turning points is nested inside the minor loop defined by the present turning points. The nesting of minor loops is also a feature known from experiments on ferroelectrics. Figure 51 illustrates this by the loops f-g and i-k, both of which are nested in loop e-h, which in turn is nested in loop c-d.

In small-signal (AC) analysis (see Small-Signal AC Analysis on page 96), a very small periodic signal is added to the DC bias. As a result, the (auxiliary) polarization at each point of the ferroelectric material changes along a very small minor loop nested in the main loop that stems from the DC variation of the bias voltage. The average slope of this minor loop is always smaller than the slope of the main loop at the point where the loops touch. Consequently, even at very low frequencies, the AC response of the system is different from what would be obtained by taking the derivative of the DC curves.

As an example of how the turning point memory works, see Figure 51. The points on the polarization curve are reached in the sequence a, b, c, d, e, f, g, f, h, i, k, i, e, c. For simplicity, a quasistationary process is assumed and, therefore, $F_{aux} = F$ and $P_{aux} = P$. Starting the simulation at point a, the newest point in memory is b (Sentaurus Device initializes it in this way). The second newest point is a negative saturation point (l), and the oldest point is a positive saturation point (u). This memory state is denoted by [blu]. For this state, a is on the decreasing field curve. The curve segment (that is, the coefficients c and P_{off}) from a to b is determined by the points l and b.

Ramping up from a makes a a turning point, so the memory becomes [ablu]. When crossing b and proceeding to c, a and b are dropped from the memory. Therefore, the memory becomes [lu]. These two points determine the curve from b to c. Turning at c, c is added to the memory, giving [clu]. From c to d, use c and l; at d, the memory becomes [dclu]; at point e, [edclu]; at f, [fedclu]; at g, [gfedclu]. Passing through f, the two newest points, f and g, are dropped and the memory is [edclu]; at h, [hedclu]; at i, [ihedclu]; at k, [kihedclu]. At i again, i and k are dropped, giving [hedclu]; at e, e and h are dropped, giving [dclu].

At the beginning of a simulation, the memory contains one turning point chosen such that the point $E_{aux} = 0$, $P_{aux} = 0$ is on the minor loop so defined (for example, point b in Figure 51 on page 797). The nature of the model is such that it is not possible to have a state of the system that is completely symmetric. In particular, even for a symmetric device and at the very beginning of the simulation, $P(E) \neq -P(-E)$. This asymmetry is most prominent for the virginal curves (for example, a-b in Figure 51) of the ferroelectric, which are different for different signs of voltage ramping.

Ginzburg–Landau Model

Under the correct conditions, ferroelectric material operates in a negative differential capacitance region, which results in an amplification effect of the gate bias. This effect can produce a body factor $m < 1$ that leads to $SS < 60\,\text{mV/dec}$. To model this effect, the standard approach is to use the Ginzburg–Landau equation [3]:

$$\rho \frac{dP}{dt} + \nabla_P U = 0 \tag{913}$$

where the free energy U of the ferroelectric is:

$$U = \alpha P^2 + \beta P^4 + \gamma P^6 - g|\nabla P|^2 - E \cdot P \tag{914}$$

With Eq. 913 and Eq. 914, you have the electric field–polarization relation:

$$E = 2\alpha P + 4\beta P^3 + 6\gamma P^5 - 2g\Delta P + \rho \frac{dP}{dt} \tag{915}$$

Here, E is the electric field in units of V/cm, and P is the polarization in units of C/cm^2. Parameters of the model are:

- α, β, and γ are ferroelectric material parameters typically extracted from measurements.
- ρ is the viscosity that represents the finite time required for the polarization to switch.
- g is the strength of the polarization gradient.

Table 141 Parameters and their default values for Ginzburg–Landau equation

Name	Description	Default value	Unit
alpha	α parameter	–4e9	cm/F
beta	β parameter	–5e16	cm^5/(FC^2)
gamma	γ parameter	5e25	cm^9/(FC^4)
rho	ρ viscosity	2.25e4	Ωcm

Table 141   Parameters and their default values for Ginzburg–Landau equation (Continued)

Name	Description	Default value	Unit
g	Gradient term	0	cm³/F
direction	Polarization direction	x	1

Using the Ginzburg–Landau Model

To activate the Ginzburg–Landau model, you must add the keyword `FEPolarization` to the global or regionwise `Physics` section in the input command file:

```
Physics (region = "FEregion1") {
   FEPolarization (
      direction=x alpha=-4e9 beta=-5e16 gamma=5e25 rho=2.25e4 g=0
   )
}
```

Here, `x` defines the switchable polarization component that is solved.

> **NOTE**   Polarization is solved only along the specified direction, which is the direction perpendicular to the gate, given the fact that the polarization vector can switch only along this direction. To solve tri-gate structures or FinFETs, you can define different ferroelectric regions and specify the proper direction in each region.

> **NOTE**   In Version N-2017.09, parameters of the ferroelectric polarization model are specified in the `Physics` section of the input file. In Version O-2018.06, ferroelectric parameter specifications will move into parameter files to allow for material-specific default settings and mole fraction dependency for composite materials.

The `g` term represents the extra energy for forming the polarization domain wall, which should be nonzero whenever polarization is not uniform. Typical values of `g` range from 10^{-6} to 10^{-2} cm³/F.

In the `Solve` section of the input file, you must add the ferroelectric equation as follows:

```
Solve{
   Coupled (Poisson Electron Hole FEPolarization...)
}
```

To simulate a ferroelectric using the Ginzburg–Landau model, it is suggested to use a `Transient` simulation that represents the physical process that finds the free energy minimum of the system. Convergence improves when the ferroelectric operates close to its critical field.

Even for `QuasiStationary` simulations, it is suggested to start with a `Transient` simulation with a very small bias ramp such that the system finds its initial stable state.

The following example ramps the voltage to 0.001 with a `Transient` simulation, such that it guarantees the ferroelectric system reaches its stable state, and then performs a `QuasiStationary` simulation:

```
Transient (
   MaxStep=1e-1 InitialStep=1e-2 MinStep=1e-3
   InitialTime=0 FinalTime=1e-4 Increment=1.2
   Goal { name=Top voltage=0.001 }
) { Coupled (Poisson Electron Hole FEPolarization) }

NewCurrentFilePrefix="quasi_"

QuasiStationary (
   MaxStep=0.01 InitialStep=0.002 MinStep=1e-4
   Goal { name=Top voltage=2 }
) { Coupled (Poisson Electron Hole FEPolarization) }
```

The polarization is stored in the dataset `FEPolarization`. To plot `FEPolarization`, specify:

```
Plot {
   FEPolarization
}
```

References

[1]   B. Jiang *et al.*, "Computationally Efficient Ferroelectric Capacitor Model for Circuit Simulation," in *Symposium on VLSI Technology*, Kyoto, Japan, pp. 141–142, June 1997.

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Ferromagnetism and Spin
Transport

This chapter introduces the physics of spin transfer torque (STT)
devices and describes the models used to simulate their behavior in
Sentaurus Device.

A Brief Introduction to Spintronics

Conventional semiconductor devices are based on charge transport. Electrons are treated as charged particles whose motion gives rise to current flow. In addition to their charge, electrons carry an intrinsic angular momentum called the electron *spin*. A charged particle with angular momentum acts as a magnetic dipole. In the absence of spatial ordering of the individual magnetic moments, their magnetic fields cancel out, and the effect of spin on electronic transport is small.

In ferromagnetic materials, however, the net magnetic moments of the inner electrons (typically, d- or f-orbitals) at neighboring lattice sites are aligned in parallel by the *exchange interaction*: Extended magnetic *domains* form, and the resulting magnetic field gives rise to a large difference in the energy of the state of conduction electrons depending on the relative orientation of magnetization and the spin direction.

The interaction between the spin of conduction electrons and the magnetization of ferromagnetic regions incorporated into the device structure gives rise to a whole class of *spintronics* devices. For example, the tunneling current between two ferromagnetic regions separated by a thin insulator becomes a function of the angle between the magnetization directions on either side of the barrier (the tunneling magnetoresistance effect). Conversely, the flow of spin-polarized electrons is accompanied by the transport of angular momentum (the spin current), and the absorption of spin current in a ferromagnetic region may change the magnetization direction (the spin transfer torque effect) [1].

The following sections describe models in Sentaurus Device for the modeling of spintronics devices, in particular, for spin-selective tunneling through magnetic tunnel junctions (MTJs) and for the magnetization dynamics in ferromagnetic regions.

A simulation example for magnetization switching in an MTJ is available from the Applications Library [2].

Transport Through Magnetic Tunnel Junctions

The magnetic direct tunneling model describes the charge and spin currents flowing through a thin barrier layer sandwiched between two ferromagnetic regions. In contrast to a nonmagnetic tunnel junction, the current across an MTJ depends on both the applied voltage across the junction and the magnetization direction on either side of the barrier. This effect is called *tunneling magnetoresistance*.

Magnetic Direct Tunneling Model

The magnetic direct tunneling model assumes the barrier layer to consist of a single material and treats the tunneling barrier as trapezoidal. Figure 52 shows a schematic band diagram of such an MTJ.

Figure 52   Schematic band diagram of an MTJ

The current and spin transmission amplitudes for the MTJ are obtained by solving the Schrödinger equation with open boundary conditions. This can be done by applying the formalism of the non-equilibrium Green's function (NEGF) [3][4]. However, for the situation shown in Figure 52, finding the numeric solution to the open boundary may be accelerated by an analytic ansatz: In the ferromagnetic regions (zero field), the spinor components of the wavefunction may be expressed as linear combinations of forward- and backward-propagating plane waves. In the barrier region (constant field), Airy functions (of the first and second kind) are used instead.

At the interfaces, continuity of probability density and conservation of probability density flux are enforced. The resulting model resembles the regular `DirectTunneling` model used in Sentaurus Device to study the gate leakage currents of transistors (see Direct Tunneling on

page 718). However, instead of scalar wavefunctions, spinors are used to handle the spin degree of freedom, and the integral over the crystal momentum component parallel to the interface is retained.

Under certain restrictions ($\Delta = 0$; equal masses in metal and barrier regions, moderate bias), the results of the magnetic direct tunneling model reduce to those of the regular `DirectTunneling` model (see Direct Tunneling on page 718). The Airy function formulation of magnetic tunneling has been validated by direct comparison to an in-house NEGF implementation. In the lattice-converged limit, there is exact agreement between the NEGF and the Airy function results.

Using the Magnetic Direct Tunneling Model

The magnetic direct tunneling model is activated by specifying:

```
Tunneling(DirectTunneling(MTJ))
```

in the `Physics` section for the interface between the ferromagnetic and barrier materials in the command file:

```
Physics (MaterialInterface="CoFeB/MgO") {
   Tunneling(DirectTunneling(MTJ))
}
```

Physics Parameters for Magnetic Direct Tunneling

The parameters for the magnetic direct tunneling model are defined in the `DirectTunneling` section of the parameter file pertaining to the required material (or region) interface, for example:

```
MaterialInterface="CoFeB/MgO" {
   DirectTunneling {
      m_M = 0.73
      m_dos = 0.73, 0            # hole m_dos must be zero
      m_ins = 0.16, 999          # hole value is ignored
      E_F_M = 2.25
      E_barrier = 3.285, 999     # hole value is ignored
      D_spin = 2.15
   }
}
```

The parameters for the magnetic direct tunneling model are described in Table 142. Relative to the nonmagnetic direct tunneling, there is one additional parameter: the spin-energy splitting Δ. The ferromagnetic materials are assumed to be metals; therefore, the semiconductor effective mass parameter m_S is not used, and only electron tunneling is considered. Hole parameter values are ignored, but dummy values are required for correct parsing of the parameter file.

Table 142   Coefficients for direct tunneling (values for MgO on CoFeB from [4][5])

Symbol	Parameter name	Electrons	Holes	Unit	Description
E_F	E_F_M	2.25	-/-	eV	Fermi energy in ferromagnet (relative to conduction band).
Δ	D_spin	2.15	-/-	eV	Energy splitting between spin-up and spin-down electrons in ferromagnet.
U_B	E_barrier	3.185	<ignored>	eV	Energy barrier (difference of conduction band edge in ferromagnet and barrier).
m_{FM}	m_M	0.73	-/-	m_0	Effective mass in ferromagnet.
m_{ox}	m_ins	0.16	<ignored>	m_0	Effective mass in barrier.
m_{dos}	m_dos	0.73	0	m_0	The density-of-states mass parallel to the interface; the hole value *must* be zero.

NOTE   The parameters on either side of the barrier must be the same.

NOTE   The image-force effective barrier model has not been tested in the context of the magnetic direct tunneling model. It is disabled by default.

Math Parameters for Magnetic Direct Tunneling

The evaluation of the MTJ tunneling integrals as well as the value caching and interpolation strategy for reusing previous results can be controlled by an MTJ statement in the Math section of the command file, for example:

```
Math {
    MTJ(interpolate(kT(order=1 Grid=1e-3)))
}
```

Table 143 on page 809 summarizes the available parameters. Parameter names are subdivided by a slash (/) to reflect the hierarchical structure of the MTJ statement. For example, the order parameter in the preceding example is listed as interpolate/kT/order.

Table 143   Math parameters for magnetic direct tunneling model

Parameter name	Default	Unit	Description
`interpolate/Voltage/Grid`	1e-3	V	Grid spacing for interpolation or snapping of the voltage across the MTJ.
`interpolate/Voltage/order`	2	–	Interpolation order for the applied voltage: `0`: Simple value snapping `1`: Piecewise linear interpolation `2`: Piecewise parabolic interpolation
`interpolate/kT/Grid`	1e-8	eV	Grid spacing for interpolation or snapping of the temperature (multiplied by k_B) at both ends of a tunneling edge.
`interpolate/kT/order`	0	–	Interpolation order for the junction temperature: `0`: Simple value snapping `1`: Bilinear interpolation
`dE`	0.01	eV	Interval size for (total) energy integration.
`dEp`	0.01	eV	Interval size for energy integration (contribution from surface parallel k-vector).
`digits`	10	–	Number of significant digits in the tunneling integral.

Magnetization Dynamics

This section discusses the modeling of the magnetization dynamics inside a free ferromagnetic layer in the presence of STT. The Landau–Lifshitz–Gilbert (LLG) equation is introduced with a discussion of the expression used for the *effective magnetic field* in the macrospin approximation. It is based on the presentation of magnetization dynamics and spin-current interaction in [6][7].

Spin Dynamics of a Free Electron in a Magnetic Field

The spin angular momentum $\vec{S}$ and the magnetic moment $\vec{\mu}$ of a free electron are related by the gyromagnetic ratio:

$$\gamma = \frac{|\vec{\mu}|}{|\vec{S}|} = -2.0023 \cdot \underbrace{\frac{e}{m_e} \cdot \frac{\hbar}{2}}_{\mu_B} < 0 \tag{916}$$

The energy $\hat{H}$ of a magnetic moment $\vec{\mu}$ in a local field $\vec{B} = \mu_0 \vec{H}$ is given by $\hat{H} = -\vec{\mu} \cdot \vec{B}$.

This Hamiltonian gives rise to the dynamic equation:

$$\frac{d}{dt}\vec{S} = \frac{i}{\hbar}[\hat{H},\vec{S}] = -\frac{i}{\hbar}\gamma\mu_0[\vec{S}\cdot\vec{H},\vec{S}] = \gamma\mu_0\vec{S}\times\vec{H} \tag{917}$$

which describes the precession of the electron spin around the direction of the local magnetic field. This may be expressed equivalently in terms of the magnetic moment instead of the spin angular momentum as:

$$\frac{d}{dt}\vec{\mu} = -\gamma_0\vec{\mu}\times\vec{H}, \text{where } \gamma_0 = |\gamma|\mu_0 \tag{918}$$

Magnetization Dynamics in a Ferromagnetic Layer

The magnetization vector $\vec{M}$ can be interpreted as a volume density N/V of magnetic dipoles $\vec{\mu}$. In the absence of damping terms, the magnetization vector will precess around an effective magnetic field $\vec{H}_{\text{eff}}$ according to:

$$\frac{d}{dt}\vec{M} = -\gamma_0\vec{M}\times\vec{H}_{\text{eff}} \tag{919}$$

where the effective field is obtained by taking the derivative of the magnetic energy density U with respect to the local magnetization:

$$\vec{H}_{\text{eff}} = -\frac{1}{\mu_0}\nabla_{\vec{M}}U \tag{920}$$

The LLG equation accounts for the observation that, over time, the magnetization aligns itself with the effective magnetic field, by adding a phenomenological *viscous* damping term [8]:

$$\frac{d}{dt}\vec{M} = -\gamma_0\vec{M}\times\vec{H}_{\text{eff}} + \underbrace{\frac{\alpha}{M_s}\vec{M}\times\frac{d}{dt}\vec{M}}_{\text{Gilbert damping}} \tag{921}$$

where $M_s = |\vec{M}|$ is the saturation magnetization (assumed to be a material constant), and α is a phenomenological damping parameter.

In the presence of spin-polarized currents, the rate at which angular momentum is absorbed by the ferromagnetic layer also needs to be taken into account.

The spin current $\vec{Q}$ is defined as the rate at which angular momentum is injected into the ferromagnetic layer (the magnetic direct tunneling model provides both the charge current I and the spin current $\vec{Q}$).

It is assumed that the spin direction of the injected conduction electrons is aligned rapidly to the magnetization of the ferromagnetic layer. During this process, the normal component:

$$\vec{\Gamma}_s = \vec{Q} - \frac{1}{M_s^2}\vec{M}(\vec{M} \cdot \vec{Q}) = \frac{1}{M_s^2}\vec{M} \times (\vec{Q} \times \vec{M}) \tag{922}$$

of the injected angular momentum is transferred from the conduction electrons to the core electrons of the ferromagnet and exerts an additional torque on the magnetization. This is the eponymous spin transfer torque of STT-RAM:

$$\frac{d}{dt}\vec{M} = -\gamma_0 \vec{M} \times \vec{H}_{\text{eff}} + \frac{\alpha}{M_s}\vec{M} \times \frac{d}{dt}\vec{M} + \underbrace{\frac{\gamma_0 \vec{\Gamma}_s}{\mu_0 V}}_{\text{STT}} \tag{923}$$

In terms of the magnetization direction $\vec{m} = \vec{M}/|M_s|$ and after the elimination of the time derivative on the RHS of Eq. 923, the LLG equation with STT takes the form:

$$(1 + \alpha^2)\frac{d}{dt}\vec{m} = -\gamma_0\left(\vec{m} \times \left(\vec{H}_{\text{eff}} + \frac{\alpha\vec{\Gamma}_s}{\mu_0 M_s V}\right) + \alpha\vec{m} \times (\vec{m} \times \vec{H}_{\text{eff}}) + \frac{\vec{\Gamma}_s}{\mu_0 M_s V}\right) \tag{924}$$

Contributions of the Magnetic Energy Density

As shown in Eq. 920, p. 810, the effective magnetic field that drives the magnetization dynamics is related to the energy density U. In general, the magnetization may be a position and a time-dependent vector field $\vec{M}(\vec{x}, t)$. Then, the energy density U may be written as:

$$U = U_X + U_{\text{demag}} + U_{\text{aniso}} + U_{\text{ext}} \tag{925}$$

with contributions due to the following effects:

- Exchange interaction: $U_X = A \sum_{i = x, y, z} \left(\frac{\partial m_i}{\partial x_i}\right)^2$.

  This term favors parallel alignment of nearby spins in a ferromagnet ($A < 0$). If this term dominates, a single magnetic domain may span the entire sample.

- Stray/demagnetizing field: $U_{\text{demag}} = -\frac{\mu_0}{2}\vec{M} \cdot \vec{H}_{\text{demag}}$.

  The demagnetizing field is the magnetic field caused by the sum of all magnetic moments in the sample. In sufficiently large samples, the energy content of the demagnetizing field can be reduced by the formation of multiple magnetic domains. In smaller samples, this

term favors aligning the magnetization direction along the longest extension of the sample (like in a *compass needle*).

■ Magnetocrystalline anisotropy: U_{aniso}.

In crystalline materials, the magnetic energy may depend on the direction of the magnetization relative to the crystal axes.

■ Zeeman energy: $U_{\text{ext}} = -\vec{M} \cdot \vec{B}_{\text{ext}}$.

Energy of the magnetic moments in an external magnetic field.

Energy Density and Effective Field in Macrospin Approximation

In the macrospin approximation, each magnetic region is considered to consist of a single, perfectly aligned, magnetic domain. This removes the position dependency from the magnetization vector field $\vec{M}(\vec{x}, t)$ of the previous section and reduces it to a single time-dependent magnetization vector $\vec{M}(t)$.

The macrospin approximation models the dominance of the exchange term over the remaining terms in the energy density (a single perfect domain). Since there is no more position dependency in the magnetization direction inside the sample, U_X vanishes.

In addition, the energy density U and, therefore, the effective magnetic field $\vec{E}_{\text{eff}}$ are treated as local functions of $\vec{M}$. This implies the assumption of a position-independent demagnetizing field inside the ferromagnetic layer. It can be shown that, in an infinite thin film as well as in an ellipsoidal [9] ferromagnetic sample, the demagnetizing field is exactly constant and parallel to the magnetization direction. For a cylindrical thin-film geometry, this is still approximately true.

At the level of the macrospin approximation, the effects of magnetocrystalline anisotropy and the demagnetizing field become indistinguishable and are grouped together into a single *effective anisotropy* term.

In Sentaurus Device, the energy density associated with this effective anisotropy is divided into the *uniaxial anisotropy*:

$$U_K = K(1 - m_z^2) \tag{926}$$

where:

$$K = \frac{1}{2}\mu_0 M_s H_k \tag{927}$$

and H_k is the Stoner–Wohlfarth switching field, and the *easy-plane anisotropy*:

$$U_P = K_P m_x^2 \qquad (928)$$

with:

$$K_P = \frac{1}{2}\mu_0 M_s M_{\text{eff}} \qquad (929)$$

where M_{eff} is used as a parameter to account for deviations from the ideal thin-film geometry ($M_s = M_{\text{eff}}$).

Using Magnetization Dynamics in Device Simulations

Magnetization dynamics is included in the simulation if the equation name `LLG` is specified in the `Solve` section of the command file. Usually, transient simulations are required for STT devices.

To solve magnetizations, the current flow in metals, and the electrostatic potential simultaneously, you must solve the LLG equation, the contact equation, and the Poisson equation as a system of coupled equations. Therefore, a typical `Solve` statement for an STT device simulation would be:

```
Transient (InitialTime=0 FinalTime=12e-9 maxstep=1.0e-11) {
   Coupled { Poisson Contact LLG }
}
```

The time-step size must be limited to ensure that the high-frequency oscillations typical of magnetization dynamics are captured.

Domain Selection and Initial Conditions

The definition of fixed and pinned regions, and of initial conditions for the magnetization direction is handled by the `Magnetism` statement in the region-specific `Physics` sections:

```
Physics(Region="AnodeWell") {
   Magnetism(PinnedMagnetization Init(phi=0.0 theta=0.0))
}

Physics(Region="CathodeWell") {
   Magnetism(Init(phi=0.0 theta=3.14))
}
```

Here, the magnetization in the region `AnodeWell` is pinned at $\vartheta = \varphi = 0$ ($m_z = 1$); whereas, the magnetization in the region `CathodeWell` is free with initial conditions of $\varphi = 0$ and $\vartheta = 3.14$ (close to $m_z = -1$).

An external magnetic field $\vec{H}_{ext}$ (in A/m) may be specified in the `Magnetism` statement as `H_ext = (<Hx>, <Hy>, <Hz>)`.

Plotting of the Time-Dependent Magnetization

In the macrospin approximation, the magnetization is constant across each region. Then, the full time evolution of the magnetization can be captured by plotting the average direction of the magnetization vector in the free layer. In the simulation example [2], the free layer is called `CathodeWell`, and plotting of the magnetization direction is triggered by the following `CurrentPlot` section:

```
CurrentPlot { MagnetizationDir/Vector3D(average(Region="CathodeWell")) }
```

In addition to the magnetization direction in Cartesian coordinates, you can plot the magnetization of the zenith angle `Magnetization_theta` and the azimuth `Magnetization_phi` of the magnetization direction ($\vartheta = \varphi = 0$ corresponds to the positive z-direction).

Parameters for Magnetization Dynamics

The parameters for magnetization dynamics (LLG equation) are defined in the `Magnetism` section of the corresponding material or region in the parameter file. Table 144 summarizes the available parameters.

Table 144   Parameters for LLG equation (typical values shown)

Symbol	Parameter name	Value	Unit	Description
M_s	`SaturationMagnetization`	8.0e5	A/m	Saturation magnetization of the ferromagnetic material.
α	`alpha`	0.01	1	Gilbert damping coefficient.
H_K	`Hk`	7957.75	A/m	Stoner–Wohlfarth switching field (depends on layer geometry).

Table 144   Parameters for LLG equation (typical values shown) (Continued)

Symbol	Parameter name	Value	Unit	Description
M_{eff}	Meff	5e5	A/m	Effective magnetization for parameterizing the easy-plane anisotropy (geometry dependent).
A	A	1e-11	J/m	Exchange stiffness of the ferromagnetic material (only used if macrospin is disabled; see Magnetization Dynamics Beyond Macrospin: Position-Dependent Exchange and Spin Waves on page 817).

Time-Step Control for Magnetization Dynamics

To improve time-step control during the transient solution of the LLG equation, you can restrict the maximum change of the magnetization direction during the simulation that may occur during a single time step. If this limit is exceeded, the update is rejected, and the time step Δt is reduced until the limit is met.

For example, a maximum local change of the Cartesian components of the magnetization of 0.1 per time step is requested in the `Math` section of the command file like this:

```
Math {
    Magnetism(dxyz=0.1))
}
```

The default value for `dxyz` is 0.15.

Thermal Fluctuations

The magnetization dynamics may be influenced by thermal fluctuations. This effect may be included in the analysis by replacing the deterministic effective field $\vec{H}_{\text{eff}}$ with $\vec{H}_{\text{eff}} + \vec{H}_{\text{T}}$, where the *thermal fluctuation field* $\vec{H}_{\text{T}}$ is a stochastic field with the autocorrelation function [10]:

$$\langle H_T^i(t) H_T^j(t') \rangle = \frac{2kT\alpha}{\gamma_0 \mu_0 M_s V} \delta_{i,j} \delta(t - t') \tag{930}$$

Using Thermal Fluctuations

Modeling of thermal fluctuations is activated by adding the `ThermalFluctuations` keyword to the `Magnetism` statement of the `Physics` section:

```
Physics {
  Magnetism(ThermalFluctuations)
}
```

The magnitude of the thermal fluctuation field may be modified by multiplication with the optional parameter `H_th_scaling_factor` (default: 1). The syntax for suppressing $\vec{H}_T$ by a factor of 2 (which corresponds to dividing the temperature by 4) is:

```
Physics {
   Magnetism(ThermalFluctuations H_th_scaling_factor=0.5)
}
```

Parallel and Perpendicular Spin Transfer Torque

In an MTJ, it is customary to decompose the STT $\vec{\Gamma}_s$ (Eq. 922, p. 811) into *perpendicular* and *parallel* (or *in-plane*) components, relative to the plane spanned by the magnetization directions on both sides of the tunneling barrier.

If $\vec{n} = \vec{m}_1 \times \vec{m}_2$ is the unit normal vector of this plane, the perpendicular torque is defined as:

$$\vec{\Gamma}_\perp = \left(\vec{n} \cdot \vec{\Gamma}_s \right) \vec{n} \tag{931}$$

The in-plane torque is defined as:

$$\vec{\Gamma}_\| = -\vec{n} \times \left(\vec{n} \times \vec{\Gamma}_s \right) = \vec{\Gamma}_s - \vec{\Gamma}_\perp \tag{932}$$

Sometimes, it may be instructive to be able to modify the relative strength of the in-plane and the perpendicular torque components. For this purpose, user-accessible scaling factors $\varepsilon_\|$ and $\varepsilon_\perp$ are provided. If they are modified from their default values of 1, the STT $\vec{\Gamma}_s$ in the LLG equation (Eq. 924, p. 811) is replaced with an effective torque:

$$\vec{\Gamma}_{s,\,\text{eff}} = \varepsilon_\| \vec{\Gamma}_\| + \varepsilon_\perp \vec{\Gamma}_\perp \tag{933}$$

In the command file, these scaling factors can be accessed from the `Physics` section:

```
Physics {
   Magnetism(parallel_torque_scaling_factor=<double>)        # ε‖
   Magnetism(perpendicular_torque_scaling_factor=<double>)   # ε⊥
}
```

Magnetization Dynamics Beyond Macrospin: Position-Dependent Exchange and Spin Waves

The macrospin approximation is based on the assumption that the effect of the exchange interaction is much stronger than all other magnetic effects. Therefore, the most energetically favorable magnetization configuration is a single perfectly aligned domain that spans the entire ferromagnet.

In many structures, however, there is competition between the exchange interaction, which favors single-domain behavior, and the demagnetizing field, which tries to break down domains to reduce the energy content of the stray field. The nonlocality of the demagnetizing field has not yet been implemented in Sentaurus Device. However, even without it, restoring the vector-field character to the magnetization direction $\vec{m}(\vec{x}, t)$ and adding the exchange field:

$$\vec{H}_X = \frac{2A}{\mu_0 M_s} \nabla^2 \vec{m} \tag{934}$$

to the effective field $\vec{H}_{\text{eff}}$ of the LLG equation (Eq. 924, p. 811) leads to interesting phenomena such as spin waves. This allows, for example, the modeling of the nonlocal switching behavior of devices such as the spin-torque majority gate suggested in [11].

Figure 53 on page 818 shows a snapshot of the position-dependent magnetization direction in a spin-torque majority gate.

Figure 53   Snapshot of position-dependent magnetization in a spin-torque majority gate; the pinned layer is split into four pieces, and the MTJs with different applied voltages compete for switching of the cross-shaped free layer

Using Position-Dependent Exchange

The exchange term becomes active as soon as the node-merging mechanism of the macrospin approximation is disabled:

```
Physics (Region="CathodeWell") {
   Magnetism(-MacroSpin)              # disable the macrospin approximation
}
```

User-Defined Contributions to the Effective Magnetic Field of the LLG Equation

Additional contributions to the $\vec{H}_{\text{eff}}$ field of the LLG equation (Eq. 924, p. 811) can be defined using the physical model interface (PMI). See Chapter 38 on page 1043 for general information on the PMI and Ferromagnetism and Spin Transport on page 1294 for detailed information on spintronics-specific PMI models.

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CHAPTER 31 Modeling Mechanical Stress Effect

This chapter presents an overview of the importance of stress in device simulation.

Stress engineering is a key point to ensuring the high performance of CMOS devices. Mechanical stress can affect workfunction, band gap, effective mass, carrier mobility, and leakage currents. The stress is generated by many technological processes due to different process temperatures and material properties. In addition, it can be added (such as silicon layers onto SiGe bulk) to improve device performance.

Overview

Mechanical distortion of semiconductor microstructures results in a change in the band structure and carrier mobility. These effects are well known, and appropriate computations of the change in the strain-induced band structure are based on the deformation potential theory [1]. The implementation of the deformation potential model in Sentaurus Device is based on data and approaches presented in the literature [1][2][3][4]. Other approaches [5][6] implemented in Sentaurus Device focus more on the description of piezoresistive effects.

Stress and Strain in Semiconductors

Generally, the stress tensor $\bar{\sigma}$ is a symmetric 3×3 matrix. Therefore, it only has six independent components, and it is convenient to express it in a contracted six-component vector notation:

$$\bar{\sigma} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{bmatrix} \rightarrow \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} \tag{935}$$

where pairs of indices are contracted using:

$$11 \rightarrow 1, 22 \rightarrow 2, 33 \rightarrow 3, 23 \rightarrow 4, 13 \rightarrow 5, 12 \rightarrow 6 \tag{936}$$

The contracted tensor notation simplifies tensor expressions. For example, one of the options for computing the strain tensor $\bar{\varepsilon}$ (which is needed for the deformation potential model) is given by the generalized Hooke's law for anisotropic materials:

$$\varepsilon_{ij} = \sum_{k=1}^{3} \sum_{l=1}^{3} S_{ijkl}\sigma_{kl} \tag{937}$$

where S_{ijkl} is a component of the elastic compliance tensor S. The elastic compliance tensor is symmetric, which allows Eq. 937 to be written in a simplified contracted form:

$$\varepsilon_i = \sum_{j=1}^{6} S_{ij}\sigma_j \tag{938}$$

In addition to index contraction (Eq. 936), the following contraction rules for ε_{ij} and S_{ijkl} were used to obtain this result [7]:

$$
\begin{aligned}
\varepsilon_p &= \varepsilon_{ij} && , \text{if } p < 4 \\
&= 2\varepsilon_{ij} && , \text{if } p > 3 \\
\\
S_{pq} &= S_{ijkl} && , \text{if } p < 4 \text{ and } q < 4 \\
&= 4S_{ijkl} && , \text{if } p > 3 \text{ and } q > 3 \\
&= 2S_{ijkl} && , \text{otherwise}
\end{aligned}
\tag{939}
$$

Note that ε_4, ε_5, and ε_6 are often called *engineering shear-strain components* and are related to the double-subscripted shear components that are used in the model equations by:

$$
\begin{aligned}
\varepsilon_4 &= 2\varepsilon_{23} = 2\varepsilon_{32} \\
\varepsilon_5 &= 2\varepsilon_{13} = 2\varepsilon_{31} \\
\varepsilon_6 &= 2\varepsilon_{12} = 2\varepsilon_{21}
\end{aligned}
\tag{940}
$$

In crystals with cubic symmetry such as silicon, the number of independent coefficients of the elastic compliance tensor (as well as with other material property tensors) reduces to three by rotating the coordinate system parallel to the high-symmetric axes of the crystal [8]. This gives the following (contracted) compliance tensor S:

$$
\bar{S} = \begin{bmatrix}
S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\
S_{12} & S_{11} & S_{12} & 0 & 0 & 0 \\
S_{12} & S_{12} & S_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & S_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & S_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & S_{44}
\end{bmatrix}
\tag{941}
$$

where the coefficients S_{11}, S_{12}, and S_{44} correspond to parallel, perpendicular, and shear components, respectively.

In Sentaurus Device, the stress tensor can be defined in the stress coordinate system $(\vec{e}_1, \vec{e}_2, \vec{e}_3)$. To transfer this tensor to another coordinate system (for example, the crystal system $(\vec{e}'_1, \vec{e}'_2, \vec{e}'_3)$, which is a common operation, the following transformation rule between two coordinate systems is applied:

$$\sigma'_{ij} = \sum_{k=1}^{3} \sum_{l=1}^{3} a_{ik} a_{jl} \sigma_{kl} \tag{942}$$

where $\bar{a}$ is the rotation matrix:

$$a_{ik} = \frac{\vec{e}'_i \cdot \vec{e}_k}{|\vec{e}'_i||\vec{e}_k|} \tag{943}$$

Using Stress and Strain

Stress-dependent models are selected in the `Physics{Piezo()}` section of the command file. Components of the stress and strain tensors (if they are constant over the device or region) also are specified here, as well as the components $\vec{e}_1$ `OriKddX` and $\vec{e}_2$ `OriKddY` of the coordinate system where stress and strain are defined (see Table 145):

```
Physics {
   Piezo (
      Stress = (XX, YY, ZZ, YZ, XZ, XY)
      Strain = (XX, YY, ZZ, YZ, XZ, XY)
      OriKddX = (1,0,0)
      OriKddY = (0,1,0)
      Model (...)
   )
}
```

Table 145   General keywords for Piezo

Parameter	Description
`Stress=(XX, YY, ZZ, YZ, XZ, XY)`	Specifies uniform stress [Pa] if the `Piezo` file is not given in the `File` section.
`Strain=(XX, YY, ZZ, YZ, XZ, XY)`	Specifies uniform strain [1].
`OriKddX = (1,0,0)`	Defines Miller indices of the stress system relative to the simulation system.

Table 145   General keywords for Piezo (Continued)

Parameter	Description
`OriKddY = (0,1,0)`	Defines Miller indices of the stress system relative to the simulation system.
`Model(<options>)`	Selects stress-dependent models in `<options>` (see sections from Deformation of Band Structure on page 826 to Mobility Modeling on page 838).

NOTE The stress system is always defined relative to the simulation coordinate system of Sentaurus Device (in the `Piezo` section of the command file). The simulation coordinate system is defined relative to the crystal orientation system by default but, in the parameter file (see below), it is possible to define the crystal system relative to the simulation system. By default, all three coordinate systems coincide.

Stress Tensor

Apart from specifying a constant stress tensor in the `Piezo` section of the command file, Sentaurus Device also provides different ways to define position-dependent stress values:

■ A field of stress values [Pa] (as obtained by mechanical structure analysis) is read by specifying the `Piezo` entry in the `File` section:

```
File {
    Piezo = <piezofile>
}
```

Sentaurus Device recognizes stress either as a single symmetric second-order tensor of dimension 3 (`Stress`), or as six scalar values (`StressXX`, `StressXY`, `StressXZ`, `StressYY`, `StressYZ`, and `StressZZ`).

■ A physical model interface can be used for stress specification (see Stress on page 1186).

■ The `Mechanics` command in the `Solve` section can update the stress tensor in response to changes in bias conditions. In particular, the stress tensor can be computed as a function of lattice temperature and electric field. This is described in Mechanics Solver on page 890.

NOTE Stress values in all these stress specifications should be in Pa ($1\,\mathrm{Pa} = 10\,\mathrm{dyn/cm^2}$) and tensile stress should be positive according to convention.

Strain Tensor

The strain tensor can be computed in one of the following ways:

■ According to the generalized Hooke's law, strain can be obtained from stress through the elastic compliance tensor S (see Eq. 937, p. 822).

- A constant strain tensor can be specified in the `Piezo` section of the command file (see Table 145 on page 823).

- Sentaurus Device can read the strain tensor $\bar{\varepsilon}$ from the TDR file (`ElasticStrain` field). This requires that a `Piezo` file is specified in the `File` section.

By default, the strain tensor will be computed by Hooke's law. If necessary, the required option can be selected as follows in the `Piezo` section of the command file:

```
Physics {
  Piezo (
    Strain = Hooke
    Strain = (XX, YY, ZZ, YZ, XZ, XY)
    Strain = LoadFromFile
  )
}
```

Stress Limits

Extremely high stress values can sometimes cause stress-dependent models to produce nonphysical results. As an option, you can limit stress values read from files or specified in the command file to a user-specified maximum. This is accomplished by specifying the `StressLimit` parameter in the `Math` section of the command file:

```
Math {
  StressLimit = 4e9   #[Pa]
}
```

The magnitude of all stress components at each semiconductor vertex is limited to the specified value, but the sign of the stress value is retained. For example, with the above specification, a stress value of $\sigma_{yy} = -8.2 \times 10^9$ read from a file is limited to $\sigma_{yy} = -4 \times 10^9$.

Crystallographic Orientation and Compliance Coefficients

The simulation coordinate system relative to the crystal coordinate system can be defined by the `X` and `Y` vectors in the `LatticeParameters` section of the parameter file. The defaults are:

```
LatticeParameters {
  X = (1, 0, 0)
  Y = (0, 1, 0)
}
```

The simulation system is defined relative to the crystal system. Alternatively, there is an option to represent the crystal system relative to the Sentaurus Device simulation system. In this case, the keyword `CrystalAxis` must be in the `LatticeParameters` section, and the `X` and `Y` vectors will represent the $\langle 100 \rangle$ and $\langle 010 \rangle$ axes of the crystal system in the Sentaurus Device simulation system.

The elastic compliance coefficients S_{ij} [10^{-12} cm^2/dyn] can be specified in the field `S[i][j]` in the `LatticeParameters` section of the parameter file. If the cubic crystal system is selected (by specifying `CrystalSystem=0`), it is sufficient to specify S_{11}, S_{12}, and S_{44}. For a hexagonal crystal system (`CrystalSystem=1`), S_{33} and S_{13} must also be specified. Otherwise, all unspecified coefficients are set to 0.

The following section of the parameter file shows the defaults for silicon:

```
LatticeParameters {
* Crystal system and elasticity.
 X = (1, 0, 0)          # [1]
 Y = (0, 1, 0)          # [1]
 S[1][1] = 0.77         # [1e-12 cm^2/dyn]
 S[1][2] = -0.21        # [1e-12 cm^2/dyn]
 S[4][4] = 1.25         # [1e-12 cm^2/dyn]
 CrystalSystem = 0      # [1]
}
```

Deformation of Band Structure

In deformation potential theory [2][9], the strains are considered to be relatively small. The change in energy of each carrier valley or band, caused by the small deformation of the lattice, is a linear function of the strain.

For silicon, Bir and Pikus [9] proposed a model for the strain-induced change in the energy of carrier valleys or bands (three Δ_2 electron valleys, heavy-hole, and light-hole bands are considered) where they ignore the shear strain for electrons and suggest nonlinear dependence for holes (which corresponds to 6×6 k · p theory [12]):

$$\Delta E_{C, i} = \Xi_d(\varepsilon'_{11} + \varepsilon'_{22} + \varepsilon'_{33}) + \Xi_u \varepsilon'_{ii}$$

$$\Delta E_{V, i} = a(\varepsilon'_{11} + \varepsilon'_{22} + \varepsilon'_{33}) \pm \delta E$$

$$\delta E = \sqrt{\frac{b^2}{2}((\varepsilon'_{11} - \varepsilon'_{22})^2 + (\varepsilon'_{22} - \varepsilon'_{33})^2 + (\varepsilon'_{11} - \varepsilon'_{33})^2) + d^2(\varepsilon'^2_{12} + \varepsilon'^2_{13} + \varepsilon'^2_{23})}$$

(944)

where Ξ_d, Ξ_u, a, b, d are deformation potentials, i corresponds to the carrier band number, and ε'_{ij} are the components of the strain tensor in the crystal coordinate system (see Stress and Strain in Semiconductors on page 821 for a description of tensor transformations). The sign $\pm$ separates heavy-hole and light-hole bands of silicon.

The stress-induced change of the Δ_2 electron valley energy in Eq. 944 corresponds to a simple form of the linear deformation model. The model applied to arbitrary ellipsoidal bands (for example, as for four L-electron valleys in germanium or Γ-electron valley in III-V materials) could be expressed as [10]:

$$\Delta E_{\mathrm{i}} = \left[\Xi_d \bar{1} + \Xi_u \left\{ \vec{e}_i \vec{e}_i^T \right\} \right] : \bar{\varepsilon}' \tag{945}$$

where:

- Ξ_d, Ξ_u are linear deformation potentials.
- $\bar{1}$ is a unit 3×3 matrix.
- $\bar{\varepsilon}'$ is the strain tensor in the crystal coordinate system.
- $\vec{e}_i$ is the unit vector parallel to the **k**-vector of the main axis of the ellipsoidal valley i.

> **NOTE** The dyadic product is defined as $\bar{a}:\bar{b} = \sum_i \sum_j a_{ij} b_{ij}$.
>
> For spherical bands such as, for example, the Γ-electron valley with isotropic effective mass, the deformation potential Ξ_u should be equal to zero in Eq. 945.

As previously mentioned, the linear deformation potential model (Eq. 945) is limited to small strain and some specific band structures. For silicon, other models provide nonlinear corrections.

Using a degenerate $\mathrm{k \cdot p}$ theory at the zone boundary X-point, the authors of [11] and [13] derived an additional shear term for the Δ_2 electron valleys in Eq. 944:

$$\Delta E_{\mathrm{C}, i} = \Xi_d(\varepsilon'_{11} + \varepsilon'_{22} + \varepsilon'_{33}) + \Xi_u \varepsilon'_{ii} + \begin{cases} -\dfrac{\Delta}{4}\eta_i^2 & , \ |\eta_i| \leq 1 \\ -(2|\eta_i| - 1)\dfrac{\Delta}{4} & , \ |\eta_i| > 1 \end{cases} \tag{946}$$

where:

- $\eta_i = \dfrac{4\Xi_{u'}\varepsilon'_{jk}}{\Delta}$ is a dimensionless off-diagonal strain with $j \neq k \neq i$.
- ε'_{jk} is a shear strain component.
- Δ is the band separation between the two lowest conduction bands.
- $\Xi_{u'}$ is the deformation potential responsible for the band-splitting of the two lowest conduction bands [11]: $(E_{\Delta_1} - E_{\Delta'_2})\big|_{X[001]} = 4\Xi_{u'}\varepsilon'_{jk}$.

The strain-induced shifts of valence bands can be computed using 6x6 $\mathrm{k \cdot p}$ theory for the heavy-hole, light-hole, and split-off bands as described in [12]. The specification of the

deformation potentials for these models and is described in Using Deformation Potential Model on page 829.

Using the stress tensor $\overline{\sigma}$ from the command file, Sentaurus Device recomputes it from the stress coordinate system to the tensor $\overline{\sigma}'$ in the crystal system by Eq. 942. The strain tensor $\overline{\varepsilon}'$ is a result of applying Hooke's law Eq. 938 to the stress $\overline{\sigma}'$. Using Eq. 945, Eq. 946, or solving the cubic equation from [12], the energy band change can be computed for each conduction and valence carrier bands.

By default, Sentaurus Device does not modify the effective masses, but instead it computes strain-induced conduction and valence band-edge shifts, ΔE_C and ΔE_V, using an averaged value of the individual band-edge shifts:

$$
\begin{aligned}
\frac{\Delta E_C}{kT_{300}} &= -\ln\left[\frac{1}{n_C}\sum_{i=1}^{n_C}\exp\left(\frac{-\Delta E_{C,i}}{kT_{300}}\right)\right] \\
\frac{\Delta E_V}{kT_{300}} &= \ln\left[\frac{1}{n_V}\sum_{i=1}^{n_V}\exp\left(\frac{\Delta E_{V,i}}{kT_{300}}\right)\right]
\end{aligned}
\tag{947}
$$

where n_C and n_V are the number of subvalleys considered in the conduction and valence bands, respectively, and $T_{300} = 300\,\text{K}$.

Alternatively, a more accurate representation of the band gap can be obtained by using the minimum and maximum of the individual conduction and valence band shifts, respectively, as follows:

$$
\begin{aligned}
\Delta E_C &= \min(\Delta E_{C,i}) \\
\Delta E_V &= \max(\Delta E_{V,i})
\end{aligned}
\tag{948}
$$

In this case, however, the strain dependency of the effective mass and the density-of-states should be accounted for (see Strained Effective Masses and Density-of-States on page 830).

The band gap and affinity can be modified:

$$
\begin{aligned}
E_g &= E_{g0} + \Delta E_C - \Delta E_V \\
\chi &= \chi_0 - \Delta E_C
\end{aligned}
\tag{949}
$$

where the index '0' corresponds to the affinity and bandgap values before stress deformation.

Using Deformation Potential Model

To activate the deformation potential models Eq. 944–Eq. 946 with $k \cdot p$ models for electrons and holes, and Eq. 948 for the conduction band and valence band energy shifts, the following must be specified in the `Piezo` section of the command file:

```
Physics (Region = "StrainedSilicon") {
   Piezo(
      Model(DeformationPotential(ekp hkp minimum)
   )
}
```

NOTE   Usage of `DeformationPotential` without the `ekp` and `hkp` options is not recommended because an unsupported way of setting deformation potentials in Eq. 944 will be used.

To modify the deformation potentials of these models, the following parameters in the section `LatticeParameters` should be used:

```
LatticeParameters {
* Deformation potentials of k.p model for electron bands
 xis = 7    # [eV]
 dbs = 0.53 # [eV]
 xiu = 9.16 # [eV]
 xid = 0.77 # [eV]
 Mkp = 1.2  # [1]
* Deformation potentials of k.p model for hole bands
 adp =  2.1   # [eV]
 bdp = -2.33  # [eV]
 ddp = -4.75  # [eV]
 dso =  0.044 # [eV]
* Deformation potentials and energy (in ref. to Delta-valley) for L-valleys
 xiu_l =  11.5 # [eV]
 xid_l = -6.58 # [eV]
 e_l   =  1.1  # [eV]
* Deformation potential and energy (in ref. to Delta-valley) for Gamma-valley
 xid_gamma = -7.0 # [eV]
 e_gamma   =  2.3 # [eV]
}
```

This example shows the default parameter values for silicon. The parameters `xis`, `dbs`, `xiu`, and `xid` correspond to the deformation potentials $\Xi_{u'}, \Delta, \Xi_u, \Xi_d$ of the Δ_2 electron valleys in Eq. 946. The parameters `xiu_l` and `xid_l` define the deformation potentials of the L-valleys in Eq. 945, and `e_l` sets the relaxed energy difference between the L and Δ_2 electron valleys in the conduction band. The parameter `xid_gamma` defines the deformation potential of the Γ-valley, and the parameter `e_gamma` sets the relaxed energy difference between the Γ and Δ_2

electron valleys. The other parameters are the valence-band deformation potentials described in [12]:

- `adp` is the hydrostatic deformation potential.
- `bdp` is the shear deformation potential.
- `ddp` is the deformation potential.
- `dso` is the spin-orbit splitting energy.

Using Δ_2-valleys, L-valleys, and Γ-valley for the conduction band representation, and 6×6 $k \cdot p$ hole bands for the valence band, you can describe various semiconductor band structures. Sentaurus Device provides default band-structure parameters for silicon, germanium, SiGe, and several III–V materials in the `LatticeParameters` section. All parameters in this section can be mole fraction dependent.

In applications where the multivalley model is used (see Multivalley Band Structure on page 835), there is a possibility to use the option `DeformationPotential(multivalley)` as an alternative to the other options. This option checks whether the multivalley model is activated in the `Physics` section (if not, the `multivalley` option will be ignored) and, if so, uses all the valleys specified in the model (including $k \cdot p$ and analytic ones with the deformation potentials) to define the change to the band edge. This option allows you to propagate the `Multivalley` bandgap and `Affinity` change to other models, such as generation–recombination models.

> **NOTE** Specifying `DeformationPotential(minimum ekp hkp multivalley)` with, for example, the `eMultivalley` model activated will overwrite the options (`minimum ekp`) for electrons and will use only the valleys of the `eMultivalley` specification to define the change to the conduction band edge (accounting for the minimum energy of each valley). The same specification without, for example, the `hMultivalley` model means that the options (`minimum hkp`) will be used to define the change to the valence band edge.

To see the changes to the conduction band and valence band edges related to the `DeformationPotential` model separately, specify the following in the `Plot` section:

```
Plot {
   eDeformationPotential hDeformationPotential
}
```

Strained Effective Masses and Density-of-States

Sentaurus Device provides options for computing strain-dependent effective mass for both electrons and holes and, consequently, the strain-dependent conduction band and valence band effective density-of-states (DOS).

Strained Electron Effective Mass and DOS

The conduction band in silicon is approximated by three pairs of equivalent Δ_2 valleys. Without stress, the DOS of each valley is:

$$N_{C,i} = \frac{N_C}{3}, \qquad i = 1, 3 \tag{950}$$

where N_C can be defined by two effective mass components m_1 and m_t (see Eq. 182, p. 262).

As described in Deformation of Band Structure on page 826, an applied stress induces a relative shift of the energy $\Delta E_{C,i}$ that is different for each Δ_2 valley. In addition, in the presence of shear stress, there is a large effective mass change for electrons. An analytic derivation for this mass change can be found in [13] and is based on a two-band $k \cdot p$ theory. To simplify the final expressions, the same dimensionless off-diagonal strain introduced in Eq. 946 is used here:

$$\eta_i = \frac{4\Xi_{u'}\varepsilon'_{jk}}{\Delta}, \qquad j \neq k \neq i \tag{951}$$

Note that the ε'_{jk} strain affects only the Δ_2 valley along the i-axis, where $i = 1, 2,$ or 3 represents the [100], [010], or [001] axis, respectively.

When the $k \cdot p$ model [13] is evaluated at the band minima of the first conduction band, two different branches for the transverse effective mass are obtained where $m_{t1,i}$ is the mass across the stress direction, and $m_{t2,i}$ is the mass along the stress direction:

$$m_{t1,i}/m_t = \begin{cases} \left(1 - \dfrac{\eta_i}{M}\right)^{-1} & , \; |\eta_i| \leq 1 \\[2ex] \left(1 - \dfrac{\mathrm{sign}(\eta_i)}{M}\right)^{-1} & , \; |\eta_i| > 1 \end{cases} \tag{952}$$

$$m_{t2,i}/m_t = \begin{cases} \left(1 + \dfrac{\eta_i}{M}\right)^{-1} & , \; |\eta_i| \leq 1 \\[2ex] \left(1 + \dfrac{\mathrm{sign}(\eta_i)}{M}\right)^{-1} & , \; |\eta_i| > 1 \end{cases} \tag{953}$$

$$m_{1,i}/m_1 = \begin{cases} (1 - \eta_i^2)^{-1} & , \; |\eta_i| < 1 \\[2ex] \left(1 - \dfrac{1}{|\eta_i|}\right)^{-1} & , \; |\eta_i| > 1 \end{cases} \tag{954}$$

In the above equations, M is a $k \cdot p$ model parameter that has been adjusted to provide a good fit with the empirical pseudopotential method (EPM) results.

Another result of the $k \cdot p$ model [13] is that the nonparabolicity of the Δ_2 valley changes with stress as follows:

$$\alpha = \alpha_0 \frac{1 + 2(\eta m_t / M)^2}{1 - (\eta m_t / M)^2} \tag{955}$$

where α_0 is the relaxed nonparabolicity of the Δ_2 valley. Such stress-induced change of the nonparabolicity in Eq. 955 can be accounted for with the `eMultivalley(kpDOS Nonparabolicity)` option (see Multivalley Band Structure on page 267).

The stress-induced change of the effective DOS for each Δ_2-valley can then be written as:

$$N_{C,i} = \sqrt{\left(\frac{m_{t1,i}}{m_t}\right)\left(\frac{m_{t2,i}}{m_t}\right)\left(\frac{m_{l,i}}{m_l}\right)} \cdot \left(\frac{N_C}{3}\right) \tag{956}$$

Accounting for the change of the stress-induced valley energy $\Delta E_{C,i}$ and the carrier redistribution between valleys, the strain-dependent conduction-band effective DOS can be derived for Boltzmann statistics:

$$N_C' = \gamma \cdot N_C \tag{957}$$

where:

$$\gamma = \frac{1}{N_C} \cdot \sum_{i=1}^{3} N_{C,i} \cdot \exp\left(\frac{\Delta E_{C,min} - \Delta E_{C,i}}{kT_n}\right) \tag{958}$$

and:

$$\Delta E_{C,min} = \min(\Delta E_{C,i}) \tag{959}$$

This is incorporated into Sentaurus Device as a strain-dependent electron effective mass using:

$$m_n' = \gamma^{2/3} \cdot m_n \tag{960}$$

and:

$$N_C' = \left(\frac{m_n'}{m_n}\right)^{3/2} N_C \tag{961}$$

For materials such as Ge and III–V, the stress-related change of the effective DOS should account for L- and Γ-electron valleys as well. The stress effect in L- and Γ-electron valleys is described by the linear deformation potential model (Eq. 945) where the valley effective mass change is not accounted for. This simplifies the model where L- and Γ-valleys are added to γ similarly as suggested by Eq. 958:

$$\gamma = \frac{1}{N_C} \cdot \left(\sum_{i=1}^{3} N_{\Delta_2, i} \cdot e^{\left(\frac{\Delta E_{C, \min} - \Delta E_{\Delta_2, i}}{kT_n}\right)} + \sum_{i=1}^{4} N_{L, i} \cdot e^{\left(\frac{\Delta E_{C, \min} - \Delta E_{L, i}}{kT_n}\right)} + N_\Gamma \cdot e^{\left(\frac{\Delta E_{C, \min} - \Delta E_\Gamma}{kT_n}\right)} \right) \tag{962}$$

where:

- $N_{\Delta_2, i}$ is the effective DOS of the Δ_2-valley (corresponds to $N_{C, i}$ in Eq. 956).
- $N_{L, i}$ is the effective DOS of each L-valley.
- N_Γ is the effective DOS of each Γ-valley.
- The Δ_2-valley, L-valley, and Γ-valley energy shifts $\Delta E_{\Delta_2, i}$, $\Delta E_{L, i}$, ΔE_Γ are in reference to the conduction band edge.
- $\Delta E_{C, \min}$ is the minimum between all energy shifts $\Delta E_{\Delta_2, i}$, $\Delta E_{L, i}$, ΔE_Γ (as in Eq. 959).
- N_C in Eq. 962 is the relaxed effective DOS of the conduction band, which is computed with an account of all Δ_2-, L-, and Γ-valleys.

Strained Hole Effective Mass and DOS

To compute the hole effective DOS mass for arbitrary strain in silicon, the band structure provided by the six-band $k \cdot p$ method is explicitly integrated assuming Boltzmann statistics [14][15]. In this approximation, the total hole effective DOS mass is given by:

$$m'_p(T) = [m_{cc,1}^{3/2} e^{-(E_3 - E_1)/(kT)} + m_{cc,2}^{3/2} e^{-(E_3 - E_2)/(kT)} + m_{cc,3}^{3/2}]^{2/3} \tag{963}$$

where E_1, E_2, and E_3 are the ordered band edges for each of the three valence valleys, and $m_{cc,1}$, $m_{cc,2}$, and $m_{cc,3}$ are the carrier-concentration masses for each of the valleys given by:

$$m_{cc}^{3/2}(T) = \frac{2}{\sqrt{\pi}} (kT)^{-3/2} \int_0^\infty dE\, m_{DOS}^{3/2}(E) \sqrt{E} e^{-E/(kT)} \tag{964}$$

The energy-dependent DOS mass of each valley, m_{DOS}, is given by:

$$m_{DOS}^{3/2}(E) = \frac{\sqrt{2}\pi^2\hbar^3}{\sqrt{E}} \frac{1}{(2\pi)^3} \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin(\theta) \left[\left|\frac{\partial k}{\partial E}\right| k^2\right]_{\varphi, \theta, E} \tag{965}$$

The band structure–related integrand is computed from the inverse six-band $k \cdot p$ method in polar k-space coordinates. The integrals in Eq. 964 and Eq. 965 are evaluated using optimized quadrature rules.

The six-band $k \cdot p$ method is controlled by seven parameters:

- Three Luttinger–Kohn parameters (γ_1, γ_2, γ_3) that determine the band dispersion.
- The spin-orbit split-off energy (Δ_{so}).
- Three deformation potentials (a, b, d) that determine the strain response.

The Luttinger–Kohn parameters and Δ_{so} have been set to reproduce the DOS mass for relaxed silicon, m_p, as given by Eq. 185, p. 263 as a function of temperature. The default deformation potentials have been taken from the literature [16].

The strain-dependent valence-band effective DOS is then calculated from:

$$N_V' = \left(\frac{m_p'}{m_p}\right)^{3/2} N_V \tag{966}$$

Using Strained Effective Masses and DOS

The strain-dependent effective mass and DOS calculations can be selected by specifying `DOS(eMass)`, `DOS(hMass)`, or `DOS(eMass hMass)` as an argument to `Piezo(Model())` in the `Physics` section of the command file. For example:

```
Physics {
   Piezo (
      Model (
         DOS (eMass hMass)
      )
   )
}
```

Currently, these models have been calibrated only for strained silicon, germanium, SiGe, and several III–V materials. Most of the model parameters are defined in the `LatticeParameters` section of the parameter file. Parameters affecting the `DOS(eMass)` model for Δ_2 valleys include the deformation potentials of the $k \cdot p$ model for electron bands (`xis`, `dbs`, `xiu`, `xid`) and the Sverdlov $k \cdot p$ parameter (`Mkp`). Parameters affecting the `DOS(eMass)` model for L-valleys include the deformation potentials (`xiu_l` and `xid_l`), the relaxed energy difference between Δ_2 valleys and L-valleys (`e_l`), and the effective masses (`me_l0_l` and `me_l0_t`) defined in the `StressMobility` section (the masses define the effective DOS of one L-valley $N_{L,i}$ in Eq. 962). Parameters affecting the `DOS(eMass)` model for Γ-valleys include the deformation potential (`xid_gamma`), the relaxed energy difference between Δ_2- and Γ-valleys (`e_gamma`), and the effective mass (`me0_gamma`) defined in the `StressMobility` section (the mass defines the effective DOS of one Γ-valley N_Γ in

Eq. 962). Parameters affecting the `DOS(hMass)` model include the deformation potentials of the $k \cdot p$ model for hole bands (`adp`, `bdp`, `ddp`, `dso`) and the Luttinger parameters (`gamma_1`, `gamma_2`, `gamma_3`). These parameters can be specified in the `LatticeParameters` section of the parameter file and can be mole fraction dependent.

The `DOS(hMass)` model involves stress-dependent and lattice temperature–dependent numeric integrations that can be very CPU intensive. For simulations at a constant lattice temperature, you should only observe this CPU penalty once, usually at the beginning of the simulation. For nonisothermal thermal simulations, these integrations would usually have to be repeated for every lattice temperature change during the solution, resulting in a very prohibitive simulation.

As an alternative, Sentaurus Device provides an option for modeling the lattice temperature dependency of the strain-affected hole mass with analytic expressions that are fit to the full numeric integrations for each stress in the device. A CPU penalty will still be observed at the beginning of the simulation while fitting parameters are determined, but the remainder of the simulation should proceed as usual since the analytic expression evaluations are very fast.

By default, the analytic lattice temperature fit is used with thermal simulations and numeric integration is used for isothermal simulations. These defaults can be overridden by using the `AnaltyicLTFit` or `NumericalIntegration` options for `DOS(hMass)`:

```
DOS(eMass hMass(NumericalIntegration))
DOS(eMass hMass(AnalyticLTFit))
```

Multivalley Band Structure

The multivalley model is an alternative that accounts for the carrier population in various valleys presented in the semiconductor band structure where the stress effect is accounted for in each valley separately. Therefore, this model does not require to have effective corrections applied to the conduction and valence band edge-energy and DOS. Based on such detailed consideration of the carrier repopulation between valleys, this model gives a possibility to account for the stress effect in both the carrier density and mobility consistently.

For a general description of the multivalley model and its implementation, see Multivalley Band Structure on page 267. The multivalley model accounts for the stress effect in the band structure by stress-induced change of the energy and effective masses in each valley.

The stress-induced change in the valley energy is described in Deformation of Band Structure on page 826. It is accounted for in both $k \cdot p$ bands [12][13] and arbitrary valleys defined in the parameter file (see Using Multivalley Band Structure on page 270).

The stress-induced change in the valley effective mass is accounted for in the two-band $k \cdot p$ model [13] for electrons and the 6×6 $k \cdot p$ model [12] for holes by a computation of the

effective DOS factors $g_{n,i}$, $g_{p,i}$ in Eq. 198, p. 267 and Eq. 199, p. 267. The stress-induced change of the effective DOS masses for each valley is described in Strained Effective Masses and Density-of-States on page 830.

Referring to Eq. 956 and Eq. 963, and using their variables, the effective DOS factors of each Δ_2 valley can be expressed as follows if only k · p bands are defined in the multivalley model:

$$g_{n,i} = \frac{1}{3}\sqrt{\left(\frac{m_{t1,i}}{m_t}\right)\left(\frac{m_{t2,i}}{m_t}\right)\left(\frac{m_{l,i}}{m_l}\right)} \qquad g_{p,i} = \left(\frac{m_{cc,i}}{m_p}\right)^{3/2} \tag{967}$$

For a general case, where both k · p bands and arbitrary valleys are defined, the effective DOS factors are computed similarly to Eq. 207, p. 274.

In most III–V materials, the electron transport in the Γ-valley must be accounted for properly. Usually, this valley is strongly nonparabolic and its properties are affected by the stress.

According to the k · p perturbation theory [17], the electron Γ-valley mass m_Γ could be represented as $m_0/m_\Gamma - 1 = (P^2/3)(2/E_\Gamma + 1/(E_\Gamma + \Delta_0))$ where:

- E_Γ is the Γ-valley energy in reference to the valence band energy.
- m_0 is the free electron mass.
- Δ_0 is the valence band spin-orbit splitting energy.
- P^2 is the squared conduction-to-valence momentum matrix element.

An assumption that P^2 does not depend on the stress gives the following expression for the stress-dependent Γ-valley mass m'_Γ:

$$R_m = \left(\frac{\dfrac{2}{E_\Gamma} + \dfrac{1}{E_\Gamma + \Delta_0}}{\dfrac{2}{E'_\Gamma} + \dfrac{1}{E'_\Gamma + \Delta_0}} - 1\right)A_m + 1$$
$$\frac{m'_\Gamma}{m_0} = \frac{R_m}{\dfrac{m_0}{m_\Gamma} + R_m - 1} \tag{968}$$

where $E'_\Gamma = E_\Gamma + \Delta E_\Gamma$, ΔE_Γ is the stress-related energy shift of the Γ-valley, A_m is a fitting parameter where, if $A_m = 0$, there is no stress effect in the Γ-valley mass.

Similarly, based on [18], the stress-dependent band nonparabolicity α'_Γ of the Γ-valley could be expressed as follows:

$$R_\alpha = \left(\left| \frac{E_\Gamma}{E'_\Gamma} \frac{1 - \frac{m'_\Gamma}{m_0}}{1 - \frac{m_\Gamma}{m_0}} \right|^2 - 1 \right) A_\alpha + 1$$

$$\alpha'_\Gamma = \alpha_\Gamma R_\alpha$$

(969)

where α_Γ is the relaxed band nonparabolicity of the Γ-valley, A_α is a fitting parameter where, if $A_\alpha = 0$, there is no stress effect in the Γ-valley nonparabolicity.

Using Multivalley Band Structure

The multivalley model is activated with the keyword `MultiValley` in the `Physics` section. If the model must be activated only for electrons or holes, the keywords `eMultiValley` and `hMultiValley` can be used. All options of the multivalley model can be used in stress simulations (see Using Multivalley Band Structure on page 270).

> **NOTE** Although the multivalley model works together with any `DeformationPotential` model (it recomputes all valley energy shifts with reference to the band edges defined by the deformation potential model), Sentaurus Device stops with an error message if the `DOS` statement is used (see Strained Effective Masses and Density-of-States on page 830).

For the carrier density computation, all parameters of arbitrary valleys can be changed in the `MultiValley` section of the parameter file (see Using Multivalley Band Structure on page 270). However, for k · p bands, you should use the `LatticeParameters` section of the parameter file (see Using Deformation Potential Model on page 829).

In III–V materials, the band nonparabolicity plays an important role in the carrier density and mobility. To account for it in the multivalley model, use `MultiValley(Nonparabolicity)` in the `Physics` section. To activate the stress-dependent Γ-valley mass and the nonparabolicity models, as in Eq. 968 and Eq. 969, the keywords `m0` and `alpha0` must be used instead of `m` and `alpha` in the valley specification (see Using Multivalley Band Structure on page 270). Such an option is possible only for valleys with isotropic mass. For example, for InAs, it could be as follows:

```
eValley"Gamma"(m0=0.0244 energy=0.0 alpha0=1.39 degeneracy=1 xid=-10.2)
```

The fitting parameters A_m and A_α from Eq. 968 and Eq. 969 can be specified globally for all valleys as follows in the `Multivalley` section of the parameter file:

```
Multivalley{
    BandgapMassFactor = A_m
    BandgapAlphaFactor = A_α
}
```

The default value of both the fitting parameters A_m and A_α is equal to 1.

The multivalley band structure can be used to compute the stress-induced change in the carrier mobility with the advanced mobility models, which account for the carrier interface quantization in each valley (see Multivalley Electron Mobility Model on page 839 and Multivalley Hole Mobility Model on page 849). For these models, additional band structure–related parameters can be changed in the `StressMobility` section of the parameter file. To have better flexibility and to use other than the multivalley MLDA quantization model in the carrier density (see Quantization Models on page 283), there is an option to exclude the multivalley model from the carrier density computation, but still have it in the stress-induced mobility models. For that, use `Multivalley(-Density)`.

Mobility Modeling

The presence of mechanical stress in device structures results in anisotropic carrier mobility that must be described by a mobility tensor. The electron and hole current densities under such conditions are given by:

$$\vec{J}_\alpha = \left(\frac{\bar{\mu}_\alpha}{\mu_{\alpha 0}}\right)\vec{J}_{\alpha 0}, \quad \alpha = n, p \tag{970}$$

where:

- $\bar{\mu}_\alpha$ is the stress-dependent mobility tensor.
- $\mu_{\alpha 0}$ denotes the isotropic mobility without stress (the reference mobility in the specific transport direction).
- $\vec{J}_{\alpha 0}$ is the carrier current density without stress.

NOTE Eq. 970 is a general expression that is used to correct the carrier current density $\vec{J}_{\alpha 0}$. The mobility model corrections $\bar{\mu}_\alpha / \mu_{\alpha 0}$ described in this section account for detailed semiconductor band structure, interface and channel orientations effects, interface and geometric quantizations, and so on. Therefore, these models are not limited to only stress problems and can be used in other applications where such effects are important. As a result, not related to stress problems, if the geometric quantization

model is used (with the `ThinLayer` keyword; see Nonparabolic Bands and Geometric Quantization on page 303), the relative isotropic mobility $\mu_{\alpha 0}$ is computed without the geometric quantization effect. This allows you to account for a dependency of the carrier current density $\vec{J}_{\alpha}$ on the layer thickness due to the geometric quantization effect.

The following sections describe options available in Sentaurus Device for including the effects of stress, interface or channel orientation, and geometric confinement in thin layers on the carrier mobilities $\bar{\mu}_{\alpha}$ and $\mu_{\alpha 0}$.

NOTE For a general case that does not require you to consider any specific transport direction in the reference mobility, you can use a full tensor reference mobility $\bar{\bar{\mu}}_{\alpha 0}$. In this case, Eq. 970 must be rewritten as follows $\vec{J}_{\alpha} = \bar{\bar{\mu}}_{\alpha} \times (\bar{\bar{\mu}}_{\alpha 0})^{-1} \vec{J}_{\alpha 0}$. Such an option can be time consuming, specially for holes.

Multivalley Electron Mobility Model

To calculate stress-induced electron mobility, Sentaurus Device considers several approaches [6][13][20][21] for the mobility approximation, and it computes the mobility ratio (3×3 tensor), which corrects the relaxed current density in Eq. 970. The simplest approach [6] focuses on the modeling of the mobility changes due to the carrier redistribution between bands in silicon. As a known example, the electron mobility is enhanced in a strained-silicon layer grown on top of a thick, relaxed SiGe layer. Due to the lattice mismatch (which can be controlled by the Ge mole fraction), the thin silicon layer appears to be 'stretched' (under biaxial tension).

The origin of the electron mobility enhancement can be explained [6] by considering the six-fold degeneracy in the conduction band. The biaxial tensile strain lowers two perpendicular valleys (Δ_2) with respect to the four-fold in-plane valleys (Δ_4). Therefore, electrons are redistributed between valleys and Δ_2 is occupied more heavily. It is known that the perpendicular effective mass is much lower than the longitudinal one. Therefore, this carrier redistribution and reduced intervalley scattering enhance the electron mobility.

The model consistently accounts for a change of band energy as described in Deformation of Band Structure on page 826, that is, a modification of the deformation potentials in Eq. 906, p. 793 will affect the strain-silicon mobility model. In the crystal coordinate system, the model gives only the diagonal elements of the electron mobility matrix.

Based on the model [6] that accounts only for carrier occupation, the following expressions have been suggested for the electron mobility:

$$\mu_{n,ii} = \mu_{n0}\left[1 + \frac{1 - m_{n1}/m_{nt}}{1 + 2(m_{n1}/m_{nt})}\left(\frac{F_{1/2}\left(\frac{F_n - E_C - \Delta E_{C,i}}{kT}\right)}{F_{1/2}\left(\frac{F_n - E_C - \Delta E_C}{kT}\right)} - 1\right)\right] \tag{971}$$

where:

- μ_{n0} is electron mobility without the strain.
- m_{n1} and m_{nt} are the electron longitudinal and transverse masses in the subvalley, respectively.
- $\Delta E_{C,i}$ and ΔE_C are computed by Eq. 906 and Eq. 947 or Eq. 948, respectively.
- The index i corresponds to a direction (for example, $\mu_{n,11}$ is the electron mobility in the direction of the x-axis of the crystal system and, therefore, $\Delta E_{C,1}$ should correspond to the two-fold subvalley along the x-axis).
- F_n is quasi-Fermi level of electrons.

  NOTE For the carrier quasi-Fermi levels, as for Eq. 971, there are two options to be computed: (a) assuming the charge neutrality between carrier and doping, and it gives only the doping dependence of the model and (b) using the local carrier concentration (see Using Multivalley Electron Mobility Model on page 846).

Derivation of Eq. 971 is based on consideration of the change in the stress-induced band energy in bulk silicon. However, in MOSFETs, there is an additional influence of a quantization that appears in the carrier channel at the silicon–oxide interface. For example, there is a reduction of the stress effect with applied gate voltage. Partially, this is due to the Fermi-level dependency on the carrier concentration, as well as to the quantization in the channel gives a different carrier redistribution between electron bands (see Inversion Layer on page 844).

Intervalley Scattering

Another effect of the stress-induced mobility change is intervalley scattering, which is considered in [20] for the bulk case. According to that model, the total relaxation time in valley i is expressed as follows:

$$\frac{1}{\tau_i} = \frac{1}{\tau^g} + \frac{1}{\tau_i^f} + \frac{1}{\tau^l} \tag{972}$$

where:

- τ^g denotes the momentum relaxation time due to acoustic intravalley scattering and intervalley scattering between equivalent valleys (g-type scattering).
- τ^I is the impurity scattering relaxation time.
- τ_i^f is the relaxation time for intervalley scattering between nonequivalent valleys (f-type scattering).

The intervalley scattering rate for electrons to scatter from initial valley i to final valley j can be defined as [20]:

$$S(\varepsilon, \Delta_{ij}) = C\left[(\varepsilon - \Delta_{ij}^{\mathrm{emi}})^{1/2} + \exp\left(\frac{\hbar\omega_{\mathrm{opt}}}{kT}\right)(\varepsilon - \Delta_{ij}^{\mathrm{abs}})^{1/2}\right]$$

$$\Delta_{ij}^{\mathrm{emi}} = \Delta E_{C,\,j} - \Delta E_{C,\,i} - \hbar\omega_{\mathrm{opt}} \tag{973}$$

$$\Delta_{ij}^{\mathrm{abs}} = \Delta E_{C,\,j} - \Delta E_{C,\,i} + \hbar\omega_{\mathrm{opt}}$$

where $\hbar\omega_{\mathrm{opt}}$ is the phonon energy and C is a constant. The relaxation time for this scattering event can be defined as follows:

$$\frac{1}{\tau^f(i \to j)} = \int_0^\infty S(\varepsilon, \Delta_{ij}) f(\varepsilon, F_n) d\varepsilon \tag{974}$$

where $f(\varepsilon, F_n)$ is the electron distribution function.

Using the Fermi–Dirac distribution function and considering that electrons from the valley i can be scattered into two valleys j and l ($1/\tau_i^f = 1/\tau^f(i \to j) + 1/\tau^f(i \to l)$), a ratio between unstrained and strained relaxation times for this intervalley scattering in valley i can be written as:

$$h_i = \frac{\tau^{f0}}{\tau_i^f} = \frac{F_{1/2}\left(\frac{\eta - \Delta_{ij}^{\mathrm{emi}}}{kT}\right) + F_{1/2}\left(\frac{\eta - \Delta_{il}^{\mathrm{emi}}}{kT}\right) + \exp\left(\frac{\hbar\omega_{\mathrm{opt}}}{kT}\right)\left[F_{1/2}\left(\frac{\eta - \Delta_{ij}^{\mathrm{abs}}}{kT}\right) + F_{1/2}\left(\frac{\eta - \Delta_{il}^{\mathrm{abs}}}{kT}\right)\right]}{2\left[F_{1/2}\left(\frac{\eta + \hbar\omega_{\mathrm{opt}}}{kT}\right) + \exp\left(\frac{\hbar\omega_{\mathrm{opt}}}{kT}\right)F_{1/2}\left(\frac{\eta - \hbar\omega_{\mathrm{opt}}}{kT}\right)\right]} \tag{975}$$

where $\eta = F_n - E_C$.

NOTE The authors in [20] used the Boltzmann distribution function to express h_i. As a result, Eq. 20 of [20] does not have any carrier concentration (or doping) dependence, but Eq. 975 does have it through the Fermi level F_n.

Considering undoped/doped and unstrained/strained cases, the paper [20] derives an expression for total mobility change in valley i, which is based on a doping-dependent mobility model. With simplified doping dependence, a ratio between strained and unstrained total relaxation times for the valley i can be expressed as follows:

$$\frac{\tau_i}{\tau_0} = \frac{1}{1 + (h_i - 1)\dfrac{1 - \beta^{-1}}{1 + \left(\dfrac{N_{\text{tot}}}{N_{\text{ref}}}\right)^\alpha}}$$

(976)

where N_{tot} is the sum of donor and acceptor impurities, and $\beta = 1 + \tau^g / \tau^{f0}$ is a fitting parameter [20] as both others N_{ref} and α.

The final modification of the mobility along valley i (in Eq. 971), which includes the stress-induced carrier redistribution and change in the intervalley scattering, is:

$$\mu_{n,\,ii} = \frac{3\mu_{n0}}{1 + 2(m_{n1}/m_{nt})} \cdot \frac{\dfrac{\tau_i}{\tau_0}F_{1/2}\left(\dfrac{\eta - \Delta E_{C,\,i}}{kT}\right) + \dfrac{\tau_j m_{n1}}{\tau_0 m_{nt}}F_{1/2}\left(\dfrac{\eta - \Delta E_{C,\,j}}{kT}\right) + \dfrac{\tau_l m_{n1}}{\tau_0 m_{nt}}F_{1/2}\left(\dfrac{\eta - \Delta E_{C,\,l}}{kT}\right)}{F_{1/2}\left(\dfrac{\eta - \Delta E_{C,\,i}}{kT}\right) + F_{1/2}\left(\dfrac{\eta - \Delta E_{C,\,j}}{kT}\right) + F_{1/2}\left(\dfrac{\eta - \Delta E_{C,\,l}}{kT}\right)}$$

(977)

NOTE The model (Eq. 975 and Eq. 976) was developed originally for the bulk case. However, in MOSFET channels, to obtain an agreement with experimental data, the model and parameter β, responsible for the unstressed ratio between g-type and f-type scatterings, must be modified (see Inversion Layer on page 844).

Effective Mass

It is known that the effective mass of electrons does not change significantly if the stress is applied along the crystal axis, and it allows you to write the stress-induced mobility change in the form of Eq. 971 and Eq. 977. However, an analysis based on the empirical nonlocal pseudopotential theory [21] shows that, for the stresses applied along $\langle 110 \rangle$, the effective mass changes strongly and it affects the electron mobility. The literature [21] suggests a simple empirical polynomial approximation for the dependency of the effective mass on stress applied along $\langle 110 \rangle$. Later, the two-band $k \cdot p$ theory [13] was developed for electrons with the main analytic results for the effective masses described in Strained Electron Effective Mass and DOS on page 831.

To formulate the stress-induced change of the mobility generally (accounting for arbitrary channel and interface orientations), the inverse conductivity mass tensor for the valley i is represented in the following very general form:

$$(\overline{m}_{\text{cond},i})^{-1} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon^i(\vec{k})}{\partial k_j \partial k_l}$$

(978)

where:

- $\varepsilon^i(\vec{k})$ is the energy dispersion of valley i defined by the two-band k · p theory.
- k_j, k_l are the wavevectors.
- The inverse mass tensor $(\overline{m}_{\text{cond},i})^{-1}$ is computed in the valley energy minima, which is a good approximation for electron conductivity masses in silicon.

Near an interface, you can assume zero current perpendicular to the interface. This assumption and a consideration of the carrier quantization near the interface [22] suggest that the 3x3 inverse conductivity mass tensor of Eq. 978 should be recomputed into a 2x2 in-plane tensor. For the inverse conductivity mass tensor in the interface coordinate system (with components w_{ij}) where the perpendicular axis has an index *3*, the following recomputation into the 2x2 in-plane symmetric tensor should be performed:

$$w'_{11} = w_{11} - \frac{w_{13}^2}{w_{33}}$$

$$w'_{22} = w_{22} - \frac{w_{23}^2}{w_{33}}$$

(979)

$$w'_{12} = w_{12} - \frac{w_{13}w_{23}}{w_{33}}$$

Setting $w'_{13} = w'_{23} = 0$ and $w'_{33} = w_{33}$, this tensor is rotated back to the crystal coordinate system and is used as $(\overline{m}_{\text{cond},i})^{-1}$. Such a recomputation has an effect for cases where the valley ellipsoid in *k*-space is not aligned to the interface.

Another optional mass transformation can be performed for 1D carrier transport that appears, for example, in nanowires. The 1D mass transformation is performed in the vicinity of the interface and with a specified direction of the 1D carrier transport. This direction (the user-defined vector in the simulation coordinate system) is projected on to the interface plane. The projected in-plane vector and the normal vector to the interface define a coordinate system where the tensor from Eq. 979 (with 2D transport mass transformation) is rotated. Assuming that the index 1 of the rotated tensor is along the 1D transport direction, the corresponding inverse mass tensor component can be written as:

$$w''_{11} = w'_{11} - \frac{(w'_{12})^2}{w'_{22}}$$

(980)

Similar to Eq. 979, when setting $w''_{12} = w''_{13} = w''_{23} = 0$ and $w''_{22} = w'_{22}$, $w''_{33} = w'_{33}$, this diagonal tensor is rotated back to the crystal coordinate system and is used as $(\bar{m}_{\text{cond},\,i})^{-1}$.

To account for such stress-induced mass change, Eq. 971 and Eq. 977 are generalized as stated in the next section, Inversion Layer.

Inversion Layer

Generally, using only the valley data, the total mobility tensor could be written in the following general form, which generalizes Eq. 971, and Eq. 977:

$$\bar{\mu}_n = q\tau_0 \sum_i \frac{n_i}{n} \frac{\tau_i}{\tau_0} (\bar{m}_{\text{cond},\,i})^{-1} \tag{981}$$

where:

- n_i/n is a local valley occupation.
- τ_i/τ_0 is the ratio of stressed and unstressed relaxation times as it is in Eq. 976.
- $(\bar{m}_{\text{cond},\,i})^{-1}$ is the inverse conductivity mass tensor Eq. 978.

To use Eq. 981 in Sentaurus Device stress modeling, the mobility tensor $\bar{\mu}_n$ should be divided by unstressed mobility μ_{n0} because the stress effect is accounted for as a multiplication factor to TCAD mobility (for example, the Lombardi model) used in the device simulation. Therefore, the unstressed mobility μ_{n0} also is computed by Eq. 981, but with zero stress.

In the multivalley representation, Eq. 981 is general enough to describe the mobility for both bulk and MOSFET inversion layer cases, but a difference between these cases is in the n_i/n and τ_i/τ_0 terms. For inversion layers, the quantization effect must be accounted for in each valley separately.

At this point, only the multivalley MLDA model gives such a possibility (see MLDA Model on page 300). Therefore, for the inversion layer mobility, the local valley occupation is computed by the multivalley MLDA model where the quantization mass m_q in the perpendicular direction to the interface is computed using stressed k · p bands (by a rotation of the inverse mass tensor $(\bar{m}_{\text{cond},\,i})^{-1}$ to an interface coordinate system).

NOTE The multivalley MLDA model accounts for arbitrary interface orientation automatically (see Interface Orientation and Stress Dependencies on page 301), which complements the general inverse mass tensor $(\bar{m}_{\text{cond},\,i})^{-1}$ in Eq. 978, and it gives users an automatic option that accounts for both channel and interface orientations simultaneously.

For the inversion layer mobility model, there are some changes to the scattering ratio τ_i/τ_0 in Eq. 975. First, the DOS used in Eq. 973 is a parabolic bulk DOS, which makes such a scattering model mostly applicable to the bulk case. The MLDA quantization model (Eq. 234) gives an MLDA DOS $D^i(\varepsilon, z)$ that becomes the bulk DOS at a distance from the interface where the quantum effect is small. Second, Eq. 973 accounts only for the intervalley optical phonon scattering, but Eq. 982 includes both intervalley and intravalley scattering with acoustic and optical phonons.

In addition, this equation takes into account an effect of the interface quantization in the scattering by the following use of both MLDA and bulk DOS:

$$
\begin{aligned}
\frac{\sum_j D^j(\varepsilon, z)}{\tau_{ac}^i(\varepsilon, z)} &= \frac{2\pi kT}{\bar{h}\rho}\left(\frac{D_{ac}}{c_1}\right)^2 \sum_j \sum_k D_{bulk}^j(\varepsilon) D_{bulk}^k(\varepsilon - \Delta\varepsilon_0^{k,i}) \\[2mm]
\frac{\sum_j D^j(\varepsilon, z)}{\tau_{ope}^i(\varepsilon, z)} &= \frac{\pi\bar{h}D_{op}^2}{\rho\hbar\omega_{opt}}(N_{op} + 1) \sum_j \sum_k D_{bulk}^j(\varepsilon) D_{bulk}^k(\varepsilon - \hbar\omega_{opt} - \Delta\varepsilon_0^{k,i}) \\[2mm]
\frac{\sum_j D^j(\varepsilon, z)}{\tau_{opa}^i(\varepsilon, z)} &= \frac{\pi\bar{h}D_{op}^2}{\rho\hbar\omega_{opt}}N_{op} \sum_j \sum_k D_{bulk}^j(\varepsilon) D_{bulk}^k(\varepsilon + \hbar\omega_{opt} - \Delta\varepsilon_0^{k,i}) \\[2mm]
S^i(\varepsilon, z) &= \frac{1}{\tau_{ac}^i(\varepsilon, z)} + \frac{1}{\tau_{ope}^i(\varepsilon, z)} + \frac{1}{\tau_{opa}^i(\varepsilon, z)}
\end{aligned}
\tag{982}
$$

where:

- $D_{bulk}^i(\varepsilon) = \dfrac{2}{(2\pi)^3} \oint_{\varepsilon^i(\vec{k}) = \varepsilon} \dfrac{dS}{\left|\nabla_k \varepsilon^i(\vec{k})\right|}$ is the electron bulk DOS of the valley i.

- $\Delta\varepsilon_0^{k,i} = \Delta E_{C,k} - \Delta E_{C,i}$ is a valley minimum energy difference between valleys i and k.
- $\dfrac{D_{ac}}{c_1}$ is the ratio of the acoustic-phonon deformation potential and the sound velocity.
- ρ is the mass density.
- $\hbar\omega_{opt}$ is the optical-phonon energy.
- D_{op} is the optical-phonon deformation potential.
- $N_{op} = [\exp(\hbar\omega_{opt}/kT) - 1]^{-1}$ is the phonon number.

  NOTE   For the bulk case, $D^j(\varepsilon, z) = D_{bulk}^j(\varepsilon)$ and, therefore, Eq. 982 can be simplified to regular bulk scattering rate equations. Eq. 982 accounts for both interband and intraband phonon scattering with the same deformation potentials, but there is an option to control the interband scattering factor.

Using Eq. 982 will activate a numeric integration in Eq. 974 with Gauss–Laguerre quadratures as described in Nonparabolic Band Structure on page 268. Another change in the scattering ratio τ_i / τ_0 is based on comparisons to various stress- and orientation-dependent experimental data. It gives the new user-defined parameter β for the inversion layer (see Using Multivalley Electron Mobility Model on page 846).

For the bulk case, the unstressed mobility μ_{n0} computed by Eq. 981 is always isotropic. However, for the MOSFET on a (110) silicon substrate, it is not. In this case, Eq. 981 without stress gives anisotropic unstressed electron mobility, and a ratio between the mobilities of the <100> and <110> channel orientations is equal to approximately 1.1. This ratio is in reasonable agreement to experimentally observed data where the ratio changes from 1.2 to 1.1 for a high-gate electric field.

> **NOTE** By default, the unstressed mobility μ_{n0} (in Eq. 970) is always computed for a <110> channel orientation and for a substrate orientation that corresponds to the auto-orientation Lombardi option (see Auto-Orientation for Lombardi Model on page 337). Such a default requires you to have calibrated the Lombardi model parameters for the <110> channel (critical for MOSFETs on (110) substrate where the unstressed mobility is anisotropic).

Using Multivalley Electron Mobility Model

The stress-induced mobility model can be activated regionwise or materialwise. To activate the inversion layer model (see Inversion Layer on page 844), the eMultivalley(MLDA) statement must be specified in the Physics section. In this case, all valleys defined by the multivalley model (for example, with eMultivalley(kpDOS parfile); see Multivalley Band Structure on page 267) will be used in the model. However, currently, it is calibrated for silicon, germanium, and SiGe band structures (with Δ_2- and L-valleys), and for InGaAs materials where the Γ-valley carrier transport is mostly important. The keyword MLDA activates the multivalley MLDA quantization model (see MLDA Model on page 300), which is applied to both the density and the inversion layer stress-induced mobility models. To use another quantization model in the density computation, specify the -Density option in the eMultivalley statement (see MLDA Application Notes on page 308). To ensure that electron stress-related models are consistent and physically correct, the Physics section should contain the following:

```
Physics {
   eMultiValley(MLDA)
   Piezo(Model(Mobility(eSubband(Fermi EffectiveMass Scattering(MLDA)))))
}
```

> **NOTE** If the model is used without options, as eSubband, then the recommended options are activated, and this is equivalent to eSubband(Doping EffectiveMass Scattering(MLDA)).

The keyword `Fermi` defines that the Fermi–Dirac distribution function is used in the mobility models Eq. 971, Eq. 977, and Eq. 981 with the carrier self-consistent quasi-Fermi energy. To activate only doping-dependent quasi-Fermi energy, use `eSubband(Doping)`. If neither `Fermi` nor `Doping` is used, the Boltzmann distribution function is used, which illuminates the quasi-Fermi energy dependency.

To activate the model for a stress-induced change of the electron effective mass (see Effective Mass on page 842, Eq. 978), use the keywords `Mobility(eSubband(EffectiveMass))`. If this keyword is not present, the unit diagonal (and stress-independent) tensor is used as $(\overline{m}_{\mathrm{cond},i})^{-1}$ in Eq. 981.

Using `EffectiveMass(-Transport)` excludes the 2D inverse conductivity mass tensor recomputation (Eq. 979). With the option `EffectiveMass(Transport<vector>)`, you can activate the 1D transport mass recomputation (Eq. 980) where `<vector>` represents the direction of 1D carrier transport in the simulation coordinate system.

The unstressed longitudinal and perpendicular effective masses m_l and m_t for this model (to be used in two-band $\mathrm{k} \cdot \mathrm{p}$ theory; see Strained Electron Effective Mass and DOS on page 831) are defined as follows:

```
StressMobility {
   me_l0 = 0.914      # [1]
   me_t0 = 0.196      # [1]
}
```

Usually for III–V materials, the two-band $\mathrm{k} \cdot \mathrm{p}$ model for Δ_2-valleys should not be used, and all valleys must be defined in the `Multivalley` section of the parameter file with all needed masses, energy shifts, deformation potentials, and so on. For some III–V materials such as InGaAs, GaAs, and InAs, all valleys of the semiconductor band structure are defined by the default in the parameter file. For such materials (where the electron Γ-valley is the lowest), the band nonparabolicity, the stress-induced Γ-valley mass change, and the geometric quantization effects in thin layers are important.

To activate the related models, the following statement must be used:

```
eMultiValley(MLDA Nonparabolicity ThinLayer)
```

See Nonparabolic Bands and Geometric Quantization on page 303 and Multivalley Band Structure on page 835.

The statement `Scattering(MLDA)` means that the scattering rate is computed with Eq. 982. If the keyword `Scattering` is not present, then τ_i/τ_0 is unit and stress independent in Eq. 977 and Eq. 981. The keyword `MLDA` in the `Scattering` statement defines that the MLDA DOS is used in the scattering rate as this is in Eq. 982. However, using only the keyword `Scattering` (without `MLDA`) activates the simplified bulk scattering rate of Eq. 973.

For III–V materials, the statement `Scattering(MLDA2)` might be used, which replaces the bulk DOS $D_{\text{bulk}}^j(\varepsilon)$ by the MLDA DOS $D^j(\varepsilon, z)$ in Eq. 982.

The parameters of the intervalley scattering model can be specified in the same `StressMobility` section of the parameter file, as this is below for silicon:

```
StressMobility {
    Ephonon = 0.06              # [eV]
    Dop = 1.25e9                # [eV/cm]
    Dac_cl = 1.027e-5           # [eVs/cm]
    beta = 1.22                 # [1]
    beta_mlda = (1.5,1.5,1.5)   # [1]
    Nref = 3e19                 # [cm^-3]
    alpha = 0.65                # [1]
}
```

where `Ephonon` is $\hbar\omega_{\text{opt}}$ in Eq. 973 and Eq. 982, `Dop` is D_{op}, and `Dac_cl` is D_{ac}/c_1, in Eq. 982. The parameters `Nref` and `alpha` correspond to the impurity scattering parameters N_{ref}, α in Eq. 976. The fitting parameter `beta` in Eq. 976 is β for the bulk case, and `beta_mlda` defines β for the inversion layer case for three interface orientations (100), (110), and (111). This gives additional calibration flexibility to users. Although, as described for Eq. 976, the parameter β was initially introduced specifically for silicon, but generally, it is an estimation of the ratio of the total scattering rate to the scattering rate of scattering events that do not depend on the stress and layer thickness in the device, with no stress and no geometric confinement.

> **NOTE** The inversion layer mobility model ($\bar{\mu}_n$ in Eq. 970) is designed to work with arbitrary channel and interface orientations. This orientation is simply defined by a specification of only the `X` and `Y` simulation coordinate axes in reference to the crystal coordinate system in the `LatticeParameters` section (see Using Deformation Potential Model on page 829).

> **NOTE** The reference isotropic mobility (μ_{n0} in Eq. 970), by default, is computed for the <110> channel direction. Such a default requires you to have calibrated the Lombardi model parameters for the <110> channel (critical for (110) interface orientation where the unstressed mobility is anisotropic). However, if you want to use <100>/(110) Lombardi model parameters, the keyword `-RelChDir110` must be used inside the `eSubband` statement. For a general case of the tensor reference mobility ($\bar{\mu}_{n0}$), the keyword `-AutoOrientation` must be used instead.

All parameters of the `StressMobility` model can be mole fraction dependent. You can check this in the SiGe material parameter file.

Multivalley Hole Mobility Model

Similar to the electron stress-induced mobility model (Eq. 981), the total hole mobility tensor can be written in the following general form, which can be applied to both bulk and inversion layer cases [23]:

$$\bar{\mu}_p = q\tau_0 \sum_i \frac{p_i}{p} \frac{\tau}{\tau_0} (\bar{m}_{\text{cond}, i})^{-1} \tag{983}$$

where:

- p_i/p is a local hole-band occupation.
- τ/τ_0 is a ratio of the stressed and unstressed valence-band relaxation times.
- $(\bar{m}_{\text{cond}, i})^{-1}$ is the inverse conductivity hole mass tensor.

The model accounts for the six-band $k \cdot p$ hole band structure [14] in all of the above three terms of Eq. 983. In the case of the inversion layer, the model computes the six-band $k \cdot p$ MLDA DOS of each band as described in MLDA Model on page 300 and, correspondingly, it affects all terms of Eq. 983. Finally, the model computes the mobility ratio (3×3 tensor), which corrects the relaxed current density in Eq. 970.

Effective Mass

The inverse mass tensor $(\bar{m}_{\text{cond}, i})^{-1}$ of the band i in Eq. 983 is based on an averaging of the reciprocal mass tensor in **k**-space and energy space. If the reciprocal mass tensor at any **k**-vector is expressed as follows:

$$w_{jl}^i(\vec{k}) = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_i(\vec{k})}{\partial k_j \partial k_l} \tag{984}$$

then the averaging in **k**-space is performed in accordance to the DOS computation (Eq. 237, p. 302), which for the inversion layer can be formulated as:

$$w_{jl}^i(\varepsilon, z) = \frac{\dfrac{2}{(2\pi)^3} \oint\limits_{\varepsilon^i(\vec{k}) = \varepsilon} \dfrac{w_{jl}^i(\vec{k})}{|\nabla_k \varepsilon^i(\vec{k})|} \left[1 - \exp\left(i2z\gamma_{\text{kp}} \sum_j k_j \dfrac{w_{j3}(\vec{k})}{w_{33}(\vec{k})} \right) \right] dS}{D^i(\varepsilon, z)} \tag{985}$$

Finally, the inverse mass tensor of the band i is computed as an averaged value over the energy space with the carrier distribution function $f(\varepsilon, F_p)$ accounted:

$$(\overline{m}_{\text{cond}, i})^{-1} = \frac{\displaystyle\int_0^\infty D^i(\varepsilon, z) w_{jl}^i(\varepsilon, z) f(\varepsilon, F_p) d\varepsilon}{p_i} \tag{986}$$

where:

- p_i is a hole-band concentration ($p_i(F_p, z) = \int_0^\infty D^i(\varepsilon, z) f(\varepsilon, F_p) d\varepsilon$).
- $(\overline{m}_{\text{cond}, i})^{-1}$ is a symmetric 3×3 tensor, which depends on the quasi-Fermi energy F_p and the distance from interface z (for the inversion layer case).

Similar to the computation of the hole-band concentration p_i, the integral over the energy in Eq. 986 is computed using Gauss–Laguerre quadratures and, for that, the energy-dependent reciprocal mass tensor (Eq. 985) is computed on a predefined energy mesh (same as for the DOS $D^i(\varepsilon, z)$).

Optionally, you can account for the 2D (in the vicinity of interfaces) or the 1D (in nanowires) carrier transport nature in the inverse mass tensor $(\overline{m}_{\text{cond}, i})^{-1}$. This is similar to recomputation of the electron transport effective masses (Eq. 979 and Eq. 980). However, for holes, it is performed for all considered energies and, correspondingly, it uses the inverse mass tensor components $w_{jl}^i(\varepsilon, z)$.

Scattering

The scattering model defines the ratio of the stressed and unstressed valence-band momentum relaxation times τ/τ_0. The model considers four scattering mechanisms (which are affected by the stress) for holes in each band assisted by: acoustic phonon, optical phonon emission, optical phonon absorption, and simplified impurity scattering.

The phonon-assisted relaxation times can be expressed as follows for the band i in the case of the inversion layer:

$$\frac{\displaystyle\sum_j D^j(\varepsilon, z)}{\tau_{\text{ac}}^i(\varepsilon, z)} = \frac{2\pi kT}{\overline{h}\rho}\left(\frac{D_{\text{ac}}}{c_1}\right)^2 \sum_j \sum_k D_{\text{bulk}}^j(\varepsilon) D_{\text{bulk}}^k(\varepsilon - \Delta\varepsilon_0^{k, i})$$

$$\frac{\displaystyle\sum_j D^j(\varepsilon, z)}{\tau_{\text{ope}}^i(\varepsilon, z)} = \frac{\pi\overline{h}D_{\text{op}}^2}{\rho\varepsilon_{\text{op}}}(N_{\text{op}} + 1) \sum_j \sum_k D_{\text{bulk}}^j(\varepsilon) D_{\text{bulk}}^k(\varepsilon - \varepsilon_{\text{op}} - \Delta\varepsilon_0^{k, i}) \tag{987}$$

$$\frac{\displaystyle\sum_j D^j(\varepsilon, z)}{\tau_{\text{opa}}^i(\varepsilon, z)} = \frac{\pi\overline{h}D_{\text{op}}^2}{\rho\varepsilon_{\text{op}}} N_{\text{op}} \sum_j \sum_k D_{\text{bulk}}^j(\varepsilon) D_{\text{bulk}}^k(\varepsilon + \varepsilon_{\text{op}} - \Delta\varepsilon_0^{k, i})$$

where:

- $D_{bulk}^i(\varepsilon) = \dfrac{2}{(2\pi)^3} \oint\limits_{\varepsilon^i(\vec{k})\,=\,\varepsilon} \dfrac{dS}{\left|\nabla_k \varepsilon^i(\vec{k})\right|}$ is the hole bulk DOS of the band i.

- $\Delta\varepsilon_0^{k,i}$ is a band minimum energy difference between bands i and k.

- $\dfrac{D_{ac}}{c_{1.}}$ is a ratio of the acoustic-phonon deformation potential by the sound velocity.

- ρ is the mass density.

- ε_{op} is the optical-phonon energy.

- D_{op} is the optical-phonon deformation potential.

- $N_{op} = \left[\exp(\varepsilon_{op}/kT) - 1\right]^{-1}$ is the phonon number.

> **NOTE** For the bulk case, $D^j(\varepsilon, z) = D_{bulk}^j(\varepsilon)$ and, therefore, Eq. 987 can be simplified to regular bulk scattering rate equations. Eq. 987 accounts for both interband and intraband phonon scattering with the same deformation potentials, but you have an option to control the interband scattering factor.

Based on Eq. 987, the total phonon-limited hole-scattering rate in the band i is written as:

$$\frac{1}{\tau_{ph}^i(\varepsilon, z)} = \frac{1}{\tau_{ac}^i(\varepsilon, z)} + \frac{1}{\tau_{ope}^i(\varepsilon, z)} + \frac{1}{\tau_{opa}^i(\varepsilon, z)} \tag{988}$$

Therefore, the macroscopic phonon-limited momentum relaxation time of the full valence band can be expressed similarly for electrons (Eq. 975):

$$\frac{1}{\tau^{ph}} = \frac{\displaystyle\sum_i \int_0^\infty D^i(\varepsilon, z)\frac{1}{\tau_{ph}^i(\varepsilon, z)} f(\varepsilon, F_p)\,d\varepsilon}{p} \tag{989}$$

where τ^{ph} depends on the quasi-Fermi energy F_p and the distance from interface z (for the inversion layer case). The impurity scattering is introduced also similarly to how it is performed for electrons in Eq. 976, and the ratio of the stressed and unstressed valence-band relaxation times in Eq. 983 is expressed as follows:

$$\frac{\tau}{\tau_0} = \frac{1}{1 + \left(\dfrac{\tau_0^{ph}}{\tau^{ph}} - 1\right)\dfrac{1 - \beta^{-1}}{1 + \left(\dfrac{N_{tot}}{N_{ref}}\right)^\alpha}} \tag{990}$$

where:

- τ_0^{ph} is the phonon-limited momentum relaxation time in the valence band for zero stress computed using Eq. 988 and Eq. 989.

- N_{tot} is the doping concentration.

- N_{ref}, α are fitting parameters of the impurity scattering model.

- β is a fitting parameter that can be represented as $\beta = 1 + \tau^{indep}/\tau_0^{ph}$, where τ^{indep} is a relaxation time of other scattering mechanisms that are not accounted for in Eq. 987 and that are independent of the stress. Therefore, for example, if the stress-independent scattering rate (not accounted for in Eq. 987) is much higher than $1/\tau_0^{ph}$, then $\beta = 1$ and therefore $\tau/\tau_0 = 1$. However, if this rate is negligible, then $\beta^{-1} = 0$.

> **NOTE** The default value of the parameter β is different for the bulk and inversion layer simulations. Some fitting of this parameter was performed to obtain a reasonable agreement of the model (Eq. 983) to multiple stress and orientation data.

Using Multivalley Hole Mobility Model

The stress-induced hole mobility model can be activated with `hMultivalley(kpDOS)` because the model uses the six-band $k \cdot p$ valence band structure. The model works in two modes: bulk and inversion layer (in the presence of `hMultivalley(MLDA kpDOS)` and inside semiconductor–insulator interface vicinity). Generally, all valleys defined by the multivalley model (for example, with `hMultivalley(kpDOS parfile)`; see Multivalley Band Structure on page 267) will be used in the model. However, currently, it is calibrated only for silicon, germanium, and SiGe band structures with the six-band $k \cdot p$ model. With `hMultivalley(MLDA)`, the multivalley MLDA quantization model (see MLDA Model on page 300) is applied to both the density and the inversion layer stress-induced mobility model. To use another quantization model in the density computation, specify the `-Density` option in the `hMultivalley` statement (see MLDA Application Notes on page 308).

The model can be used regionwise or materialwise and, typically, for PMOSFET stress simulations, it can be activated with the following keyword in the `Mobility` statement of the `Piezo` model:

```
Physics {
   hMultivalley( MLDA kpDOS )
   Piezo( Model(Mobility(hSubband(Fermi EffectiveMass Scattering(MLDA)))) )
}
```

The keyword `Fermi` defines that the Fermi–Dirac distribution function is used in Eq. 986 and Eq. 989 with the carrier self-consistent quasi-Fermi energy. To activate only doping-dependent quasi-Fermi energy, the keywords `hSubband(Doping)` should be used. If neither of these keywords (`Fermi` and `Doping`) is used, the Boltzmann distribution function is used and this illuminates the quasi-Fermi energy dependency in the mobility model (Eq. 983).

> **NOTE** If the model is used without options, as `hSubband`, then the recommended options are activated, and this is equivalent to `hSubband(Doping EffectiveMass Scattering(MLDA))`.

The keyword `EffectiveMass` means that the inverse mass tensor (Eq. 986) is computed. If this keyword is not present, the unit diagonal (and stress-independent) tensor is used as $(\bar{m}_{cond,\,i})^{-1}$ in Eq. 983. Using `EffectiveMass(Transport)` activates the 2D inverse conductivity mass tensor recomputation (similar to Eq. 979 for electrons). With the option `EffectiveMass(Transport<vector>)`, you can activate the 1D transport mass recomputation (similar to Eq. 980 for electrons) where `<vector>` represents the direction of 1D carrier transport in the simulation coordinate system.

The statement `Scattering(MLDA)` means that the scattering model (Eq. 987–Eq. 990) is used. If the keyword `Scattering` is not present, then τ/τ_0 is unit and stress independent in Eq. 983. The keyword `MLDA` in the `Scattering` statement defines that MLDA DOS is used in the scattering rate (exactly as it is in Eq. 987), but using only the keyword `Scattering` (without `MLDA`) gives the bulk scattering rates ($D^j(\varepsilon, z) = D^j_{bulk}(\varepsilon)$ in Eq. 987).

The scattering model parameters (see Eq. 987 and Eq. 990) can be specified in the parameter file in the `StressMobility` section as follows:

```
StressMobility {
    Ephonon_h = 0.0612          # [eV]
    Dop_h = 7.47e8              # [eV/cm]
    Dac_cl_h = 7.5e-6           # [eVs/cm]
    beta_h = 1e10               # [1]
    beta_mlda_h = (6.5,1.2,2.5) # [1]
    Nref_h = 3e19               # [cm^-3]
    alpha_h = 0.85              # [1]
}
```

where `Ephonon_h` corresponds to ε_{op} used in Eq. 987, `Dop_h` is D_{op} and `Dac_cl_h` is D_{ac}/c_l in Eq. 987, `beta_h` is β in Eq. 990 for the bulk case, and `beta_mlda_h` defines β for the inversion layer case for three interface orientations (100), (110), (111). These β values are a result of the calibration of the stress effect in mobility produced by the model in comparison to measurement and other simulation data. The parameters `Nref_h` and `alpha_h` correspond to the impurity scattering parameters N_{ref}, α in Eq. 990.

All conductivity mass–related parameters (used to compute $(\bar{m}_{cond,\,i})^{-1}$ in Eq. 986) are defined by the six-band $\mathbf{k \cdot p}$ model and must be specified in the `LatticeParameter` section (see Using Strained Effective Masses and DOS on page 834).

NOTE   By default, the unstressed mobility μ_{p0} (in Eq. 970) is always computed for a <110> channel orientation and for substrate orientation, which corresponds to the auto-orientation Lombardi option (see Auto-Orientation for Lombardi Model on page 337). Such a default requires you to have calibrated the Lombardi model parameters for the <110> channel (critical for (110) interface orientation where the unstressed mobility is anisotropic). However, if you want to use <100>/(110) Lombardi model parameters, the keyword `-RelChDir110` must be used inside the `hSubband` statement.

NOTE   For a general case of the tensor reference mobility ($\bar{\mu}_{p0}$), the keyword `-AutoOrientation` must be used inside the `hSubband` statement. This option can be time consuming because additional tensor operations and mobility computations must be performed for each mesh node.

All parameters of the `StressMobility` model can be mole fraction dependent. You can check this in the SiGe material parameter file.

Intel Stress-Induced Hole Mobility Model

Intel [24] suggested a mobility model for strained PMOS devices based on the occupancy of different parts of the topmost valence band. As shown in Figure 54, under zero stress, the topmost valence band has a fourfold symmetry with arms along $\langle 110 \rangle$ and $\langle \bar{1}10 \rangle$. Each ellipsoid is characterized by a transverse mass m_t and a longitudinal mass m_l.

Figure 54   Sketch of Intel two-ellipsoid model; one ellipsoid is aligned along <110> and the other along <−110>

As compressive uniaxial stress along $\langle 110 \rangle$ is applied, one of the arms shrinks and the band becomes a single ellipsoidal band. In Figure 54, this modification of the band structure is modeled as the splitting and change in curvature of two ellipsoidal bands. With applied stress, the maximum energy associated with each of these bands splits with carriers preferentially

occupying the upper valley. In addition, the transverse and longitudinal effective masses of each of these two valleys change with stress.

Under zero stress, the occupancies of the two ellipsoids are assumed equal and the mobility is isotropic with a value:

$$\mu_0 = q \langle \tau \rangle \left[\frac{0.5}{m_{t0}} + \frac{0.5}{m_{l0}} \right] \tag{991}$$

where $\langle \tau \rangle$ is the scattering time and the index '0' in effective masses corresponds to the unstressed case.

Accounting for stress-induced reoccupation of these ellipsoids f_1 and f_2, and assuming that the scattering time $\langle \tau \rangle$ is the same for both valleys and is independent of stress, the relative change in mobility is given by a diagonal tensor in the $\langle 110 \rangle$, $\langle \bar{1}10 \rangle$ coordinate system as [24]:

$$\begin{bmatrix} 1 + \dfrac{\Delta\mu_{110}}{\mu_0} \\[2ex] 1 + \dfrac{\Delta\mu_{-110}}{\mu_0} \end{bmatrix} = \frac{2m_{l0}m_{t0}}{m_{l0} + m_{t0}} \begin{bmatrix} \dfrac{f_1}{m_{t1}} + \dfrac{f_2}{m_{l2}} & 0 \\[2ex] 0 & \dfrac{f_1}{m_{l1}} + \dfrac{f_2}{m_{t2}} \end{bmatrix} \tag{992}$$

Denoting the energy split between the two values as Δ, the occupancies for the two valleys are given by:

$$f_1 = \frac{1}{1 + \exp(-\Delta/kT)}$$
$$f_2 = 1 - f_1 \tag{993}$$

where T is the lattice temperature.

Stress Dependencies

Intel decomposes the planar stress tensor in the crystallographic coordinate system as:

$$S = \begin{bmatrix} b + a & s \\ s & b - a \end{bmatrix} \tag{994}$$

where b is the biaxial component, a is the anti-symmetric component, and s is the shear component. The basic model parameters ($1/m_t$ and Δ) are expanded in powers of these components. The longitudinal mass m_l is assumed to be stress independent, that is, $m_{l1} = m_{l2} = m_{l0}$.

The symmetry of the top valence band enforces some consistency relations on the basic parameters and its power-law expansions. For example, the mobility enhancement along $\langle 110 \rangle$, when uniaxial stress along $\langle 110 \rangle$ is applied, must be equal to the enhancement along $\langle \bar{1}10 \rangle$ when uniaxial stress along $\langle \bar{1}10 \rangle$ is applied. In addition, when biaxial stress is applied, the mobility enhancements along $\langle 110 \rangle$ and $\langle \bar{1}10 \rangle$ must be the same. Enforcing these symmetries, the following expressions can be written:

$$\Delta = d_1 s$$
$$\frac{1}{m_{t1}} = \frac{1}{m_{t0}}(1 + s_{t1}s + s_{t2}s^2 + b_{t1}b + b_{t2}b^2)$$
$$\frac{1}{m_{t2}} = \frac{1}{m_{t0}}(1 - s_{t1}s + s_{t2}s^2 + b_{t1}b + b_{t2}b^2)$$

(995)

where the fitting parameters $d_1, s_{t1}, s_{t2}, b_{t1}, b_{t2}$ can be specified in the `StressMobility` section of the parameter file. The default values of these parameters are based on fitting the model to various PMOSFET stress data described in the literature [25].

Generalization of Model

The original Intel model considered only 2D planes. Therefore, it was extended and generalized in several issues: the three-dimensional case, doping dependence, and carrier redistribution between more than two valleys.

To generalize the model for the three-dimensional case, three $\langle 100 \rangle$ planes where the model is applied separately are considered. It is assumed that the valence band is a sum of six ellipsoids and this is consistent with the model suggested in the literature [26]. Sentaurus Device transforms the stress tensor into the crystal system and then, considering these three $\{100\}$ planes, it selects only the corresponding components of the stress tensor. For example, for the $[100], [010]$ plane, Sentaurus Device takes only the s_1, s_2, and s_6 stress components and recomputes them into a, b, and s of Eq. 994. Additionally, a modification of the effective mass perpendicular to the plane (parallel to the $[001]$ direction) was introduced to account better for $\langle 001 \rangle$ simulation cases: $1/m_{t\langle 001 \rangle} = (1 + b_{tt}b)/m_{t0}$, where the parameter b_{tt} can be modified in the parameter file.

With this modification, the diagonal tensor of the stress-induced mobility change in the $\langle 110 \rangle$, $\langle \bar{1}10 \rangle$, $\langle 001 \rangle$ coordinate system can be written as:

$$\begin{bmatrix} \Delta\mu_{110} \\ \Delta\mu_{-110} \\ \Delta\mu_{001} \end{bmatrix} = \mu_0 \begin{bmatrix} \left(\frac{f_1}{m_{t1}} + \frac{f_2}{m_{12}}\right)\bigg/\left(\frac{0.5}{m_{t0}} + \frac{0.5}{m_{10}}\right) - 1 & 0 & 0 \\ 0 & \left(\frac{f_1}{m_{11}} + \frac{f_2}{m_{t2}}\right)\bigg/\left(\frac{0.5}{m_{t0}} + \frac{0.5}{m_{10}}\right) - 1 & 0 \\ 0 & 0 & m_{t0}/m_{t\langle 001 \rangle} - 1 \end{bmatrix}$$

(996)

Next, the relative change of the mobility is computed independently for each plane and it is summed in the crystal system. Finally, the mobility change tensor is transformed from the crystal system to the simulation one.

The carrier occupation of the two valleys (see Eq. 993) is derived assuming Boltzmann statistics and the same density-of-states in both these valleys. To obtain a doping dependence, it is necessary to consider Fermi–Dirac statistics and, in this case, the following expression is obtained:

$$f_1 = \frac{1}{1 + F_{1/2}\left(\frac{E_V - F_p - \Delta}{kT}\right) / F_{1/2}\left(\frac{E_V - F_p}{kT}\right)}$$

$$f_2 = 1 - f_1$$

(997)

where F_p is the hole quasi-Fermi level that is computed either assuming charge neutrality between carrier and doping, which gives only the doping dependency of the model or using carrier local concentration.

As previously discussed, the generalized model considers six ellipsoids and, therefore, the carrier reoccupation between all these valleys must be accounted for. This is not a simple problem because the stress-induced energy shift of each valley must be accounted for.

As an experimental option, Sentaurus Device gives the following simplified expressions:

$$f_1 = \frac{F_{1/2}\left(\frac{E_V - F_p}{kT}\right)}{(N_e - 1)F_{1/2}\left(\frac{E_V - F_p}{kT}\right) + F_{1/2}\left(\frac{E_V - F_p - \Delta}{kT}\right)}$$

$$f_2 = \frac{F_{1/2}\left(\frac{E_V - F_p - \Delta}{kT}\right)}{(N_e - 1)F_{1/2}\left(\frac{E_V - F_p}{kT}\right) + F_{1/2}\left(\frac{E_V - F_p - \Delta}{kT}\right)}$$

(998)

where N_e is equal to the number of ellipsoids that you want to consider. The value of N_e can be specified in the parameter file. The default value is 2, which transforms Eq. 998 into Eq. 997.

> **NOTE** For this multi-ellipsoid option and $N_e > 2$, the sum $f_1 + f_2 < 1$ even without the stress. Therefore, Eq. 996 is slightly modified also to account for this different initial occupation.

Using Intel Mobility Model

To select the Intel stress-induced hole mobility model, you must include the following keyword in the `Mobility` statement of the `Piezo` model:

```
Physics {
   Piezo( Model(Mobility(hSixBand)) )
}
```

The keyword `hSixBand` assumes Boltzmann statistics and, in this case, Eq. 993 will be activated. To have doping dependence (see Eq. 997), the keyword `hSixBand(Doping)` should be specified, but to have carrier concentration dependency (Fermi statistics), use the keywords `hSixBand(Fermi)`. The model parameters (see Eq. 995) can be specified in the `StressMobility` section of the parameter file as follows:

```
StressMobility {
   mh_l0 = 0.48        # [1]
   mh_t0 = 0.15        # [1]
   ne = 2              # [1]
   d1 = -6.0000e-11    # [eV/Pa]
   st1 = -9.4426e-10   # [1/Pa]
   st2 = 4.3066e-19    # [1/Pa^2]
   bt1 = -1.0086e-10   # [1/Pa]
   bt2 = 6.5886e-21    # [1/Pa^2]
   btt = 1.2000e-10    # [1/Pa]
}
```

PMOS transistors are usually oriented in the direction to have maximum stress effect. To define this direction for the x-axis of a Sentaurus Device simulation, the following parameter set can be specified for the 2D case:

```
LatticeParameters {
   X = (1, 0, 1) #[1]
   Y = (0, 1, 0) #[1]
}
```

The `hSixBand` carrier occupancies f_1 and f_2 are calculated in the crystallographic coordinate system for each band. To plot these values, use the following keywords in the `Plot` section of the command file:

- `f1BandOccupancy001` = Occupancy of the $\langle \bar{1}10 \rangle$ ellipsoid in the (001) plane
- `f2BandOccupancy001` = Occupancy of the $\langle 110 \rangle$ ellipsoid in the (001) plane
- `f1BandOccupancy010` = Occupancy of the $\langle \bar{1}10 \rangle$ ellipsoid in the (010) plane
- `f2BandOccupancy010` = Occupancy of the $\langle 110 \rangle$ ellipsoid in the (010) plane
- `f1BandOccupancy100` = Occupancy of the $\langle \bar{1}10 \rangle$ ellipsoid in the (100) plane
- `f2BandOccupancy100` = Occupancy of the $\langle 110 \rangle$ ellipsoid in the (100) plane

Piezoresistance Mobility Model

This approach [5][7][27] focuses on the modeling of the piezoresistive effect. The model is based on an expansion of the mobility enhancement tensor in terms of stress. Sentaurus Device provides options for computing either a first-order or a second-order piezoresistance mobility model. The first-order model accounts for a linear dependency on stress; whereas, the second-order model accounts for both linear and quadratic dependencies on stress.

The electron or hole mobility enhancement tensor, expanded up to second order in stress, is given by:

$$\frac{\mu_{ij}}{\mu_0} = \delta_{ij} + \sum_{k=1}^{3}\sum_{l=1}^{3}\Pi_{ijkl}\sigma_{kl} + \sum_{k=1}^{3}\sum_{l=1}^{3}\sum_{m=1}^{3}\sum_{n=1}^{3}\Pi_{ijklmn}\sigma_{kl}\sigma_{mn} \tag{999}$$

where:

- μ_{ij} is a component of the electron or hole stress-dependent mobility tensor.
- μ_0 denotes the isotropic mobility without stress.
- δ_{ij} is the Kronecker delta function.
- σ_{kl} is a component of the stress tensor.
- Π_{ijkl} is a component of the first-order electron or hole piezoconductance tensor.
- Π_{ijklmn} is a component of the second-order electron or hole piezoconductance tensor.

The piezoconductance tensors are symmetric, which allows Eq. 999 to be written in a contracted form using index contraction (Eq. 936) and conventional contraction rules (see [7], for example):

$$\frac{\mu_i}{\mu_0} = (\delta_{i1} + \delta_{i2} + \delta_{i3}) + \sum_{j=1}^{6}\Pi_{ij}\sigma_j + \sum_{j=1}^{6}\sum_{k=1}^{6}\Pi_{ijk}\sigma_j\sigma_k \tag{1000}$$

The components of the piezoconductance tensors are related to the components of the more familiar piezoresistance tensors through the following relations [7]:

$$\begin{aligned}
\pi_{ij} &= -\Pi_{ij} &\leftrightarrow\quad \Pi_{ij} &= -\pi_{ij} \\
\pi_{ijk} &= -\Pi_{ijk} + \Pi_{ij}\Pi_{ik} &\leftrightarrow\quad \Pi_{ijk} &= -\pi_{ijk} + \pi_{ij}\pi_{ik}
\end{aligned} \tag{1001}$$

where π_{ij} and π_{ijk} are components of the first-order and second-order piezoresistance tensors, respectively. When the first-order model is used (the default), only the first summation in Eq. 1000 is included in the calculation. When the second-order model is used, the full expression given by Eq. 1000 is used.

In crystals with cubic symmetry such as silicon, the number of independent coefficients of the first-order piezoresistance tensor reduces to three by rotating the coordinate system parallel to the high-symmetric axes of the crystal [8] resulting in the following 6×6 tensor:

$$[\pi_{ij}] = \begin{bmatrix} \pi_{11} & \pi_{12} & \pi_{12} & 0 & 0 & 0 \\ \pi_{12} & \pi_{11} & \pi_{12} & 0 & 0 & 0 \\ \pi_{12} & \pi_{12} & \pi_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \pi_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \pi_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \pi_{44} \end{bmatrix} \qquad (1002)$$

The second-order piezoresistance tensor has only nine independent components and can be expressed with the following $6 \times 6 \times 6$ tensor:

$$[\pi_{1jk}] = \begin{bmatrix} \pi_{111} & \pi_{112} & \pi_{112} & 0 & 0 & 0 \\ \pi_{112} & \pi_{122} & \pi_{123} & 0 & 0 & 0 \\ \pi_{112} & \pi_{123} & \pi_{122} & 0 & 0 & 0 \\ 0 & 0 & 0 & \pi_{144} & 0 & 0 \\ 0 & 0 & 0 & 0 & \pi_{166} & 0 \\ 0 & 0 & 0 & 0 & 0 & \pi_{166} \end{bmatrix} \quad [\pi_{2jk}] = \begin{bmatrix} \pi_{122} & \pi_{112} & \pi_{123} & 0 & 0 & 0 \\ \pi_{112} & \pi_{111} & \pi_{112} & 0 & 0 & 0 \\ \pi_{123} & \pi_{112} & \pi_{122} & 0 & 0 & 0 \\ 0 & 0 & 0 & \pi_{166} & 0 & 0 \\ 0 & 0 & 0 & 0 & \pi_{144} & 0 \\ 0 & 0 & 0 & 0 & 0 & \pi_{166} \end{bmatrix} \quad [\pi_{3jk}] = \begin{bmatrix} \pi_{122} & \pi_{123} & \pi_{112} & 0 & 0 & 0 \\ \pi_{123} & \pi_{122} & \pi_{112} & 0 & 0 & 0 \\ \pi_{112} & \pi_{112} & \pi_{111} & 0 & 0 & 0 \\ 0 & 0 & 0 & \pi_{166} & 0 & 0 \\ 0 & 0 & 0 & 0 & \pi_{166} & 0 \\ 0 & 0 & 0 & 0 & 0 & \pi_{144} \end{bmatrix}$$

$$[\pi_{4jk}] = \begin{bmatrix} 0 & 0 & 0 & \pi_{441} & 0 & 0 \\ 0 & 0 & 0 & \pi_{661} & 0 & 0 \\ 0 & 0 & 0 & \pi_{661} & 0 & 0 \\ \pi_{441} & \pi_{661} & \pi_{661} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \pi_{456} \\ 0 & 0 & 0 & 0 & \pi_{456} & 0 \end{bmatrix} \quad [\pi_{5jk}] = \begin{bmatrix} 0 & 0 & 0 & 0 & \pi_{661} & 0 \\ 0 & 0 & 0 & 0 & \pi_{441} & 0 \\ 0 & 0 & 0 & 0 & \pi_{661} & 0 \\ 0 & 0 & 0 & 0 & 0 & \pi_{456} \\ \pi_{661} & \pi_{441} & \pi_{661} & 0 & 0 & 0 \\ 0 & 0 & 0 & \pi_{456} & 0 & 0 \end{bmatrix} \quad [\pi_{6jk}] = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \pi_{661} \\ 0 & 0 & 0 & 0 & 0 & \pi_{661} \\ 0 & 0 & 0 & 0 & 0 & \pi_{441} \\ 0 & 0 & 0 & 0 & \pi_{456} & 0 \\ 0 & 0 & 0 & \pi_{456} & 0 & 0 \\ \pi_{661} & \pi_{661} & \pi_{441} & 0 & 0 & 0 \end{bmatrix}$$

$$(1003)$$

Since the coordinate system of the simulation is not necessarily parallel to the high-symmetric axis of the crystal, the orientations of the x-axis and y-axis of the crystal system can be specified in the command file (see Using Stress and Strain on page 823).

Doping and Temperature Dependency

A simple model for the doping and temperature variation of the first-order and second-order piezoconductance coefficients is given by [7][28]:

$$\begin{aligned} \Pi_{ij}(N, T) &= P_1(N, T)\Pi_{ij}(0, 300\text{K}) \\ \Pi_{ijk}(N, T) &= P_2(N, T)\Pi_{ijk}(0, 300\text{K}) \end{aligned} \qquad (1004)$$

where $\Pi_{ij}(0, 300\text{K})$ and $\Pi_{ijk}(0, 300\text{K})$ are piezoconductance coefficients for low-doped silicon at 300 K, and $P_1(N, T)$ and $P_2(N, T)$ are doping factors given by:

$$P_1(N, T) = \left(\frac{300\text{K}}{T}\right)\frac{F_{-1}(\eta)}{F_0(\eta)}$$

$$P_2(N, T) = \left(\frac{300\text{K}}{T}\right)^2\frac{F_{-2}(\eta)}{F_0(\eta)}$$

(1005)

In Eq. 1005, $F_r(\eta)$ is a Fermi–Dirac integral of order "r" and η is the Fermi energy measured from the band edge in units of kT ($\eta_n = (E_{\text{F}, n} - E_\text{C})/(kT)$ and $\eta_p = (E_\text{V} - E_{\text{F}, p})/(kT)$). Doping dependency is introduced by assuming charge neutrality in the calculation of the Fermi energy.

> **NOTE** For minority carriers, the doping factors $P_1(N, T)$ and $P_2(N, T)$ are equal to 1. In addition, Sentaurus Device allows the calculation to be suppressed for majority carriers when the doping is below a user-specified doping threshold (see Stress Mobility Model for Minority Carriers on page 877).

The temperature and doping variation of the piezoresistance coefficients is obtained by combining Eq. 1001 and Eq. 1004. An exception to this is when the first-order model is used. In this case, the piezoresistance coefficients are split between a constant part (associated with changes in the effective masses) and a part that varies with temperature and doping (associated with anisotropic scattering):

$$\pi_{ij}(N, T) = \pi_{ij, \text{var}}P_1(N, T) + \pi_{ij, \text{con}}$$

(1006)

The default values of the piezoresistance coefficients for low-doped silicon at 300 K are listed in Table 146 on page 862 and Table 147 on page 862. They can be changed in the parameter file as described in Using Piezoresistance Mobility Model on page 861.

Using Piezoresistance Mobility Model

The command file syntax for the piezoresistance mobility models, including options, is:

```
Physics {
  Piezo (
    Model (
      Mobility (
        Tensor (
          [FirstOrder | SecondOrder] [Enormal | <pmi_model>] [Kanda]
          [ParameterSetName= "<psname>" | AutoOrientation]
        )
      )
    )
```

```
    )
  }
```

The keyword `Tensor` selects the anisotropic tensor model for electron and hole mobility. Alternatively, the keywords `eTensor` or `hTensor` can be used to select this model for only one carrier.

The keyword `FirstOrder` or `SecondOrder` selects the first-order or second-order model, respectively. The default is `FirstOrder`. When the `FirstOrder` model is used, Sentaurus Device uses the piezoresistance coefficients shown in Table 146. These can be changed from their default values in the `Piezoresistance` section of the parameter file.

Table 146   Piezoresistance coefficients for FirstOrder model: Defaults for silicon

Symbol	Parameter name	Electrons	Holes	Unit
$\pi_{11,\,var}$	p11var	-1.026×10^{-9}	1.5×10^{-11}	Pa^{-1}
$\pi_{12,\,var}$	p12var	5.34×10^{-10}	1.5×10^{-11}	Pa^{-1}
$\pi_{44,\,var}$	p44var	-1.36×10^{-10}	1.1×10^{-9}	Pa^{-1}
$\pi_{11,\,con}$	p11con	0.0	5.1×10^{-11}	Pa^{-1}
$\pi_{12,\,con}$	p12con	0.0	-2.6×10^{-11}	Pa^{-1}
$\pi_{44,\,con}$	p44con	0.0	2.8×10^{-10}	Pa^{-1}

When the `SecondOrder` model is used, Sentaurus Device uses the piezoresistance coefficients shown in Table 147. These also can be changed from their default values in the `Piezoresistance` section of the parameter file. Note that the `SecondOrder` model uses a different set of first-order piezoresistance coefficients than the `FirstOrder` model. This allows the `FirstOrder` and `SecondOrder` models to be calibrated separately.

Table 147   Piezoresistance coefficients for SecondOrder model: Defaults for silicon

Symbol	Parameter name	Electrons	Holes	Unit
π_{11}	p11	-1.1×10^{-9}	0.0	Pa^{-1}
π_{12}	p12	4.5×10^{-10}	2.0×10^{-11}	Pa^{-1}
π_{44}	p44	2.5×10^{-10}	1.19×10^{-9}	Pa^{-1}
π_{111}	p111	6.6×10^{-19}	-4.5×10^{-19}	Pa^{-2}
π_{112}	p112	-5.5×10^{-20}	2.8×10^{-19}	Pa^{-2}
π_{122}	p122	-2.2×10^{-20}	-2.5×10^{-19}	Pa^{-2}
π_{123}	p123	8.8×10^{-19}	2.0×10^{-20}	Pa^{-2}
π_{144}	p144	1.0×10^{-20}	-3.3×10^{-19}	Pa^{-2}

Table 147 Piezoresistance coefficients for SecondOrder model: Defaults for silicon

Symbol	Parameter name	Electrons	Holes	Unit
π_{166}	p166	-6.9×10^{-19}	6.6×10^{-19}	Pa^{-2}
π_{661}	p661	6.0×10^{-21}	-3.1×10^{-19}	Pa^{-2}
π_{456}	p456	2.0×10^{-20}	-3.0×10^{-19}	Pa^{-2}
π_{441}	p441	2.0×10^{-20}	0.0	Pa^{-2}

The keyword Kanda activates the calculation of the doping factors $P_1(N, T)$ and $P_2(N, T)$ (see Eq. 1005). If Kanda is not specified, these factors are equal to 1.

Named Parameter Sets for Piezoresistance

The Piezoresistance parameter set can be named. For example, in the parameter file, you can write the following to declare a parameter set with the name myset:

```
Piezoresistance "myset" { ... }
```

To use a named parameter set, specify its name with ParameterSetName as an option to Tensor as shown in the command file syntax (see Using Piezoresistance Mobility Model on page 861).

By default, the unnamed parameter set is used.

Auto-Orientation for Piezoresistance

The piezoresistance models support the auto-orientation framework (see Auto-Orientation Framework on page 37) that switches between different named parameter sets based on the orientation of the nearest interface. This can be activated by specifying AutoOrientation as an argument to Tensor in the command file.

Enormal- and MoleFraction-Dependent Piezo Coefficients

Measured data shows that the piezoresistive coefficients can have dependencies with respect to the normal electric field $E_\perp$ or the mole fraction x or both. Sentaurus Device has a calibration option to specify these dependencies of the piezoresistive coefficients.

This model is based on the piezoresistive prefactors $P_{ij} = P_{ij}(E_\perp, x)$. The new coefficients are calculated from:

$$\pi_{ij, \text{new}} = P_{ij}(E_\perp, x) \cdot \pi_{ij} \tag{1007}$$

Sentaurus Device allows a piecewise linear or spline approximation (the third degree) of the prefactors over the normal electric field and a piecewise linear or piecewise cubic approximation over the mole fraction (see Ternary Semiconductor Composition on page 25).

Using Piezoresistive Prefactors Model

To activate this model, add the keyword `Enormal` to the subsection `{e,h}Tensor`, for example:

```
Physics {
    ...
    Piezo(
        Model(Mobility(eTensor(Kanda Enormal)))
    )
}
```

The implementation of this model is based on the PMI (see Piezoresistive Coefficients on page 1237). The keyword `Enormal` means that Sentaurus Device uses the PMI predefined model `PmiEnormalPiezoResist`. You can create your own PMI models and, in this case, the keyword `Enormal` must be replaced by the name of the PMI model (for example, `eTensor("my_pmi_model")`) and the parameter file must contain a corresponding section.

> **NOTE** Piezoresistive prefactors are only available when using the `FirstOrder` piezoresistance mobility model. In addition, named parameter sets and auto-orientation are not supported for piezoresistive prefactors.

By default, the values of all prefactors are equal to 1. These values can be changed in the section `PmiEnormalPiezoResist` of the parameter file. The following examples show how to use this section.

Example 1

This example shows the section of the parameter file for purely `Enormal`-dependent prefactors:

```
Material = "Silicon" {
* Example 1: Only Enormal dependence of piezoresistive coefficients
PmiEnormPiezoResist
{
    eEnormalFormula = 2 # cubic spline
*                 = 0 # no Enormal dependence (default)
*                 = 1 # piecewise linear approximation
*                 = 2 # cubic spline approximation

    eNumberOfEnormalNodes = 3   # number of nodes for Spline(Enormal)
```

```
    # _k is _"index of node"
eEnormal_1 = 1.0e+5 # [V/cm
   eP11_1 = 1.0     # [1]
   eP12_1 = 1.0     # [1]
   eP44_1 = 1.0     # [1]

eEnormal_2 = 4.0e+5 # [V/cm]
   eP11_2 = 0.75    # [1]
   eP12_2 = 0.75    # [1]
   eP44_2 = 0.75    # [1]

eEnormal_3 = 7.0e+5 # [V/cm]
   eP11_3 = 0.5     # [1]
   eP12_3 = 0.5     # [1]
   eP44_3 = 0.5     # [1]

hEnormalFormula = 1       # piecewise linear approximation
hNumberOfEnormalNodes = 4 # number of nodes

   # _k is _"index of the node"
hEnormal_1 = 1.0e+5 # [V/cm]
   hP11_1 = 1.0     # [1]
   hP12_1 = 1.0     # [1]
   hP44_1 = 1.0     # [1]

hEnormal_2 = 1.9e+5 # [V/cm]
   hP11_2 = 0.969625 # [1]
   hP12_2 = 0.969625 # [1]
   hP44_2 = 0.969625 # [1]

hEnormal_3 = 6.1e+5 # [V/cm]
   hP11_3 = 0.530375 # [1]
   hP12_3 = 0.530375 # [1]
   hP44_3 = 0.530375 # [1]

hEnormal_4 = 7.0e+5 # [V/cm]
   hP11_4 = 0.5     # [1]
   hP12_4 = 0.5     # [1]
   hP44_4 = 0.5     # [1]
}
}
```

Figure 55 shows the dependency of these piezo prefactors with respect to `Enormal`.

Figure 55   Example of cubic spline and piecewise linear approximation of piezo prefactors

Example 2

This example shows the section of the parameter file for purely `MoleFraction`-dependent prefactors:

```
Material = "SiliconGermanium" {
* Mole dependent material: SiliconGermanium (x=0) = Silicon
* Mole dependent material: SiliconGermanium (x=1) = Germanium
* Example 2: Only MoleFraction dependence.
PmiEnormPiezoResist
{
   eMoleFormula = 1             # piecewise linear approximation
   eMoleFractionIntervals = 1  # number of MoleFraction intervals
                               # i.e. x0=0, x1=1

     # _i is _"index of mole fraction value"
   eXmax_0 = 0
     eP11_0 = 1 # [1]
     eP12_0 = 1 # [1]
     eP44_0 = 1 # [1]
```

```
      eXmax_1 = 1
        eP11_1 = 0.5 # [1]
        eP12_1 = 0.5 # [1]
        eP44_1 = 0.5 # [1]

        hMoleFormula = 2    # piecewise cubic approximation
        hMoleFractionIntervals = 2
           # see Ternary Semiconductor Composition on page 25
           # P = P[i-1] + A[i]*dx + B[i]*dx^2 + C[i]*dx^3
           # where:
           # A[i]  = (P[i]-P[i-1])/dx[i] - B[i]*dx[i] - C[i]*dx[i]
           # dx[i] = xMax[i] - xMax[i-1]
           # dx    = x - xMax[i-1]
           # i = 1,..,nbMoleIntervals

        # _i is _"index of mole fraction value"
      hXmax_0 = 0
        hP11_0 = 1 # [1]
        hP12_0 = 1 # [1]
        hP44_0 = 1 # [1]

      hXmax_1 = 0.5
        hP11_1 = 2 # [1]
        hP12_1 = 2 # [1]
        hP44_1 = 2 # [1]

        # B and C coefficients
        hB11_1 = 4.
        hC11_1 = 0.
        hB12_1 = 4.
        hC12_1 = 0.
        hB44_1 = 4.
        hC44_1 = 0.

      hXmax_2 = 1
        hP11_2 = 3 # [1]
        hP12_2 = 3 # [1]
        hP44_2 = 3 # [1]

        # B and C coefficients
        hB11_2 = -4.
        hC11_2 =  0.
        hB12_2 = -4.
        hC12_2 =  0.
        hB44_2 = -4.
        hC44_2 =  0.
    }
  }
```

Figure 56 shows the dependency of the `hPij` prefactors of the previous example with respect to `MoleFraction`.

Figure 56   Example of piecewise cubic approximation

Example 3

This example shows the section of the parameter file for `Enormal`- and `MoleFraction`-dependent prefactors:

```
Material = "SiliconGermanium" {
* Mole dependent material: SiliconGermanium (x=0) = Silicon
* Mole dependent material: SiliconGermanium (x=1) = Germanium

* Example 3: Enormal and MoleFraction dependent piezoresistance prefactors
* (general case)
PmiEnormPiezoResist
{

    eMoleFormula = 2          # piecewise cubic approximation
    eMoleFractionIntervals = 1  # i.e. x0=0, x1=1

# begin description for mole fraction x0=0
    eXmax_0 = 0
    eEnormalFormula_0 = 2       # cubic spline
    eNumberOfEnormalNodes_0 = 3 # number of nodes for Spline(Enormal)
```

```
    # _i_k is _"index of mole fraction value"_"index of node for Spline"
  eEnormal_0_1 = 1.0e+5 # [V/cm]
     eP11_0_1 = 1.0 # [1]
     eP12_0_1 = 1.0 # [1]
     eP44_0_1 = 1.0 # [1]

  eEnormal_0_2 = 4.0e+5 # [V/cm]
     eP11_0_2 = 0.75 # [1]
     eP12_0_2 = 0.75 # [1]
     eP44_0_2 = 0.75 # [1]

  eEnormal_0_3 = 7.0e+5 # [V/cm]
     eP11_0_3 = 0.5 # [1]
     eP12_0_3 = 0.5 # [1]
     eP44_0_3 = 0.5 # [1]
# end description for mole fraction x0=0

# begin description for mole fraction x1=1
  eXmax_1 = 1
  eEnormalFormula_1 = 1    # piecewise linear approximation
  eNumberOfEnormalNodes_1 = 2 # number of nodes

    # _i_k is _"index of mole fraction value"_"index of node for Spline"
  eEnormal_1_1 = 1.0e+5 # [V/cm]
     eP11_1_1 = 1.0 # [1]
     eP12_1_1 = 1.0 # [1]
     eP44_1_1 = 1.0 # [1]

  eEnormal_1_2 = 7.0e+5 # [V/cm]
     eP11_1_2 = 0.5 # [1]
     eP12_1_2 = 0.5 # [1]
     eP44_1_2 = 0.5 # [1]

     # B and C coefficients
     hB11_1 = 3.
     hC11_1 = -2.
     hB12_1 = 3.
     hC12_1 = -2.
     hB44_1 = 3.
     hC44_1 = -2.

# end description for mole fraction x1=1

# hPij prefactors are equal to default values (i.e. 1)
}
}
```

Figure 57 shows the difference between I_d–V_g curves for a MOSFET. The parameter file section `PmiEnormPiezoResist` is the same as in Example 1 on page 864. The `Physics` section is:

```
Physics {
   Fermi
   Mobility( Phumob HighFieldsat Enormal )
   EffectiveIntrinsicDensity( BandGapNarrowing(OldSlotboom) )
   Recombination( SRH(DopingDependence) )
   Piezo(
      Model( Mobility(eTensor(Kanda Enormal)) DeformationPotential )
      Stress = (1.3e8, 0, 0, 0, 0, 0)
   )
}
```


Figure 57 I_d–V_g curve, with Enormal-dependent piezo prefactors, shifts downwards

Isotropic Factor Models

Sentaurus Device provides options for calculating stress-dependent enhancement factors that are applied to mobility as isotropic factors. These options, known as `Factor` models, can be used as an alternative to the tensor-based models and provide a robust approximate solution for cases where current in the device is predominantly in a direction parallel to one of the coordinate axes.

By default, the mobility enhancement factor γ calculated from a `Factor` model is applied to the total unstressed low-field mobility, $\mu_{low,0}$:

$$\mu_{low} = \gamma \mu_{low,0} \tag{1008}$$

where:

$$\gamma = 1 + \frac{\Delta\mu_{low}}{\mu_{low,0}} \tag{1009}$$

However, the option `ApplyToMobilityComponents` allows the enhancement factor to be applied to individual mobility components (see Factor Models Applied to Mobility Components on page 876).

The choices for isotropic `Factor` models include `FirstOrder` or `SecondOrder` piezoresistance models, `EffectiveStressModel`, a mobility stress factor PMI model, and an `SFactor` dataset or PMI model.

Using Isotropic Factor Models

The command file syntax for the isotropic `Factor` models, including options, is:

```
Physics {
  Piezo (
    Model (
      Mobility (
        Factor (
          [ FirstOrder | SecondOrder |
            EffectiveStressModel([AxisAlignedNormals]) |
            <mobility_stress_factor_pmi_model> |
            SFactor="<dataset_name-or-pmi_model_name>" ]
          [ChannelDirection=<n>] [Kanda]
          [AutoOrientation | ParameterSetName="<psname>"]
          [ApplyToMobilityComponents]
        )
      )
    )
  )
}
```

The keyword `Factor` selects an isotropic factor model for electron and hole mobility. Alternatively, the keywords `eFactor` or `hFactor` can be used to select these models for only one carrier.

Descriptions of the model choices and options are given in the following sections.

Piezoresistance Factor Models

These models are based on the full piezoresistance tensor calculations described in Piezoresistance Mobility Model on page 859.

The piezoresistance `Factor` models use one of the diagonal components of the piezoresistance mobility enhancement tensor in the simulation coordinate system (Eq. 1000 after transformation from the crystallographic coordinate system) as the isotropic factor γ that is applied to mobility. When using this option, the channel direction must be specified using the `ChannelDirection` parameter, which determines the component of the mobility enhancement tensor to use (the default is `ChannelDirection=1`):

$$\gamma = \begin{cases} \mu'_1/\mu_0 = \mu'_{xx}/\mu_0 \text{ , ChannelDirection=1} \\ \mu'_2/\mu_0 = \mu'_{yy}/\mu_0 \text{ , ChannelDirection=2} \\ \mu'_3/\mu_0 = \mu'_{zz}/\mu_0 \text{ , ChannelDirection=3} \end{cases} \tag{1010}$$

As with the piezoresistance tensor models, either a `FirstOrder` or `SecondOrder` model can be selected, and piezoresistance coefficients can be specified in the `Piezoresistance` section of the parameter file (see Table 146 on page 862 and Table 147 on page 862).

Effective Stress Model

The `EffectiveStressModel` is an isotropic `Factor` model that relates the mobility enhancement γ in a device to an effective stress parameter that is calculated from the diagonal components of the 3D stress tensor [29]:

$$\gamma = \frac{1}{\mu_0} \left(\frac{A_1 - A_2}{1 + \exp\left(\frac{S_{\text{eff}} - S_0}{t}\right)} + A_2 \right) \tag{1011}$$

where:

$$A_1 = \begin{cases} a_{10} + a_{11}\left(\frac{F_\perp}{10^6 \text{ V/cm}}\right) + a_{12}\left(\frac{F_\perp}{10^6 \text{ V/cm}}\right)^2 \text{ , } F_\perp \leq F_0 \times 10^6 \text{ V/cm} \\ a_{10} + a_{11}F_0 + a_{12}F_0^2 \qquad\qquad , F_\perp > F_0 \times 10^6 \text{ V/cm} \end{cases} \tag{1012}$$

$$A_2 = \begin{cases} a_{20} + a_{21}\left(\dfrac{F_\perp}{10^6 \text{ V/cm}}\right) + a_{22}\left(\dfrac{F_\perp}{10^6 \text{ V/cm}}\right)^2 & , F_\perp \le F_0 \times 10^6 \text{ V/cm} \\[4mm] a_{20} + a_{21}F_0 + a_{22}F_0^2 & , F_\perp > F_0 \times 10^6 \text{ V/cm} \end{cases} \tag{1013}$$

$$S_0 = \begin{cases} s_{00} + s_{01}\left(\dfrac{F_\perp}{10^6 \text{ V/cm}}\right) + s_{02}\left(\dfrac{F_\perp}{10^6 \text{ V/cm}}\right)^2 & , F_\perp \le F_0 \times 10^6 \text{ V/cm} \\[4mm] s_{00} + s_{01}F_0 + s_{02}F_0^2 & , F_\perp > F_0 \times 10^6 \text{ V/cm} \end{cases} \tag{1014}$$

$$t = t_0 + t_1\left(\frac{F_\perp}{10^6 \text{ V/cm}}\right) + t_2\left(\frac{F_\perp}{10^6 \text{ V/cm}}\right)^2 \tag{1015}$$

$F_\perp$ is the normal electric field and μ_0, a_{10}, a_{11}, a_{12}, a_{20}, a_{21}, a_{22}, s_{00}, s_{01}, s_{02}, t_0, t_1, t_2, and F_0 are model parameters.

Effective Stress

In Eq. 1011, S_{eff} is an effective stress parameter and is given by:

$$S_{\text{eff}}(\text{MPa}) = \sum_{i=1}^{3} \alpha_i\left(\frac{S_{ii}}{10^6 \text{ Pa}}\right) + \sum_{i=1}^{3}\sum_{j\ge i}^{3} \beta_{ij}\left(\frac{S_{ii}}{10^6 \text{ Pa}}\right)\left(\frac{S_{jj}}{10^6 \text{ Pa}}\right) \tag{1016}$$

where α_i and β_{ij} are model parameters, and S_{ii} is a diagonal component of the stress tensor. The subscripts in Eq. 1016 have the following meaning:

$$i, j = \begin{cases} 1 \to \text{channel direction} \\ 2 \to \text{nearest interface normal direction} \\ 3 \to \text{in-plane direction} \end{cases} \tag{1017}$$

The assignment of S_{11}, S_{22}, and S_{33} is on a vertex-by-vertex basis.

S_{11} is always assigned the diagonal component of stress that is associated with the `ChannelDirection` specification:

$$S_{11} = \begin{cases} \sigma_{xx} , \texttt{ChannelDirection=1} \\ \sigma_{yy} , \texttt{ChannelDirection=2} \\ \sigma_{zz} , \texttt{ChannelDirection=3} \end{cases} \tag{1018}$$

The assignment of S_{22} and S_{33} is performed automatically by Sentaurus Device and depends on the dimensionality of the structure, ChannelDirection, and the nearest interface normal direction.

In 2D structures with $S_{11} \neq \sigma_{zz}$:

- If $S_{11} = \sigma_{xx}$, then $S_{22} = \sigma_{yy}$ and $S_{33} = \sigma_{zz}$.
- If $S_{11} = \sigma_{yy}$, then $S_{22} = \sigma_{xx}$ and $S_{33} = \sigma_{zz}$.

In 3D structures, or 2D structures with $S_{11} = \sigma_{zz}$, the nearest interface normal may not be aligned with an axis direction. In this case, a stress transformation is made to a coordinate system (x', y', z') where x' is aligned with the channel direction, y' is aligned with the component of the nearest interface normal that is not in the channel direction, and z' is aligned with $x' \times y'$. After the stress transformation, the stress assignments are:

$$
\begin{aligned}
S_{11} &= \sigma_{x'x'} \\
S_{22} &= \sigma_{y'y'} \\
S_{33} &= \sigma_{z'z'}
\end{aligned}
\tag{1019}
$$

Alternatively, the S_{22} assignment also can be made by choosing the diagonal stress component corresponding to the direction for which the nearest interface normal has its largest component (excluding any component in the channel direction). In this case, the assignment is performed as if the interface normal is aligned along an axis. S_{33} is then taken as the component that is not assigned to S_{11} or S_{22}. To select this option, specify AxisAlignedNormals as an argument to the EffectiveStressModel.

Effective Stress Model Parameters

The EffectiveStressModel parameters can be specified in the EffectiveStressModel parameter set in the parameter file. Table 148 lists the model parameters from [29] for two different surface orientations. The (100) parameters are used by default.

Table 148 Effective stress model parameters

Symbol	Parameter name	(100)/<110> Electrons	(100)/<110> Holes	(110)/<110> Electrons	(110)/<110> Holes	Unit
α_1	alpha1	1.0	1.0	1.0	1.0	MPa
α_2	alpha2	−1.7	−0.4	0.8	−0.3	MPa
α_3	alpha3	0.7	−0.6	−1.8	−0.7	MPa
β_{11}	beta11	0.0	0.0	0.0	0.0	MPa
β_{12}	beta12	0.0	0.0	0.0	0.0	MPa
β_{13}	beta13	0.0	−0.00004	0.0	0.0	MPa

Table 148 Effective stress model parameters (Continued)

Symbol	Parameter name	(100)/<110> Electrons	(100)/<110> Holes	(110)/<110> Electrons	(110)/<110> Holes	Unit
β_{22}	`beta22`	0.0	0.00006	0.0	0.0001	MPa
β_{23}	`beta23`	0.0	–0.00018	0.0	0.0	MPa
β_{33}	`beta33`	0.0	0.00011	0.0	0.0	MPa
μ_0	`mu0`	810.0	212.0	326.0	1235.0	$cm^2/(Vs)$
a_{10}	`a10`	565.0	2460.0	270.0	505.0	$cm^2/(Vs)$
a_{11}	`a11`	–81.0	0.0	0.0	–365.0	$cm^2/(Vs)$
a_{12}	`a12`	–44.0	0.0	0.0	164.0	$cm^2/(Vs)$
a_{20}	`a20`	2028.0	42.0	761.0	9136.0	$cm^2/(Vs)$
a_{21}	`a21`	–1992.0	0.0	0.0	–25027.0	$cm^2/(Vs)$
a_{22}	`a22`	920.0	0.0	0.0	24494.0	$cm^2/(Vs)$
s_{00}	`s00`	1334.0	–1338.0	799.0	–2084.0	MPa
s_{01}	`s01`	–2646.0	0.0	0.0	6879.0	MPa
s_{02}	`s02`	875.0	0.0	0.0	–6896.0	MPa
t_0	`t0`	882.0	524.0	417.0	–650.0	MPa
t_1	`t1`	–987.0	0.0	0.0	0.0	MPa
t_2	`t2`	604.0	0.0	0.0	0.0	MPa
F_0	`F0`	10^{10}	10^{10}	10^{10}	0.5	1
F_{fixed}	`F_fixed`	–1	–1	–1	–1	MV/cm

By default, the F_{fixed} parameter is ignored. Specifying $F_{\text{fixed}} \geq 0$ causes a fixed value of the normal field to be used in the evaluation of γ instead of the actual normal field. This is useful for calibration or examination of model behavior.

Mobility Stress Factor PMI Model

A mobility stress factor PMI model (see Mobility Stress Factor on page 1193) created by the user can be utilized to obtain a mobility enhancement factor. In addition to stress, this type of PMI model allows a dependency on the normal electric field.

If specified, the `Factor` options `ChannelDirection=<n>`, `AutoOrientation`, and `ParameterSetName="<psname>"` are passed as parameters to the mobility stress factor PMI model (`AutoOrientation` is passed as `AutoOrientation=1`).

SFactor Dataset or PMI Model

The `SFactor` parameter can be used to obtain an isotropic mobility enhancement factor from a dataset or a PMI model.

If `SFactor="<dataset_name>"` is used, the vertex values of γ are taken directly from the specified dataset name, which can include the PMI user fields `PMIUserField0` through `PMIUserField299`.

If `SFactor="<pmi_model_name>"` is used, the vertex values of γ are calculated from a space factor PMI model (see Space Factor on page 1190). If specified, the `Factor` options `ChannelDirection=<n>`, `AutoOrientation`, and `ParameterSetName="<psname>"` are passed as parameters to the space factor PMI model (`AutoOrientation` is passed as `AutoOrientation=1`).

Isotropic Factor Model Options

Kanda Parameter

The `Kanda` parameter can be specified for all isotropic factor models to include a doping and temperature dependency in the enhancement factor calculation. In the case of the `FirstOrder` and `SecondOrder` piezoresistance models, this is included as described in Doping and Temperature Dependency on page 860. For the `EffectiveStressModel` and `SFactor` models, the enhancement factor given by Eq. 1009 is modified to include the $P_1(N, T)$ factor (see Eq. 1005):

$$\gamma = 1 + P_1(N, T)\frac{\Delta\mu_{\text{low}}}{\mu_{\text{low},0}} \tag{1020}$$

Named Parameter Sets and Auto-Orientation

The piezoresistance models and the `EffectiveStressModel` support the use of named parameter sets (see Named Parameter Sets on page 36) and the auto-orientation framework (see Auto-Orientation Framework on page 37). To use one of these capabilities, specify `ParameterSetName="<psname>"` or `AutoOrientation` as an argument to `Factor` in the command file.

Factor Models Applied to Mobility Components

By default, the isotropic mobility enhancement factor γ calculated by a `Factor` model is applied to total low-field mobility. However, the calculated enhancement factor can be applied to select mobility components (for example, only to acoustic phonon mobility or surface roughness mobility in the `Lombardi` model) by specifying the option

`ApplyToMobilityComponents`. When this option is selected, mobility models that support this feature apply an enhancement factor γ_i to the ith mobility component for which a stress scaling factor a_i is available:

$$\gamma_i = 1 + a_i(\gamma - 1) \tag{1021}$$

If $a_i = 1$, then $\gamma_i = \gamma$. If $a_i = 0$, then $\gamma_i = 1$ and no stress enhancement factor is applied to this component. In most cases, the stress scaling factors have a value of 0 or 1, but intermediate values are allowed.

The a_i parameters are specified in the parameter file in the parameter set associated with the mobility model. The mobility models that support this feature and the available stress scaling parameters are shown in Table 149.

Table 149   Mobility models that support the ApplyToMobilityComponents feature

Model	Parameter set name	Available stress scaling parameters
Coulomb2D	Coulomb2DMobility	a_{C}
IALMob	IALMob	$a_{\text{ph,2D}}$, $a_{\text{ph,3D}}$, $a_{\text{C,2D}}$, $a_{\text{C,3D}}$, a_{sr}
Lombardi	EnormalDependence	a_{ac}, a_{sr}
NegInterfaceCharge	NegInterfaceChargeMobility	a_{C}
PosInterfaceCharge	PosInterfaceChargeMobility	a_{C}
RCS	RCSMobility	a_{rcs}
RPS	RPSMobility	a_{rps}
ThinLayer	ThinLayerMobility	a_{bp}, a_{sp}, a_{tf}

Stress Mobility Model for Minority Carriers

Measured data shows that the stress dependency of minority carrier mobility (like the mobility of carriers in the channel of a MOSFET) is different from the stress dependency of majority carrier mobility. For example, the stress effect for minority carriers may have a dependency on electric field and, perhaps, a different (or smaller) doping dependency.

As a calibration option, Sentaurus Device provides an additional factor β for the stress effect applied to minority carrier mobility:

$$\bar{\mu} = \mu_0\left(\bar{1} + \beta\frac{\Delta\bar{\mu}_{\text{stress}}}{\mu_0}\right) \tag{1022}$$

where $\Delta\bar{\mu}_{stress}$ is the stress-induced change of the mobility tensor for any stress model described in this chapter. The minority carrier factor β can be specified (the default value is equal to 1) in the `Piezo` section of the command file using the keywords `eMinorityFactor` and `hMinorityFactor` for electrons and holes, respectively, for example:

```
Physics {
   Piezo( Model(Mobility(eMinorityFactor = 0.5 hMinorityFactor = 0.5) ) )
}
```

In some cases, it is useful to switch off the doping dependency of the stress models and also to have the minority carrier factor β applied to portions of the device where the carrier is actually a majority carrier (for example, in low-doped parts of MOSFET source/drain regions). This can be achieved by specifying the parameter `DopingThreshold=`N_{th} as an argument to `eMinorityFactor` or `hMinorityFactor`, for example:

```
Physics {
   Piezo( Model(Mobility(eMinorityFactor(DopingThreshold=1e18) = 0.5
                         hMinorityFactor(DopingThreshold=-1e18) = 0.5) ) )
}
```

When `DopingThreshold=`N_{th} is specified, the behavior of the program depends on the relation of N_{th} to the local net doping, $N_D - N_A$:

$$\mu_n: N_D - N_A < N_{th} \;\rightarrow\; \text{eMinorityFactor} = \beta \text{ is applied, stress model doping dependency is switched off}$$
$$\mu_p: N_D - N_A > N_{th} \;\rightarrow\; \text{hMinorityFactor} = \beta \text{ is applied, stress model doping dependency is switched off}$$
(1023)

> **NOTE** `DopingThreshold=0` corresponds to the regular definition of minority and majority carriers. To apply the factor β to a portion of the majority carrier mobility, specify $N_{th} > 0$ for electrons and $N_{th} < 0$ for holes.

> **NOTE** When the `DopingThreshold` condition is met (and the doping dependency of the stress models is switched off), the `Tensor(Kanda)` model will behave like `Tensor()`, the `eSubBand(Doping)` model will behave like `eSubBand()`, and the `hSixBand(Doping)` model will behave like `hSixBand()`.

> **NOTE** Specifying `eMinorityFactor=0.5` is not the same as specifying `eMinorityFactor(ThresholdDoping=0)=0.5` because, in the latter case, the stress model doping dependency is switched off for carriers where this factor is applied.

Dependency of Saturation Velocity on Stress

Eq. 1022 can be rewritten in the following form (see Current Densities on page 786):

$$\bar{\mu} = \mu_0 Q \begin{bmatrix} 1 + t_1 & 0 & 0 \\ 0 & 1 + t_2 & 0 \\ 0 & 0 & 1 + t_3 \end{bmatrix} Q^{\mathrm{T}} \tag{1024}$$

where:

- t_i are eigenvalues of the tensor $\beta \dfrac{\Delta\bar{\mu}_{\text{stress}}}{\mu_0}$.
- Q is the orthogonal matrix from eigenvectors (main directions) of this tensor.

In high electric fields, the mobility along the main directions is proportional to the saturation velocity: $\mu_i \sim \dfrac{v_{\text{sat}}}{F}(1 + t_i)$. Therefore, the dependence of the saturation velocity on stress is similar to the mobility (with the factor $1 + t_i$). However, measured data shows that saturation velocity can have a different stress effect or no stress effect. Sentaurus Device has a calibration option to modify the dependency of saturation velocity on stress in the following form for the main directions:

$$v_{\text{sat},\,i} = v_{\text{sat},\,0} \cdot \frac{(1 + \alpha \cdot t_i)}{(1 + t_i)} \tag{1025}$$

where $v_{\text{sat},\,0}$ is the stress-independent saturation velocity and α is a user-defined scalar factor. This factor can be specified using the keyword `SaturationFactor` in the `Piezo` section of the command file. For example:

```
Physics {
   Piezo( Model( Mobility(SaturationFactor = 0.5) ) )
}
```

This parameter can be specified separately for electrons and holes, for example:

```
Physics {
   Piezo( Model( Mobility(eSaturationFactor = 0.5 hSaturationFactor = 0) ) )
}
```

The default value for α is 1. This is equivalent to applying the stress enhancement factor to total mobility with $v_{\text{sat},\,i} = v_{\text{sat},\,0}$. Using $\alpha = 0$ with a Caughey–Thomas-type mobility (see Eq. 340, p. 363) is equivalent to applying the stress enhancement factor only to the low-field mobility, μ_{low}, with $v_{\text{sat},\,i} = v_{\text{sat},\,0}$. Figure 58 on page 880 shows how the I_d–V_d curves depend on the parameter `SaturationFactor`.

Figure 58   Dependency of I_d–V_d curves on SaturationFactor, with V_g = 1.5 V,
and Stress = (0.6e9, 0, 0, 0, 0, 0)

Mobility Enhancement Limits

With high stress values, the stress-dependent mobility models in Sentaurus Device can sometimes cause the mobility to become negative or, in some cases, to become unrealistically large. This is particularly true for the piezoresistance mobility models. To prevent this, minimum and maximum stress enhancement factors for both electron and hole mobility can be specified in the `Piezoresistance` section of the parameter file. The following example shows the default values for `MinStressFactor` and `MaxStressFactor`:

```
Piezoresistance {
   MinStressFactor = 1e-5 , 1e-5 # [1]
   MaxStressFactor = 10   , 10   # [1]
}
```

NOTE   Although these parameters are specified in the `Piezoresistance` section of the parameter file, these limits are applied to all stress-dependent mobility models.

Plotting Mobility Enhancement Factors

The mobility multiplication tensor ($\bar{\mu}/\mu_0$) can be plotted on the mesh nodes. This tensor is a symmetric 3×3 matrix and, therefore, has six independent values. To plot these values on the mesh nodes for electron and hole mobilities, use the keywords:

- `eMobilityStressFactorXX, eMobilityStressFactorYY,`
  `eMobilityStressFactorZZ`

- `eMobilityStressFactorYZ, eMobilityStressFactorXZ,`
  `eMobilityStressFactorXY`

- `hMobilityStressFactorXX, hMobilityStressFactorYY,`
  `hMobilityStressFactorZZ`

- `hMobilityStressFactorYZ, hMobilityStressFactorXZ,`
  `hMobilityStressFactorXY`

Numeric Approximations for Tensor Mobility

Tensor Grid Option

Due to an applied mechanical stress, the mobility can become a tensor. The numeric approximation of the transport equations with tensor mobility is complicated (see Chapter 28 on page 779). However, if the mesh is a tensor one, the approximation is simpler. For this option, off-diagonal mobility elements are not used and, therefore, there are no mixed derivatives in the approximation. Such an approximation gives an M-matrix property for the Jacobian and it permits stable stress simulations. Very often, critical regions are simple and the mesh constructed in such regions can be close to a tensor one.

> **NOTE**   The off-diagonal elements of the mobility tensor appear only if there is
> a shear stress or the simulation coordinate system of Sentaurus Device
> is different from the crystal system.

To activate this simple tensor-grid approximation, the keyword `TensorGridAniso` in the `Math` section must be specified.

By default, Sentaurus Device uses the `AverageAniso` approximation (see AverageAniso on page 780) which is based on a local transformation of an anisotropic task (stress-induced mobility tensor) to an isotropic one.

The `StressSG` approximation (see StressSG on page 781) gives the most accurate results and is independent of the mesh orientation. Convergence, however, may be worse than for `TensorGridAniso`.

> **NOTE** All approximation options do not guarantee a correct solution for arbitrary mesh and stress. Experiments with these options can give an estimation of ignored terms.

Stress Tensor Applied to Low-Field Mobility

In all the previous models, the stress tensor factor was a linear factor applied to high-field mobility. Sentaurus Device allows also to apply the following diagonal mobility tensor factor to the low-field mobility:

$$
\mu_{\text{high}} =
\begin{bmatrix}
\mu_{\text{high}}(\mu_{\text{low}} \cdot s_{xx}, \ldots) & 0 & 0 \\
0 & \mu_{\text{high}}(\mu_{\text{low}} \cdot s_{yy}, \ldots) & 0 \\
0 & 0 & \mu_{\text{high}}(\mu_{\text{low}} \cdot s_{zz}, \ldots)
\end{bmatrix}
\tag{1026}
$$

where:

- s_{ii} are the diagonal elements of the stress tensor factor $\left(\bar{1} + \beta \dfrac{\Delta \bar{\mu}_{\text{stress}}}{\mu_0} \right)$ in Eq. 1022, p. 877. In this model, off-diagonal elements are not used.

- $\mu_{\text{high}}(\ldots)$ is a scalar function that computes the high-field mobility (see High-Field Saturation on page 361).

This model can be specified in the `Math` section of the command file as follows:

```
Math { StressMobilityDependence = TensorFactor }
```

In this case, the dependency of saturation velocity on stress is given by:

$$
v_{\text{sat}, i} = v_{\text{sat}, 0} \cdot (1 + \alpha \cdot t_i)
\tag{1027}
$$

which results in the same dependency on `SaturationFactor` described in Dependency of Saturation Velocity on Stress on page 879 when a Caughey–Thomas-type mobility model is used.

The high-field mobility tensor (in Eq. 1026) and the corresponding factors $\mu_{\text{high}}(\mu_{\text{low}} \cdot s_{ii}, \ldots) / \mu_{\text{high}}(\mu_{\text{low}}, \ldots)$ can be plotted on the mesh nodes. To plot these values for electron and hole mobilities, use the following keywords in the `Plot` section:

- `eTensorMobilityXX, eTensorMobilityYY, eTensorMobilityZZ`

- `hTensorMobilityXX, hTensorMobilityYY, hTensorMobilityZZ`

- eTensorMobilityFactorXX, eTensorMobilityFactorYY,
  eTensorMobilityFactorZZ

- hTensorMobilityFactorXX, hTensorMobilityFactorYY,
  hTensorMobilityFactorZZ

Piezoelectric Polarization

Sentaurus Device provides two models (`strain` and `stress`) to compute polarization effects in GaN devices. They can be activated in the `Physics` section of the command file as follows:

```
Physics {
   Piezoelectric_Polarization (strain)
   Piezoelectric_Polarization (stress)
}
```

Sentaurus Device also offers a corresponding PMI model (see).

Strain Model

The piezoelectric polarization vector P can be expressed as a function of the local strain tensor $\bar{\varepsilon}$ as follows:

$$
\begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} = \begin{bmatrix} P_x^{\text{sp}} \\ P_y^{\text{sp}} \\ P_z^{\text{sp}} \end{bmatrix} + \begin{bmatrix} e_{11} & e_{12} & e_{13} & e_{14} & e_{15} & e_{16} \\ e_{21} & e_{22} & e_{23} & e_{24} & e_{25} & e_{26} \\ e_{31} & e_{32} & e_{33} & e_{34} & e_{35} & e_{36} \end{bmatrix} \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \\ \varepsilon_{xy} \end{bmatrix}
\tag{1028}
$$

Here, P^{sp} is the spontaneous polarization vector [C/cm^2], and the quantities e_{ij} denote the strain-charge piezoelectric coefficients [C/cm^2].

The quantities P^{sp} and e_{ij} are defined in the crystal system. The polarization vector is first computed in crystal coordinates and is converted to simulation coordinates afterwards.

This general model is evaluated in either of the following circumstances:

- A constant strain tensor has been specified in the `Piezo` section of the command file.

- The strain tensor is read from a TDR file. This requires the specification of both `Strain=LoadFromFile` within the `Physics{Piezo{...}}` section and `Piezo=<file>` within the `File` section of the command file.

Otherwise, the simplified model by Ambacher described in Simplified Strain Model will be selected.

Simplified Strain Model

This model is based on the work by Ambacher *et al.* [30][31]. It captures the first-order effect of polarization vectors in AlGaN/GaN HFETs: The interface charge induced is due to the discontinuity in the vertical component of the polarization vector at material interfaces.

The polarization vector is computed as follows:

$$\begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} = \begin{bmatrix} P_x^{\text{sp}} \\ P_y^{\text{sp}} \\ P_z^{\text{sp}} + P_{\text{strain}} \end{bmatrix} \tag{1029}$$

where:

- $P_{\text{strain}} = 2d_{31} \cdot \text{strain} \cdot (c_{11} + c_{12} - 2c_{13}^2/c_{33})$ for `Formula=1`.

- $P_{\text{strain}} = 2\text{strain} \cdot (e_{31} - e_{33}c_{13}/c_{33})$ for `Formula=2`.

- P^{sp} denotes the spontaneous polarization vector $[\text{C/cm}^2]$.

- d_{31} is a piezoelectric coefficient $[\text{cm/V}]$.

- c_{ij} are stiffness constants $[\text{Pa}]$.

- e_{31}, e_{33} are strain–charge piezoelectric coefficients $[\text{C/cm}^2]$. The value of strain is computed as:

$$\text{strain} = (1 - \text{relax}) \cdot (a_0 - a)/a \tag{1030}$$

where a_0 represents the strained lattice constant $[\text{Å}]$, a is the unstrained lattice constant $[\text{Å}]$, and 'relax' denotes a relaxation parameter [1].

The quantities P^{sp}, d_{ij}, c_{ij}, and e_{ij} are defined in the crystal system. The polarization vector is first computed in crystal coordinates and is converted to simulation coordinates afterwards.

Stress Model

Although, in most practical situations, there are only in-plane stress components due to lattice mismatch, the vertical and shear stress components give rise to in-plane piezopolarization components, which lead to volume charge densities and, therefore, potential variations. The stress model computes the full polarization vector in tensor form without simplifying assumptions:

$$
\begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} = \begin{bmatrix} P_x^{\mathrm{sp}} \\ P_y^{\mathrm{sp}} \\ P_z^{\mathrm{sp}} \end{bmatrix} + \begin{bmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} \end{bmatrix} \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} \tag{1031}
$$

where P^{sp} denotes the spontaneous polarization vector $[\mathrm{C/cm}^2]$, d_{ij} are the piezoelectric coefficients [cm/V], and:

$$
\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} \tag{1032}
$$

is the stress tensor [Pa].

The quantities P^{sp} and d_{ij} are defined in the crystal system. The stress tensor σ is defined in the stress system. It is first converted from stress coordinates to crystal coordinates. Then, the polarization vector is computed in crystal coordinates. Afterwards, the polarization vector is converted to simulation coordinates.

Poisson Equation

Based on the polarization vector, the piezoelectric charge is computed according to:

$$
q_{\mathrm{PE}} = -\mathrm{activation} \nabla P \tag{1033}
$$

where `activation` is a nonnegative real calibration parameter (default is 1).

This value can be defined in the `Physics` section:

```
Physics (MaterialInterface="AlGaN/GaN"){
   Piezoelectric_Polarization (strain activation=0.5)
}
```

The q_{PE} value is added to the right-hand side of the Poisson equation:

$$\nabla \varepsilon \cdot \nabla \phi = -q(p - n + N_D - N_A + q_{PE})$$

(1034)

Only the first d components of the polarization vector are used to compute the polarization charge, where d denotes the dimension of the problem.

Parameter File

The following parameters can be specified in the parameter file. All of them are mole fraction dependent, except `a0` and `relax`:

```
Piezoelectric_Polarization {
   # piezoelectric coefficients [cm/V]
   d11 = ...
   d12 = ...
   ...
   d36 = ...

   # spontaneous polarization [C/cm^2]
   psp_x = ...
   psp_y = ...
   psp_z = ...

   Formula = ...

   # stiffness constants [Pa]
   c11 = ...
   c12 = ...
   c13 = ...
   c33 = ...

   # piezoelectric coefficients [C/cm^2]
   e11 = ...
   e12 = ...
   ...
   e36 = ...

   # strain parameters [Å]
   a0 = ...
```

```
    a  = ...
    relax = ... # [1]
}
```

Coordinate Systems

The x-axis and y-axis of the simulation coordinate system are defined in the parameter file:

```
LatticeParameters {
   X = (1, 0,  0)
   Y = (0, 0, -1)
}
```

The z-axis is computed as the outer vector product of the x-axis and y-axis. The simulation system is defined relative to the crystal system. If the keyword `CrystalAxis` is present, the crystal system is defined relative to the simulation system (see Using Stress and Strain on page 823).

In the above example, the x-axis of the simulation system coincides with the x-axis of the crystal system. The y-axis of the simulation system runs along the negative z-axis of the crystal system. This is a common definition for 2D simulations.

If no `LatticeParameters` section is found in the parameter file, the following defaults take effect:

```
LatticeParameters {
   X = (1, 0, 0)
   Y = (0, 1, 0)
}
```

The x-axis and y-axis of the stress system are defined in the `Physics` section:

```
Physics {
   Piezo (
      OriKddX = (-0.96 0.28 0)
      OriKddY = (0.28 0.96 0)
   }
}
```

The z-axis is computed as the outer vector product of the x-axis and y-axis. The stress system is defined relative to the simulation system (see Using Stress and Strain on page 823).

Converse Piezoelectric Field

The values of the converse piezoelectric field are very important for applications. The dataset `ConversePiezoelectricField` can be added to the `Plot` variables (see Table 178 on page 1340). This dataset is a dimensionless tensor and is computed using the following tensor relationship:

$$
\begin{bmatrix}
\text{ConversePiezoelectricFieldXX} \\
\text{ConversePiezoelectricFieldYY} \\
\text{ConversePiezoelectricFieldZZ} \\
\text{ConversePiezoelectricFieldYZ} \\
\text{ConversePiezoelectricFieldXZ} \\
\text{ConversePiezoelectricFieldXY}
\end{bmatrix}
=
\begin{bmatrix}
d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\
d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\
d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36}
\end{bmatrix}^{t}
\begin{bmatrix}
E_x \\
E_y \\
E_z
\end{bmatrix}
\tag{1035}
$$

where d_{ij} are piezoelectric coefficients and E_k are electric-field components.

Piezoelectric Datasets

The piezoelectric polarization vector and the piezoelectric charge can be plotted by:

```
Plot {
   PE_Polarization/vector
   PE_Charge
}
```

Discontinuous Piezoelectric Charge at Heterointerfaces

Any interface has two sides (side1 and side2). If a vertex lies at the interface and heteromodels are switched on, this vertex is a double point and the piezoelectric charge has two values (q1 and q2). If the polarization vector is a constant vector, then q1 = –q2 and the total charge is equal to zero. In the case of double points, Sentaurus Device creates an output file that contains two values of the piezoelectric charge, that is, the charge distributions are interface discontinuous even in homogeneous structures. Sentaurus Device contains two datasets (continuous and discontinuous) for the piezoelectric charge:

```
Plot {
   PE_Charge    # continuous distribution in any case
   PiezoCharge  # discontinuous distribution at the interface for heteromodels
}
```

Gate-Dependent Polarization in GaN Devices

In this model, the polarization vector P has an additional term along the z-axis in the crystal system, which is dependent on the E_z component of the electric field [32]:

$$P_z^{\text{new}} = P_z + (e_{33}^2 / c_{33}) \cdot E_z \tag{1036}$$

This problem can be converted into an equivalent problem with an anisotropic permittivity tensor (z-component increased by e_{33}^2 / c_{33}):

$$\nabla \bullet \left(-\begin{bmatrix} \kappa_a E_x \\ \kappa_a E_y \\ \kappa_c E_z \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ \dfrac{e_{33}^2}{c_{33}} E_z \end{bmatrix} \right) = \nabla \bullet \left(\begin{bmatrix} \kappa_a & & \\ & \kappa_a & \\ & & \kappa_c + \dfrac{e_{33}^2}{c_{33}} \end{bmatrix} \nabla \varphi \right) = -\rho + \nabla \bullet \mathbf{P} \tag{1037}$$

where $\mathbf{P}$ is equal to Eq. 1029, p. 884 (P_{strain} is Formula 2).

The gate-dependent polarization model can be activated in the `Physics` section as follows:

```
Physics {
   Piezoelectric_Polarization (strain(GateDependent))
}
```

Two-Dimensional Simulations

For a 2D simulation, you must ensure that the anisotropic direction (defined in the crystal coordinate system) lies within the xy plane of the simulation system. You can specify explicitly the transformation from the crystal (lattice) coordinate system to the simulation (mesh) coordinate system in the `LatticeParameters` section of the parameter file (see Coordinate Systems on page 887).

If no `LatticeParameters` section is found in the parameter file, the following defaults take effect:

```
LatticeParameters {
   X = (1, 0, 0)
   Y = (0, 1, 0)
}
```

Similarly, the default anisotropic direction in a 2D simulation is the y-axis in the crystal system, which coincides with the default y-axis in the simulation system.

However, the following values of `LatticeParameters` are selected frequently for 2D simulations:

```
LatticeParameters {
   X = (1, 0, 0)
   Y = (0, 0, -1)
}
```

In this case, the y-axis in the simulation system runs along the negative z-axis in the crystal system and, therefore, it is necessary to declare the z-axis in the crystal system as the anisotropic direction:

```
Physics {
   Aniso(direction = zAxis)
}
```

Mechanics Solver

> **NOTE** The mechanics solver in Sentaurus Device is an experimental feature, and it may be modified in future releases.

During a device simulation, the stress tensor may change as a function of the solution variables, for example:

- Different materials have different thermal expansion coefficients. This thermal mismatch leads to stress changes as a function of the lattice temperature of the device. The influence of thermomechanical stress on device performance has been studied in [33] and [34].

- The electrical degradation of GaN HEMTs is described in [35]. The authors propose the formation of defects due to excessive stress associated with the inverse piezoelectric effect. In this case, the stress tensor changes as a function of the local electric field.

Sentaurus Device provides a `Mechanics` statement in the `Solve` section to recompute the stress tensor in response to changes in bias conditions:

```
Solve {
   Mechanics

   Plugin (...)
      { Poisson Electron Hole Mechanics }

   Quasistationary (...)
      { Plugin (Iterations=0 BreakOnFailure) {
         Coupled { Poisson Electron Hole }
         Mechanics
      }
   }
```

```
    Transient (...)
      { Plugin (Iterations=0 BreakOnFailure) {
        Coupled { Poisson Electron Hole }
        Mechanics
      }
    }
}
```

During a mixed-mode simulation, the `Mechanics` statement is applied by default to all the physical devices in the circuit. However, it is also possible to apply it to selected devices only:

```
Solve {
  Mechanics                            # all devices

  "mos1".Mechanics "mos2".Mechanics   # selected devices only
}
```

Sentaurus Device relies on Sentaurus Interconnect to update the stress tensor. A `Mechanics` statement in the `Solve` section performs the following operations:

- Sentaurus Device creates an input structure (TDR file) for Sentaurus Interconnect with the current solution variables, such as the electrostatic potential ϕ or the lattice temperature T, as well as a Sentaurus Interconnect command file.

- Sentaurus Device invokes Sentaurus Interconnect.

- Sentaurus Interconnect updates the mechanical stress and produces an output TDR file.

- Sentaurus Device reads the TDR file generated by Sentaurus Interconnect and updates the stress tensor.

As a consequence of this approach, the mechanical equations cannot be solved self-consistently with the device equations. Therefore, a `Mechanics` statement in the `Solve` section can only appear as an individual statement, or within a `Plugin` command. It cannot appear within a `Coupled` command.

Options for the stress solver can be specified in a `Mechanics` section within the global `Physics` section:

```
Physics {
  Mechanics (
    binary = "..."
    parameter = "..."
    command = "..."
    initial_structure = "..."
  )
}
```

The following options are supported:

- `binary = "..."`

  Name of the Sentaurus Interconnect binary. The default is `"sinterconnect -u"` (where the `-u` option switches off the log file). Use this option to select a particular release, for example:

  ```
  binary = "sinterconnect -rel N-2017.09"
  ```

  The `binary` specification also can be an option of the `Mechanics` statement in the `Solve` section:

  ```
  Solve {
     Mechanics (binary = "...")
  }
  ```

- `parameter = "..."`

  Defines Sentaurus Interconnect parameters (`pdbSet` commands). You can either specify all the parameters directly or use the Tcl `source` statement to read another file:

  ```
  parameter = "source mechanics.par"
  ```

  Sentaurus Interconnect can update the stress tensor as a function of the local electric field. To enable this option, use the following command:

  ```
  pdbSet Mechanics InversePiezoEffect 1
  ```

  By default, this option is switched off.

  The values of the piezoelectric tensor e must be specified by `pdbSetDouble` commands for each region:

  ```
  pdbSetDouble <region> Mechanics PiezoElectricTensor<ij> <value>
  ```

  where $i = 1\ldots6$, $j = 1\ldots3$. The values must be specified in units of $\mathrm{dyn}/(\mathrm{V\,cm})$, which is equivalent to $10^{-7}\mathrm{C/cm}^2$.

  The `parameter` specification also can be an option of the `Mechanics` statement in the `Solve` section:

  ```
  Solve {
     Mechanics (parameter = "...")
  }
  ```

- `command = "..."`

  This option defines the Tcl command file for Sentaurus Interconnect. You can either specify all the commands directly or use the Tcl `source` statement to read another file:

  ```
  command = "source mechanics.cmd"
  ```

Sentaurus Device defines the Tcl variables shown in Table 150 for use in the Sentaurus Interconnect command file.

Table 150 Tcl variables

Variable	Description
sdevice_load	Name of the file that must be loaded at the beginning by a Sentaurus Interconnect `init` command.
sdevice_save	Name of the file that must be saved at the end by a Sentaurus Interconnect `struct` command.
sdevice_load_temperature	Initial average device temperature in kelvin of the device defined in `$sdevice_load`.
sdevice_save_temperature	Final average device temperature in kelvin of the device to be saved in `$sdevice_save`.

To compute an updated stress tensor, a short `solve` command must be executed. The following commands represent the default for `command`:

```
init tdr= $sdevice_load !load.commands
mode mechanics
select z= PrevLatticeTemperature name= Temperature
solve time= 1<min> t.final.profile= LatticeTemperature
struct tdr= $sdevice_save
```

The `command` specification also can be an option of the `Mechanics` statement in the `Solve` section:

```
Solve {
   Mechanics (command = "...")
}
```

■ `initial_structure = "..."`

Before calling Sentaurus Interconnect, Sentaurus Device creates an input structure that contains the current solution variables, such as the electrostatic potential ϕ or the lattice temperature T. During the course of a simulation, this input structure is always based on the output structure obtained from the last call of Sentaurus Interconnect.

For the first call of Sentaurus Interconnect, the input structure is based on the TDR file specified by the `initial_structure` option. It is recommended to specify a Sentaurus Interconnect structure that still contains gas regions:

```
initial_structure = "n1_fps.tdr"
```

In this way, a remeshing in Sentaurus Interconnect can be avoided.

If this option is not specified, the initial input structure will be based on the Sentaurus Device structure specified in the `File` section.

> **NOTE** It is assumed that the stress tensor in the initial structure is identical to the stress tensor in Sentaurus Device (as loaded by the `Piezo` statement in the `File` section). If a stress tensor is missing, it will be copied from the Sentaurus Device stress tensor.

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Galvanic Transport Model

This chapter describes the model for carrier transport in magnetic fields.

Model Description

For analysis of magnetic field effects in semiconductor devices, the transport equations governing the flow of electrons and holes in the interior of the device must be set up and solved.

To this end, the commonly used drift-diffusion-based model of the carrier current densities $\vec{J}_n$ and $\vec{J}_p$ must be augmented by magnetic field–dependent terms that account for the action of the transport equations governing the flow of electrons and holes in the interior of the device, the *Lorentz force* on the motion of the carriers [1][2][3]:

$$\vec{J}_\alpha = \mu_\alpha \vec{g}_\alpha + \mu_\alpha \frac{1}{1 + (\mu_\alpha^* B)^2} [\mu_\alpha^* \vec{B} \times \vec{g}_\alpha + \mu_\alpha^* \vec{B} \times (\mu_\alpha^* \vec{B} \times \vec{g}_\alpha)] \quad \text{with} \quad \alpha = n, p \tag{1038}$$

where:

- $\vec{g}_\alpha$ is current vector without mobility (see Current Densities on page 786).
- μ_α^* is the Hall mobility.
- $\vec{B}$ is the magnetic induction vector, and B is the magnitude of this vector.

The perpendicular (transverse) components of Hall and drift mobility are related by $\mu_n^* = r_n \mu_n$ and $\mu_p^* = r_p \mu_p$, where r_n and r_p denote the Hall scattering factors. In the case of bulk silicon, typical values are $r_n = 1.1$ and $r_p = -0.7$.

Using Galvanic Transport Model

In the `Physics` section of the command file, specify the magnetic field vector using the keyword `MagneticField = (<x>,<y>,<z>)`. In the following example, a field of 0.1 Tesla is applied parallel to the z-axis:

```
Physics {...
   MagneticField = (0.0, 0.0, 0.1)
}
```

This parameter can be ramped (see Ramping Physical Parameter Values on page 78).

Discretization Scheme for Continuity Equations

Sentaurus Device uses a modified discretization scheme for continuity equations in a constant magnetic field. This scheme contains an additive term to the effective electric field in the Scharfetter–Gummel approximation, that is, in this approximation, the argument to the Bernoulli function has an additional magnetic term. This discretization scheme has good convergence and mesh stability (the new approximation does not demand a special grid).

> **NOTE** The galvanic transport model cannot be combined with the following models: hydrodynamic, impact ionization, aniso, piezo, and quantum modeling.

> **NOTE** The value of the magnetic field is a critical parameter for convergence. For doping-dependent mobility, the convergence is reliable up to $B = 10\,\mathrm{T}$. For more general mobility, the convergence has a limit of the magnetic field up to $B = 1\,\mathrm{T}$.

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Thermal Properties

This chapter describes the models that are important for lattice heating and the thermodynamic model: heat capacity, thermal conductivity, and thermoelectric power.

Heat Capacity

Table 151 lists the values of the heat capacity used in the simulator.

Table 151   Values of heat capacity c for various materials

Material	c [J/K cm^3]	Reference
Silicon	1.63	[1]
Ceramic	2.78	[2]
SiO$_2$	1.67	[2]
Poly Si	1.63	$\approx$ Si

By default, or when you specify `HeatCapacity(TempDep)` in the `Physics` section, the temperature dependency of the lattice heat capacity is modeled by the empirical function:

$$c_{\mathrm{L}} = \mathtt{cv} + \mathtt{cv\_b}T + \mathtt{cv\_c}T^2 + \mathtt{cv\_d}T^3 \tag{1039}$$

The equation coefficients can be specified in the parameter file by using the syntax:

```
LatticeHeatCapacity{
   cv = 1.63          # [J/(K cm^3)]
   cv_b = 0.0000e+00  # [J/(K^2 cm^3)]
   cv_c = 0.0000e+00  # [J/(K^3 cm^3)]
   cv_d = 0.0000e+00  # [J/(K^3 cm^3)]
}
```

All these coefficients can be mole fraction–dependent for mole-dependent materials.

To use a PMI model to compute heat capacity, specify the name of the model as a string as an option to `HeatCapacity` (see Heat Capacity on page 1177). To use a multistate configuration–dependent PMI for heat capacity, specify the model and its parameters as arguments to `PMIModel`, which, in turn, is an argument to `HeatCapacity` (see Multistate Configuration–Dependent Heat Capacity on page 1180).

To use a constant lattice heat capacity without touching the parameter file, specify
`HeatCapacity(Constant)`.

The pmi_msc_heatcapacity Model

The model may depend on state occupation probabilities of a multistate configuration (MSC). If no explicit dependency on an MSC is given, it enables a piecewise linear (pwl) dependency on the lattice temperature, that is, it reads:

$$c_{\mathrm{V}} = c_{\mathrm{V}}(T) \tag{1040}$$

If the model depends on an MSC, for each MSC state, the heat capacity can be pwl temperature–dependent. The overall heat capacity is then averaged according to:

$$c_{\mathrm{V}} = \sum_i c_{\mathrm{V},i}(T) s_i \tag{1041}$$

where the sum is taken over all MSC states, and s_i are the state occupation probabilities.

The model is activated in the `Physics` section by:

```
HeatCapacity ( PMIModel ( Name="pmi_msc_heatcapacity" MSConfig="msc0" ) )
```

Table 152   Parameters of pmi_msc_heatcapacity

Name	Symbol	Default	Unit	Range	Description
plot	–	0	–	{0,1}	Plot parameter to screen
cv	c_{V}	0.	J/Kcm^3	real	Constant value
cv_nb_Tpairs	–	0	–	>=0	Number of interpolation points
cv_Tp<int>_X	––	–	K	real	Temperature at < int >-th interpolation point
cv_Tp<int>_Y	–	–	J/Kcm^3	real	Value at < int >-th interpolation point

Table 152 lists the parameters of the model. With `cv`, you specify a constant heat capacity, which is used as a global (no MSC dependency) or default state heat capacity. However, if you specify `cv_nb_Tpairs` greater than zero, the global and default state heat capacities are piecewise linear. In that case, you must specify the interpolation points as pairs of temperature and heat capacity values by `cv_Tp<int>_X` and `cv_Tp<int>_Y`, respectively. `<int>` ranges from zero to one less than `cv_nb_Tpairs`. The global `cv_` parameters can be prefixed with:

```
<state_name>_
```

for the named MSC states to overwrite the default state behavior.

Thermal Conductivity

Sentaurus Device uses the following temperature-dependent thermal conductivity κ in silicon [3]:

$$\kappa(T) = \frac{1}{a + bT + cT^2} \tag{1042}$$

where $a = 0.03\,\text{cmKW}^{-1}$, $b = 1.56{\times}10^{-3}\,\text{cmW}^{-1}$, and $c = 1.65{\times}10^{-6}\,\text{cmW}^{-1}\text{K}^{-1}$. The range of validity is from $200\,\text{K}$ to well above $600\,\text{K}$. Values of the thermal conductivity for some materials are given in Table 153.

Table 153   Values of thermal conductivity κ of silicon versus temperature

Material	κ [W/(cm K)]	Reference
Silicon	Eq. 1042	[3]
Ceramic	0.167	[4]
SiO$_2$	0.014	[1]
Poly Si	1.5	$\approx$ Si

As additional options to the standard specification of the thermal conductivity model, there are two different expressions to define either thermal resistivity $\chi = 1/\kappa$ or thermal conductivity for any material. This is performed by using `Formula` in the parameter file or special keywords in the command file.

For `Formula=0` (thermal resistivity specification), Sentaurus Device uses:

$$\chi = \texttt{1/kappa} + \texttt{1/kappa\_b}\,T + \texttt{1/kappa\_c}\,T^2 \tag{1043}$$

For `Formula=1` (thermal conductivity specification), it is:

$$\kappa = \texttt{kappa} + \texttt{kappa\_b}\,T + \texttt{kappa\_c}\,T^2 \tag{1044}$$

NOTE   Sentaurus Device stores six independent parameters, namely, `1/kappa`, `1/kappa_b`, and `1/kappa_c` for the thermal resistivity model in Eq. 1043, and `kappa`, `kappa_b`, and `kappa_c` for the thermal conductivity model in Eq. 1044. In particular, a change of `kappa` will not modify `1/kappa` and vice versa. The same applies to both `kappa_b` and `1/kappa_b`, as well as `kappa_c` and `1/kappa_c`.

Use the following syntax in the parameter file to select the required model and to specify the coefficients:

```
Kappa{
    Formula = 0
    1/kappa = 0.03           # [K cm/W]
    1/kappa_b = 1.5600e-03   # [cm/W]
    1/kappa_c = 1.6500e-06   # [cm/(W K)]
    kappa = 1.5              # [W/(K cm)]
    kappa_b = 0.0000e+00     # [W/(K^2 cm)]
    kappa_c = 0.0000e+00     # [W/(K^3 cm))]
}
```

The `Physics` section of the command file provides more flexibility to switch these expressions by using the keywords:

```
ThermalConductivity(
    TempDep Conductivity  # Formula = 1
    Constant Conductivity # Formula = 1 without temperature dependence
    TempDep Resistivity   # Formula = 0
    Constant Resistivity  # Formula = 0 without temperature dependence
```

By default, Sentaurus Device uses `Formula` specified in the parameter file. All these coefficients in the parameter file can be mole dependent for mole-dependent materials.

Furthermore, a simple PMI and a multistate configuration–dependent PMI are available to compute thermal conductivity. See Thermal Conductivity on page 1167 and Multistate Configuration–Dependent Thermal Conductivity on page 1173 for details.

The AllDependent Thermal Conductivity Model

In general, thermal conductivity κ is a function of lattice temperature T, doping density N, layer thickness d_{Ly}, and mole fraction x. Starting with the Boltzmann transport equation for phonons and with relaxation time approximations, κ is expressed as an integral over phonon frequency [5]:

$$\kappa = \frac{1}{3} \cdot \frac{1}{2\pi^2} \cdot n_j \cdot \sum_j \int_0^{\omega_{0,j}} \frac{\tau_{\omega,j}}{v_{\omega,j}} C(\omega)\omega^2 d\omega \tag{1045}$$

$$C(x) = kx^2 e^x (e^x - 1)^{-2} \tag{1046}$$

$$x = \frac{\hbar\omega}{kT} \tag{1047}$$

For each phonon branch κ, $\omega_{0,j}$ is the peak frequency, $v_{0,j}$ is the sound velocity, and $\tau_{0,j}$ is the total relaxation time. For the longitudinal mode ($j = L$), $n_L = 1$. For the transverse mode ($j = T$), $n_T = 1$.

Bulk Thermal Conductivity Computation

The total relaxation time is calculated with given scattering mechanisms. For pure bulk material [5]:

$$\tau_{LN}^{-1} = B_L \omega^2 T^3 + \tau_I^{-1} + \tau_b^{-1}, 0 < \omega < \omega_3 \tag{1048}$$

$$\tau_{TN}^{-1} = B_T \omega T^4 + \tau_I^{-1} + \tau_b^{-1}, \omega < \omega_1 \tag{1049}$$

$$\tau_{TU}^{-1} = B_{TU} \omega^2 / \sinh x + \tau_I^{-1} + \tau_b^{-1}, \omega_1 < \omega < \omega_2 \tag{1050}$$

$$\tau_I^{-1} = A_I \omega^4 \tag{1051}$$

$$\tau_b^{-1} = \frac{v_s}{FL} \tag{1052}$$

$$v_s = \left[\frac{1}{3}(v_L^{-1} + 2v_T^{-1}) \right]^{-1} \tag{1053}$$

Eq. 1048, Eq. 1049, and Eq. 1050 represent the phonon relaxation time for the longitudinal and transverse branches. For the transverse branch, the normal (N) process and the Umklapp (U) process are solved separately. The frequencies and phonon velocities are extracted from the bulk phonon dispersion:

- ω_1 is the turning point of the transverse branch, where the U process starts to have an effect.
- ω_2 is the peak frequency of the transverse branch.
- ω_3 is the peak frequency of the longitudinal branch.
- ω_4 is the turning point of the longitudinal branch.
- v_L is the velocity of the longitudinal mode when $\omega < \omega_4$.
- v_{Lp} is the velocity of the longitudinal mode when $\omega_4 < \omega < \omega_3$.
- v_T is the velocity of the transverse mode when $\omega < \omega_1$.
- v_{TU} is the velocity of the transverse mode when $\omega_1 < \omega < \omega_2$.
- B_L, B_T, and B_{TU} are fitting parameters.

- τ_I^{-1} and τ_b^{-1} represent scattering due to point defects and the boundary, where:

    - A_I is the scattering strength due to defects.

    - L is the bulk sample dimension.

The model is activated in the command file by:

```
Physics (...) {
    ThermalConductivity ( AllDep )
}
```

Example of Parameter File Segment

```
Kappa {
    ...
    omega1 = 2.357e13    #[s^-1]
    omega2 = 2.749e13    #[s^-1]
    ...
}
```

Table 154 summarizes the parameters for bulk silicon and germanium.

Table 154   Parameters for bulk silicon and germanium

Name	Symbol	Silicon	Germanium	Unit
omega1	ω_1	2.357e13	1.322e13	1/s
omega2	ω_2	2.749e13	1.545e13	1/s
omega3	ω_3	7.463e13	4.36e13	1/s
omega4	ω_4	4.582e13	2.514e13	1/s
vL	v_L	8.48e3	4.92e3	m/s
vLp	v_{Lp}	4.24e3	2.46e3	m/s
vT	v_T	5.86e3	3.55e3	m/s
vTU	v_{TU}	2e3	1.3e3	m/s
BL	B_L	2e-24	6.9e-24	s/K^3
BT	B_T	9.3e-13	1e-11	$1/K^4$
BTU	B_{TU}	5.5e-18	5e-18	s
AI	A_I	1.32e-45	2.4e-45	s^3
Lb	L	0.716e-2	0.24e-2	m
V_h	V	12.1e-6	13.6e-6	m^3/mol

Table 154   Parameters for bulk silicon and germanium (Continued)

Name	Symbol	Silicon	Germanium	Unit
M_h	M	28	72.6	Da
R_h	R	146e-12	125e-12	m
epsilon	ε_s	11.7	16.2	1
m_c	m_e	0.9	0.9	1
m_v	m_h	0.58	0.58	1
rho	ρ	2.329e3	5.323e3	kg/m^3

> **NOTE**   To achieve good agreement with measurement, it is necessary to understand the relative contribution of the three phonon branches to κ: κ_{TU} mainly determines the high-temperature range. The absolute values of κ_T and κ_L determine the peak value of κ, while their relative ratio κ_T / κ_L affects the slope of κ at low temperatures: The lower the ratio, the larger the slope. The fitting parameters B_L, B_T, and B_{TU} are determined accordingly.

Bulk Relaxation Time With Doping

In the case of doped samples, κ decreases due to phonon scattering with impurities and free carriers. The phonon-impurity scattering is treated in a similar way to point defects [6]:

$$\tau_{\text{impurity}}^{-1} = A\omega^4 \tag{1054}$$

$$A = A_I + A_{\delta M} + A_{\delta R} + A_x \tag{1055}$$

$$A_{\delta M} = \frac{NV^2}{4\pi v_s^3} \left(\frac{M - M_{\text{doped}}}{M} \right)^2 \tag{1056}$$

$$A_{\delta R} = \frac{2NV^2}{\pi v_s^3} Q_0^2 \Upsilon^2 \left(\frac{R - R_{\text{doped}}}{R} \right)^2 \tag{1057}$$

$A_{\delta M}$ and $A_{\delta R}$ model the impact of mass and radius differences between the host atom and the impurity atom with the given doping concentration N, where:

- V is the crystal volume of the host atom.
- M is the mass of the host atom.
- M_{doped} is the mass of the impurity atom.
- R is the radius of the host atom.

- R_{doped} is the radius of the impurity atom.
- Q_0 is a constant corresponding to the impurity.
- A_x is a fitting parameter.

The impact of phonon-carrier scattering is considered with two parts: the free carriers in the metallic state and the carriers bound to the impurity center. With a given carrier concentration n, the concentrations of bound carriers N_n and metallic carriers N_m are [7]:

$$N_n = n \exp(-t_c) \tag{1058}$$

$$N_m = n[1 - \exp(-t_c)] \tag{1059}$$

$$t_c = (4\pi/3)n r_c^3 \tag{1060}$$

$$r_c = (144/\pi^2)^{1/3} a_{\text{B}} \tag{1061}$$

where the Bohr radius a_{B} is:

$$a_{\text{B}} = \left(\frac{4\pi\varepsilon_0\hbar^2}{m_0 e^2}\right)\left(\frac{\varepsilon_s}{\varepsilon_0}\right)\left(\frac{m_0}{m_e}\right) \tag{1062}$$

Here:
- ε_s is the dielectric constant.
- m_e (or m_h) is the electron (or hole) effective mass of the host atom.

The relaxation time related to bound carriers is [8]:

$$\tau_{\text{bound},j}^{-1} = \frac{\omega^4[(1/3)\Xi_u]^4}{10\pi\rho^2 v_s^2}\chi^2\left(\frac{\omega}{v_s}\right)\left[v_L^{-5}\chi^2\left(\frac{\omega}{v_L}\right) + \frac{3}{2}v_T^{-5}\chi^2\left(\frac{\omega}{v_T}\right)\right] \cdot w_j \cdot \frac{2\Delta^2}{(\Delta^2 - \hbar^2\omega^2)^2}(2N_n) \tag{1063}$$

$$\chi(q_j) = [1 + (1/4)a_{\text{B}}^2 q_j^2]^{-2} \tag{1064}$$

where:
- Ξ_u is the shear deformation potential.
- ρ is the crystal mass density.
- w_{L}, w_{T}, and w_{TU} are parameters corresponding to each phonon mode.

For carriers in metallic states, the relaxation time is [6]:

$$\tau_{\text{free}}^{-1} = \frac{(m_e E_{\text{D}})^2 \omega}{2\pi\rho\hbar^3 v_s}, q < 2k_F \tag{1065}$$

$$\tau_{\text{free}}^{-1} = \frac{bN_m(m_e E_{\text{D}})^2}{\rho\hbar^3 q^5 a_{\text{B}}^3}, q > 2k_F \tag{1066}$$

where:

- E_{D} is the deformation potential.
- b is a fitting parameter.

Eq. 1065 and Eq. 1066 are continuous at $q = 2k_F$, which imposes the following relation:

$$k_F = \left(\frac{bN_m\pi}{32a_{\text{B}}^3}\right)^{1/6} \tag{1067}$$

Eq. 1054, Eq. 1063, Eq. 1065, and Eq. 1066 are added to Eq. 1048, Eq. 1049, and Eq. 1050 to solve for $\tau_{B,j}$, which is the bulk relaxation time.

Table 155 summarizes the parameters for phosphorus and boron in silicon bulk samples.

Table 155   Parameters for phosphorus and boron in silicon bulk samples

Symbol	Name	Phosphorus	Name	Boron	Unit
M_{doped}	M_n	30.9	M_p	10.8	Da
R_{doped}	R_n	123e-12	R_p	117e-12	m
Q_0	Q0_n	4	Q0_p	15	1
Ξ_u	Eu_n	9	Eu_p	45	eV
w_{L}	wL_n	0.2	wL_p	0.02	1
w_{T}	wT_n	8	wT_p	6	1
w_{TU}	wTU_n	0.9e6	wTU_p	2e6	1

E_{D}, b, and A_x are fitted to experiments for a given doping concentration and doping material.

Table 156 summarizes the parameters for phosphorus-doped silicon samples.

Table 156   Fitting parameters for phosphorus-doped silicon bulk samples

Symbol	Name	Doping concentration [cm⁻³]						Unit
		7.5e16	2.5e17	4.7e17	1e18	2e19	1.7e20	
E_D	ED_n	0	0.05	0.22	0.5	1.33	2.33	eV
b	b	0	8	8	8	186	286	1
A_x	Ax	0	0	11.75	11.75	6.75	11.75	$\times 10^{-45}\,\mathrm{s}^3$

Table 157 summarizes the parameters for boron-doped silicon samples.

Table 157   Fitting parameters for boron-doped silicon bulk samples

Symbol	Name	Doping concentration [cm⁻³]			Unit
		1e13	4e15	4e16	
E_D	ED_p	0	0	0.5	eV
b	b	0	0	18	1
A_x	Ax	0	0	1.2	$\times 10^{-45}\,\mathrm{s}^3$

NOTE   To achieve good agreement with measurements for various doping concentrations, it is suggested to first determine w_L, w_T, and w_{TU} for low-doping concentration samples: w_{TU} mainly determines the high-temperature range, and w_L and w_T determine the peak value and their ratio w_L/w_T determines the slope of the low-temperature range. For moderate doping cases, free-carrier scattering starts to have an effect; therefore, E_D and b are used to further fit the low-temperature range. For high doping cases, bound-carrier scattering is insignificant; therefore, κ is mainly determined by E_D, b, and A_x.

In general, E_D, b, and A_x must be fitted for each doping concentration. To provide a good guess for their values, a numerical table can be defined in the parameter file:

```
Kappa {
   NumericalTable (
      ** N ED_n ED_p b Ax
      7.5e16 0 0.5 8 0
      2.5e17 0.05 0.5 8 0
      ...
   )
}
```

The numerical table defines the fitted values of `ED_n`, `ED_p`, `b`, and `Ax` for some specific doping concentrations N. For other doping concentrations, these parameters are determined by interpolating the given values in the `NumericalTable`.

Thin-Layer Relaxation Time

For thin layers with thickness d_{Ly}, the relaxation time decreases [9]:

$$\tau_{\mathrm{Ly},j} = F(\delta_j, p)\tau_{B,j} \tag{1068}$$

$$F(\delta_j, p) = 1 \Big/ \left[1 + \frac{3}{8\delta_j}(1-p) \right] \tag{1069}$$

where:

$$\delta_j = r_\delta d_{\mathrm{Ly}} / (v_j \tau_{B,j}) \tag{1070}$$

$$p = \exp\!\left(-\frac{16\pi^3\eta^2}{\lambda^2}\right) \tag{1071}$$

$$\lambda = 2\pi v_s / \omega \tag{1072}$$

where:

- d_{Ly} is the layer thickness.
- r_δ is a constant to adjust the mean free path in some situations.
- η is a fitting parameter.

The layer thickness is computed internally by setting the `LayerThickness` command in the `Physics` section (see LayerThickness Command on page 310). Alternatively, you can define the layer thickness by setting the parameter d_{Ly} if `LayerThickness` is not defined. By default, d_{Ly} is 0.3 m, which ensures $F(\delta_j, p) = 1$, thereby the bulk relaxation time is taken into account. Table 158 summarizes the parameters for thin-layer silicon samples.

Table 158 Default values for thin-layer parameters and the numeric integral

Symbol	Name	Value	Range	Unit
d_{Ly}	dLy	3e-1	real	m
r_δ	r_del	1	[0,1]	1
η	eta	1.5e-10	real	m
N_ω	Nomg	3	integer	1
ζ	order	2	integer	1

Mole Fraction–Dependent Relaxation Time

To compute κ for alloy materials such as SiGe, the parameters are interpolated according to the standard Vegard law. This is performed using the built-in `MoleFraction`-dependent functionality in Sentaurus Device. All parameters in Table 154 on page 904 are `MoleFraction`-dependent parameters. An example of the parameter file is:

```
Kappa {
   ...
   omega1(0) = 2.357e13 #[s^-1]
   omega1(1) = 1.322e13 #[s^-1]
   ...
   AI(0) = 1.32e-45 #[s^3]
   AI(1) = 2.4e-45 #[s^3]
   Xmax(1) = 1
   B(AI(1)) = -3.74e-42
}
```

> **NOTE** Impurity scattering is significant in alloy materials. Therefore, `B(AI(1))` is fitted to achieve good agreement with measurement.

Eq. 1045 involves an integral over phonon frequency. The numeric integration is solved with the Gauss quadrature method, which can be fine-tuned by adjusting the following parameters:

- N_ω is the number of integration points.
- ζ is the order of the Legendre polynomial that is used in the Gauss quadrature method.

Table 158 on page 909 lists the default values of these two parameters. More integration points and higher orders generally lead to more accurate results, while the performance decreases significantly. Nevertheless, when using $N_\omega = 3$ and $\zeta = 2$, the computed κ agrees well with measurements.

The ConnellyThermalConductivity Model

For thin layers, the scattering of acoustic phonons at interfaces reduces the mean free path and reduces thermal conductivities. In the review paper [10], an integral equation describes the geometric effect of the reduced phonon path. The actual model provides an excellent fit of the behavior. The thermal conductivity κ is given by:

$$\kappa = \kappa_{\text{bulk}} \left(\frac{t + t_0}{0.6 \Lambda + t + t_0} \right)^\eta \tag{1073}$$

where:

- t is the layer thickness extracted by the simulator for the layer.
- t_0 is the phonon penetration at interfaces.
- Λ is the phonon mean free path.
- η is the power exponent for the thickness dependency.
- κ_{bulk} is the bulk thermal conductivity.

Table 159 Parameters of the ConnellyThermalConductivity model

Name	Symbol	Default	Unit	Range	Description
plot	–	0	–	{0,1}	Plots parameter to screen
lambda	Λ	0.3	µm	real	Phonon mean free path
t0	t_0	5e-4	µm	>=0	Phonon penetration at interfaces
eta	η	0.8	1	real	Power exponent
UseLayerThicknessField	–	0	–	{0,1}	Selects layer thickness quantity
bulkmodel	–	"Kappa"	–	string	Name for bulk model parameter

Layer Thickness Computation

The layer thickness t is computed internally (see LayerThickness Command on page 310). By default, the model uses the layer thickness quantity `LayerThickness`. Setting `UseLayerThicknessField=1` selects the quantity `LayerThicknessField`.

Bulk Thermal Conductivity Computation

The bulk thermal conductivity κ_{bulk} is computed from parameters found in the section given by the `bulkmodel` parameter. It recognizes the parameters given in Table 160.

Table 160 Parameters of ConnellyThermalConductivity for bulk thermal conductivity

Name	Symbol	Default	Unit	Range	Description
Formula	–	0	–	{0,1}	Selects formula
a1	a_1	1.	W/K cm	real	see Eq. 1075
b1	b_1	0.	W/K^2 cm	real	
c1	c_1	0.	W/K^3 cm	real	
a0	a_0	1.	K cm/W	real	see Eq. 1074

Table 160   Parameters of ConnellyThermalConductivity for bulk thermal conductivity

Name	Symbol	Default	Unit	Range	Description
b0	b_0	0.	cm/W	real	
c0	c_0	0.	cm/W K	real	

Similar to the default model, for `Formula=0`:

$$\kappa_{\text{bulk}} = \frac{1}{a_0 + b_0 T + c_0 T^2} \tag{1074}$$

For `Formula=1`:

$$\kappa_{\text{bulk}} = a_1 + b_1 T + c_1 T^2 \tag{1075}$$

The model is activated in the command file by:

```
Physics (...) {
   ThermalConductivity ( "ConnellyThermalConductivity" )
}
```

Example of Parameter File Segment

```
Material = "MyMaterial" {
   ConnellyThermalConductivity {
      lambda = 0.3                    * [um]
      ...
      UseLayerThicknessField = 0    * use LayerThickness/LayerThicknessField
      bulkmodel = "MyKappa"          * bulk model name
   }
   MyKappa {                          * parameter section specified by 'bulkmodel'
      Formula = 0                    * select formula
      ...
   }
}
```

The pmi_msc_thermalconductivity Model

This model depends on the lattice temperature and the state occupation probabilities of an MSC. If it does not depend on an MSC, it enables a pwl temperature dependency and reads as:

$$\kappa = \kappa(T) \tag{1076}$$

If an explicit MSC dependency is given, the global thermal conductivity is computed as:

$$\kappa = \sum_i \kappa_i(T) s_i \tag{1077}$$

where the sum is taken over all MSC states, κ_i are the state thermal conductivities, and s_i are the state occupation probabilities.

The model is enabled in the `Physics` section by:

```
ThermalConductivity (
    PMIModel ( Name="pmi_msc_thermalconductivity" MSConfig="m0" )
)
```

Table 161   Parameters of pmi_msc_thermalconductivity

Name	Symbol	Default	Unit	Range	Description
plot	–	0	–	{0,1}	Plot parameter to screen
kappa	κ	0.	W/Kcm	real	Constant value
kappa_nb_Tpairs	–	0	–	>=0	Number of interpolation points
kappa_Tp<int>_X	–	–	K	real	Temperature at <int>-th interpolation point
kappa_Tp<int>_Y	–	–	W/Kcm	real	Value at <int>-th interpolation point

See The pmi_msc_heatcapacity Model on page 900 for an explanation of the individual parameters and how the parameters can be overwritten for individual MSC states. Only the name of the parameters (use `kappa`) and the unit changes.

Thermoelectric Power (TEP)

Sentaurus Device supports the following choices for computing the thermoelectric powers P_n and P_p in semiconductors:

- Use a tabulated set of experimental values for silicon as a function of temperature and carrier concentration.

- Use analytic formulas with two adjustable parameters κ and s.

- As a user-defined function of the carrier density and the lattice temperature (thermoelectric power PMI).

In metals, the thermoelectric power P is only allowed as a user-defined function of the electric field vector and the lattice temperature (as a PMI model).

Physical Models

Table-Based TEPower Model

By default, Sentaurus Device computes the thermoelectric powers P_n and P_p using a table of experimental values of TEPs for silicon published by Geballe and Hull [11] as functions of temperature and carrier concentration. Sentaurus Device extrapolates P_nT and P_pT linearly for temperatures between $360\,\text{K}$ and $500\,\text{K}$, thereby preserving the $1/T$ dependency of data presented at higher temperatures by Fulkerson *et al.* [12], which holds up to near the intrinsic temperature.

P_n and P_p are shown in Figure 59 as a function of temperature and carrier concentration as used in Sentaurus Device.

Figure 59   TEPs (*left*) P_n and (*right*) P_p as a function of temperature and carrier concentration

Analytic TEPower Model

As an alternative, analytic formulas as described in [13][14] can be used to compute the thermoelectric powers in nongenerate semiconductors:

$$P_n = -\kappa_n \frac{k}{q}\left[\left(\frac{5}{2} - s_n\right) + \ln\left(\frac{N_C}{n}\right)\right] \tag{1078}$$

$$P_p = \kappa_p \frac{k}{q}\left[\left(\frac{5}{2} - s_p\right) + \ln\left(\frac{N_V}{p}\right)\right] \tag{1079}$$

where you can adjust the parameters κ and s in the parameter file. Table 162 on page 915 lists the parameters and their default values.

Table 162   Parameters of analytic TEPower model

Parameter name	Symbol	Default	Unit	Range	Description
s_n	s_n	1.	–	real	See Eq. 1078
s_p	s_p	1.	–	real	See Eq. 1079
scale_n	κ_n	1.	–	real	See Eq. 1078
scale_p	κ_p	1.	–	real	See Eq. 1079

PMI_ThermoElectricPower Model

In the most general case, the TEPs in semiconductors can be computed using the thermoelectric power PMI (see Thermoelectric Power on page 1269) as functions of the lattice temperature and the carrier density. Both the standard and simplified PMI (with automatic derivatives) are supported.

Thermoelectric Power in Metals

In metals, thermoelectric power is defined as a PMI depending on the gradient of the Fermi potential $\nabla \Phi_M$ and the lattice temperature T (see Metal Thermoelectric Power on page 1274). It is used in connection with thermodynamic transport in metals (Seebeck effect).

Using Thermoelectric Power

The thermoelectric powers in semiconductors are computed automatically when the `Temperature` equation is solved and the keyword `Thermodynamic` is specified in the global `Physics` section. By default, tabulated silicon data is used.

To enable an analytic formula (Eq. 1078, p. 914, Eq. 1079, p. 914) or thermoelectric power PMI models either regionwise, or materialwise, or globally, the keyword `TEPower` with `Analytic` or the PMI name as an option must be specified in the corresponding `Physics` section. For example:

```
Physics(Region="region1") {
   TEPower(Analytic)           # analytic formula TEP model in "region1"
}

Physics(Region="region2") {
   TEPower(pmi_tepower)        # PMI in "region2"
}
```

activates an analytic formula in `"region1"`, the thermoelectric power PMI `pmi_tepower` in `"region2"`, and tabulated data interpolation in all other semiconductor regions.

For backward compatibility, the keyword `AnalyticTEP` in the `Physics` section is still available to activate an analytic formula TEP globally. It is equivalent to specifying `TEPower(Analytic)` in the global `Physics` section.

The coefficients for the thermoelectric powers defined by the analytic formula are available in the `TEPower` parameter set (see Table 153 on page 901).

The thermoelectric power in metals is activated selectively when the `Temperature` equation is solved and the keyword `Thermodynamic` is specified in the global `Physics` section. To active it regionwise, materialwise, or globally, the keyword `MetalTEPower` with the metal thermoelectric power PMI name as an option must be specified in the corresponding `Physics` sections. For example:

```
Physics(Material="Copper") {
   MetalTEPower(pmi_tepower)
}
```

activates the metal TEP computation and thermodynamic transport in the copper part of the device.

Heating at Contacts, Metal–Semiconductor and Conductive Insulator–Semiconductor Interfaces

The Peltier heat at a contact, or a metal–semiconductor interface, or a conductive insulator–semiconductor interface is modeled as:

$$Q = J_n(\alpha_n \Delta E_n + (1 - \alpha_n)\Delta\varepsilon_n) \tag{1080}$$

$$Q = J_p(\alpha_p \Delta E_p + (1 - \alpha_p)\Delta\varepsilon_p) \tag{1081}$$

where:

- Q is the heat density at the interface or contact (when $Q > 0$, there is heating; when $Q < 0$, cooling).
- J_n and J_p are the electron and hole current densities normal to the interface or contact.
- ΔE_n and ΔE_p are the energy differences for electrons and holes across the interface or at the contact.
- α_n, α_p, $\Delta\varepsilon_n$, and $\Delta\varepsilon_p$ are fitting parameters with $0 \le \alpha_n, \alpha_p \le 1$.

For the thermodynamic model, Sentaurus Device computes the energy differences for electrons and holes as:

$$\Delta E_n = \Phi_M - \beta_n(\Phi_n + \gamma_n TP_n) + (1 - \beta_n)E_C/q \tag{1082}$$

$$\Delta E_p = \Phi_M - \beta_p(\Phi_p + \gamma_p TP_p) + (1 - \beta_p)E_V/q \tag{1083}$$

where β_n, β_p, γ_n, and γ_p are fitting parameters.

For the default lattice temperature model and the hydrodynamic model, Sentaurus Device computes the energy differences for electrons and holes as:

$$\Delta E_n = \Phi_M + E_C/q \tag{1084}$$

$$\Delta E_p = \Phi_M + E_V/q \tag{1085}$$

To activate Peltier heat, the keyword `MSPeltierHeat` must be specified inside the corresponding interface or electrode `Physics` section:

```
Physics(MaterialInterface="Silicon/Metal") {
   MSPeltierHeat
   ...
}
```

or:

```
Physics(Electrode="cathode") {
   MSPeltierHeat
   ...
}
```

The fitting parameters α, β, γ, and $\Delta\varepsilon$ can be specified in the `MSPeltierHeat` parameter set of the region interface or electrode for which the Peltier heat is computed:

```
MaterialInterface = "Silicon/Metal" {
   MSPeltierHeat
   {
      alpha  = 1.0 , 1.0 # [1]
      beta   = 1.0 , 1.0
      gamma  = 1.0 , 1.0
      deltaE = 0.0 , 0.0 # [eV]
   }
}
```

Their default values are $\alpha_n = \alpha_p = \beta_n = \beta_p = \gamma_n = \gamma_p = 1$ and $\Delta\varepsilon_n = \Delta\varepsilon_p = 0 \text{ eV}$.

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Part III Physics of Light-Emitting Diodes

This part of the *Sentaurus™ Device User Guide* contains the following chapters:

CHAPTER 34 Light-Emitting Diodes

This chapter describes the physics and the models used in light-emitting diode simulations.

NOTE LED simulations present unique challenges that require problem-specific model and numerics setups. Contact TCAD Support for advice if you are interested in simulating LEDs (see Contacting Your Local TCAD Support Team Directly on page xliii).

Modeling Light-Emitting Diodes

From an electronic perspective, light-emitting diodes (LEDs) are similar to lasers operating below the lasing threshold. Consequently, the electronic model contains similar electrothermal parts and quantum-well physics as in the case of a laser simulation.

The key difference between an LED and a laser is a resonant cavity design for lasers that enhances the coherent stimulated emission at a single frequency (for each mode). An LED emits a continuous spectrum of wavelengths based on spontaneous emission of photons in the active region. However, an alternative design for LEDs with a resonant cavity – the resonant cavity LED (RCLED) – uses the resonance characteristics to cause an amplified spontaneous emission in a narrower spectrum to allow for superbright emissions.

The simulation of LEDs presents many challenges. The large dimension of typical LED structures, in the range of a few hundred micrometers, prohibits the use of standard time-domain electromagnetic methods such as finite difference and finite element. These methods require at least 10 points per wavelength and typical emissions are of the order of $1\,\mu m$. A quick estimate gives a necessary mesh size in the order of 10 million mesh points for a 2D geometry. Alternatively, the use of the raytracing method approximates the optical intensity inside the device as well as the amount of light that can be extracted from the device. In many cases, a 2D simulation is not sufficient and a 3D simulation is required to give an accurate account of the physical effects associated with the geometric design of the LED.

Innovative designs such as inverted pyramid structures, chamfering of various corners, surface roughening, and drilling holes are performed in an attempt to extract the maximum amount of light from the device. The device editor Sentaurus Structure Editor is well equipped to create complex 3D devices and provides great versatility in exploring different realistic LED designs.

Photon recycling is important because most of the light rays are trapped within the device by total internal reflection. There are two types of photon recycling: for nonactive regions and for the active region. The nonactive-region photon recycling involves absorption of photons in the nonactive regions to produce optically generated electron–hole pairs, and these subsequently join the drift-diffusion processes of the general carrier population. The active-region photon recycling is more complicated, and interested users are referred to [1][2] for its basic theory.

Coupling Electronics and Optics in LED Simulations

An LED simulation solves the Poisson equation, carrier continuity equations, temperature equation, and Schrödinger equation self-consistently. Figure 60 illustrates the coupling of the various equation systems in an LED simulation.

Figure 60   Flowchart of the coupling between the electronics and optics for an LED simulation

Single-Grid Versus Dual-Grid LED Simulation

Both single-grid and dual-grid LED simulations are possible. However, in the case of a single-grid simulation, raytracing takes a longer time for the following reason: Raytracing builds a binary tree for each starting ray. Each branch of the tree corresponds to a ray at a mesh cell boundary. If the materials in two adjoining cells are different, the ray splits into refracted and reflected rays, creating two new branches. If the materials are the same in adjoining cells, the propagated ray creates a new branch. A fine mesh increases the depth of the branching significantly. Each new branch of the binary tree is created dynamically and, if dynamic memory allocation of the machine is not sufficiently fast, the tree creation of the raytracing becomes a bottleneck in the simulation.

To overcome this problem, the grids for the electrical problem and the raytracing problem are separated. The optical grid for raytracing is meshed coarsely. The binary tree created will be smaller and raytracing is more efficient. Such a coarse mesh enables you to compute the extraction efficiency and output radiation pattern. However, the optical intensity within the device cannot be resolved well with a coarse mesh.

Electrical Transport in LEDs

Besides the drift-diffusion transport of typical semiconductor devices, the LED requires additional physical models to compute various optical effects. These physical models are described in the following sections.

Spontaneous Emission Rate and Power

In the active region, the spontaneous emission of photons depletes the carrier population. At each active vertex, the spontaneous emission (or recombination of carriers) rate (units of $\#s^{-1}m^{-3}$) is an integral of the spontaneous emission:

$$R^{sp}_{active}(x, y, z) = \int_{0}^{\infty} r^{sp}(E)\rho^{opt}(E)dE$$

(1086)

where the optical mode density is:

$$\rho^{opt}(E) = \frac{n_g^2 E^2}{\pi^2 \hbar^3 c^2}$$

(1087)

and $r^{sp}(E)$ is defined in Eq. 1113, p. 962. The total spontaneous emission power density at each active vertex (units of $Js^{-1}m^{-3}$) is:

$$\Delta P^{sp}(x, y, z) = \int_{0}^{\infty} r^{sp}(E)\rho^{opt}(E) \cdot (\hbar\omega)dE$$

(1088)

This equation is similar to Eq. 1086, except that an additional energy term, $E = \hbar\omega$, is included in the integrand to account for the energy spectrum of the spontaneous emission.

In LED simulations, the spontaneous emission spectrum, $r^{\mathrm{sp}}(E)$, broadens significantly with increasing injected carriers. The integrals in Eq. 1086 and Eq. 1088 are based on a Riemann sum and, as with numeric integration, truncates at an internally set energy value. You can change the truncation value and the Riemann integration interval with the following syntax in the command file:

```
Physics {...
   LED (...
      Optics (...)
      SponScaling = 1.0
      SponIntegration(<energyspan>,<numpoints>)
   )
}
```

where `<energyspan>` is a floating-point number (in eV) and is measured from the edge of the energy bandgap, and `<numpoints>` is an integer denoting the number of discretized intervals to use within this energy span.

The total spontaneous emission power is the volume integral of the power density over all the active vertices:

$$P_{\mathrm{total}}^{\mathrm{sp}} = \int\limits_{(\mathrm{active-region})} \Delta P^{\mathrm{sp}}(x, y, z)dV \tag{1089}$$

This is the total spontaneous emission power that is computed and output in an LED simulation.

Since you are dealing with a spectrum for the spontaneous emission, it is evident from Eq. 1086 and Eq. 1088 that the integral sum of the photon rate and the integral sum of the photon power are not simply related by a constant photon energy, that is:

$$\Delta P^{\mathrm{sp}}(x, y, z) \neq (\hbar\omega_0)R_{\mathrm{active}}^{\mathrm{sp}}(x, y, z) \tag{1090}$$

Spontaneous Emission Power Spectrum

The LED spontaneous emission power spectrum can be plotted by activating the `GainPlot` section. The syntax consists of defining the number of discretized points for the spectrum and the span of the spectrum to plot:

```
File {...
   ModeGain = "ngainplot_des"
}

GainPlot {
   Range = (<float>, <float>)     # specific range in eV
   Range = Auto                   # automatically determines range
```

```
      Intervals = <integer>        # number of discretized points
   }

   Solve {...
      PlotGain( Range=(0,1) Intervals=5 )
   }
```

In the gain file, the quantity `SponEmissionPowerPereV` (W/eV) is plotted. Integrating this quantity over the energy (eV) span recovers the total LED power.

Current File and Plot Variables for LED Simulation

When an LED simulation is run, specific LED result variables are output to the plot file. Table 163 and Table 164 on page 926 list the current file output and the plot variables valid for LED simulation.

Table 163   Current file for LED simulation

Dataset group	Dataset	Unit	Description
`LedWavelength`		nm	Average wavelength of LED simulation.
`n_Contact` `p_Contact`	`Charge`	C	
	`eCurrent`	A	
	`hCurrent`	A	
	`InnerVoltage`	V	
	`OuterVoltage`	V	
	`TotalCurrent`	A	
`Photon_Exited`		s^{-1}	Rate of photon escaping from device.
`Photon_ExtEfficiency`		1	Photon extraction efficiency.
`Photon_NetPhotonRecycle`		s^{-1}	Net photon-recycling photon rate.
`Photon_NonActiveAbsorb`		s^{-1}	Rate of photon absorption in nonactive regions.
`Photon_Spontaneous`		s^{-1}	Spontaneous emission photon rate.
`Photon_Trapped`		s^{-1}	Rate of trapped photons in device.
`Power_Absorption`		W	Absorption power.
`Power_ASE`		W	Amplified spontaneous emission power.
`Power_Exited`		W	Power escaping from device.

Table 163   Current file for LED simulation (Continued)

Dataset group	Dataset	Unit	Description
`Power_ExtEfficiency`		1	Power extraction efficiency.
`Power_NetPhotonRecycle`		W	Net photon-recycling power.
`Power_NonActiveAbsorb`		W	Power absorbed in nonactive regions.
`Power_ReEmit`		W	Re-emission power.
`Power_SpecConvertGain`		W	Net power gain of spectral conversion.
`Power_Spontaneous`		W	Spontaneous emission power.
`Power_Total`		W	Total internal optical power of LED.
`Power_Trapped`		W	Power trapped inside device.
`Time`		1 s	For quasistationary. For transient.

Table 164   Plot variables for LED simulation

Plot variable	Dataset name	Unit	Description
`DielectricConstant`		1	Dielectric profile.
`LED_TraceSource`			Influence of each active vertex on the total extracted light.
`MatGain`	`OpticalMaterialGain`	m^{-1}	Local material gain.
`RayTraceIntensity`		Wcm^{-3}	Optical intensity from raytracing.
`RayTrees`			Raytree structure. Not available for the compact memory option.
`SpontaneousRecombination`		$cm^{-3}s^{-1}$	Sum of spontaneous emission.

`LedWavelength` is computed automatically in the simulation. It is taken as the wavelength where the peak of the spontaneous spectrum occurs. Different options for computing the wavelength are available (see). For clarity, photon rate and power output results are separated into two groups:

- The photon rate group has units of s^{-1}.
- The power group has units of W.

Photon and power quantities need to be computed separately if a spectrum is involved. Suppose that the spontaneous emission coefficient is $r^{sp'}$ (units of $eV^{-1}cm^{-3}s^{-1}$). The photon rate is $\int r^{sp'}dE$ with $r^{sp'} = r^{sp}(E) \times \rho^{opt}(E)$), while the power is $\int r^{sp'} \cdot EdE$. The extraction coefficient is the ratio of the exited and internal quantities,

so the photon rate (`Photon_ExtEfficiency`) and power (`Power_ExtEfficiency`) extraction efficiencies are different.

The only case when `Photon_ExtEfficiency=Power_ExtEfficiency` is for a single wavelength simulation that does not involve a spectrum.

The total outcoupled (exited) power is then (`Power_ExtEfficiency` x (`Power_Total-Power_NonActiveAbsorb`)), where the total internal optical power is:

$$Power\_Total = Power\_Spontaneous + Power\_NetPhotonRecycle + \\ Power\_SpecConvertGain \tag{1091}$$

The photon rate extraction efficiency has been computed using:

$$Photon\_ExtEfficiency = Photon\_Exited / (Photon\_Spontaneous + \\ Photon\_NetPhotonRecycle - Photon\_NonActiveAbsorb) \tag{1092}$$

For power conservation in a nonactive photon-recycling case, you have:

$$Power\_Total = Power\_Spontaneous \\ = Power\_Exited + Power\_Trapped + \\ Power\_NonActiveAbsorb \tag{1093}$$

`Power_Trapped` refers to the power of the photons that are trapped (by total internal reflection or possibly nonconverging raytracing) indefinitely in the raytracing simulation. In a realistic scenario, the trapped photons decay in the device by some mechanism.

> **NOTE** Users are responsible for introducing losses within the device (perhaps by introducing nonzero extinction coefficients in appropriate regions) to ensure proper treatment of the trapped photons.

> **NOTE** The `Power_NetPhotonRecycle`, `Power_SpecConvertGain`, and `Photon_NetPhotonRecycle` quantities pertain only to the active-region photon-recycling model. These quantities are zero if the active-region photon-recycling model is not activated.

LED Wavelength

There are different ways of computing or inputting the LED wavelength:

- `AutoPeak`: A robust algorithm based on the multisection method is used to search for the peak of the spontaneous emission rate spectrum ($r^{sp'}$ versus E-curve). Then, the energy of the peak $r^{sp'}$ is translated into the LED wavelength.

- `AutoPeakPower`: The same algorithm as for `AutoPeak` is used on the spontaneous emission power spectrum ($r^{sp'}E$ versus E-curve).

■ `Effective`: An effective wavelength is computed such that:

$$\text{LED power} = \text{LED photon rate x photon\_energy} \qquad (1094)$$

where photon_energy is a direct inverse function of the effective wavelength.

■ User inputs a fixed LED wavelength.

The keywords for activating the various LED wavelength options are:

```
Physics {...
   LED (...
      Optics (...
         RayTrace (...
            Wavelength = <float> | AutoPeak | Effective | AutoPeakPower
         )
      )
   )
}
```

> **NOTE** If no `Wavelength` keyword is specified, the old peak wavelength
> search algorithm is used.

Optical Absorption Heat

Photon absorption heat in semiconductor materials can be simplified into two processes:

■ *Interband absorption*: When a photon is absorbed across the forbidden band gap in a semiconductor, it is absorbed to create an electron–hole pair. The excess energy (photon energy minus the band gap) of the new electron–hole pair is assumed to thermalize, resulting in eventual lattice heating.

■ *Intraband absorption*: A photon can be absorbed to increase the energy of a carrier. The excess energy relaxes eventually, contributing to lattice heating.

In both processes, it is assumed that the eventual lattice heating (in a quasistationary simulation) occurs in the locality of photon absorption.

In LEDs, the extraction efficiency ranges between 40% and 60% commonly. This means a significant portion of the spontaneous light power is trapped within the device. The trapped light is ultimately absorbed and becomes the source of photon absorption heat.

Other keywords in the `Physics` section have been added. As far as possible, the syntax has been kept similar to that of the `QuantumYield` model (see Quantum Yield Models on page 544):

```
Plot {...
   OpticalAbsorptionHeat          # units of [W/cm^3]
}

Physics {...
   LED(...)
   OpticalAbsorptionHeat (
      StepFunction (
         Wavelength = float        # um
         Energy = float            # eV
         Bandgap                   # auto-checking of band gap
         EffectiveBandgap          # auto-checking of band gap
      )
      ScalingFactor = float        # default is 1.0
   )
}
```

Some comments about the different `StepFunction` choices:

- When the keyword `Wavelength` or `Energy` is used, the wavelength or energy of the photons is checked against this value. If the photon wavelength or energy is smaller or larger than this cutoff value, convert the optical generation totally into optical absorption heat, and set optical generation at the vertex to 0.

- The keywords `Bandgap` and `EffectiveBandgap` refer to the cutoff energy of the step function at $E_g - E_{bgn}$ and $(E_g - E_{bgn} + 2 \cdot (3/2)kT)$, respectively. If the photon energy is greater than the cutoff energy (interband absorption), deduct the band gap to obtain the excess energy but do not deduct the optical generation. If the photon energy is less than the cutoff energy (intraband absorption), set the excess energy to the photon energy. In both cases, the excess energy will be converted to a heat source term for the lattice temperature equation.

- A `ScalingFactor` is introduced to allow for flexible fine-tuning.

- The `OpticalAbsorptionHeat` statement can be specified globally in the `Physics` section or the materialwise or regionwise `Physics` section.

Quantum Well Physics

The physics in the quantum well (QW) is described in detail in Chapter 35 on page 961. Due to the size of the LED structure, it is recommended that you start with representing quantum wells as bulk active regions, and then contact TCAD Support for assistance in the more advanced settings (see Contacting Your Local TCAD Support Team Directly on page xliii).

The scattering transport into QWs is approximated with thermionic emission for the best convergence behavior. The corrections of the carrier densities due to quantizations of the QW can be taken into account in the localized QW model (see Localized Quantum-Well Model on page 978).

Accelerating Gain Calculations and LED Simulations

The computation bottleneck in LED simulations with gain tables is the calculation of the spontaneous emission rate at every Newton step. The spontaneous emission rate (unit is s^{-1}) is an energy integral of the spontaneous emission coefficient (unit is $s^{-1}eV^{-1}cm^{-3}$), and the integration is performed as a Riemann sum. To accelerate this calculation, a Gaussian quadrature integration can be used instead.

All gain calculations (with or without the gain tables) can be accelerated by specifying the following syntax in the `Math` section of the command file:

```
Math {...
   BroadeningIntegration ( GaussianQuadrature ( Order = 10 ) )
   SponEmissionIntegration ( GaussianQuadrature ( Order = 5 ) )
}
```

The Gaussian quadrature numeric integration then is used in all parts of the gain calculations including broadening effects.

The order can be from 1 to 20. This order refers to the order of the Legendre polynomial that is used to fit the spontaneous emission spectrum in the energy range of the integration. The Gaussian quadrature integration is exact for any spectrum that can be expressed as a polynomial.

> **NOTE** Convergence issues can be experienced in some situations. In such cases, switch off the Gaussian quadrature integration for `SponEmissionIntegration` and `BroadeningIntegration` in the `Math` section.

Discussion of LED Physics

Many physical effects manifest in an LED structure. Current spreading is important to ensure that the current is channeled to supply the spontaneous emission sources at strategic locations that will provide the optimal extraction efficiency.

Changes to the geometric shape of the LED are made to extract more light from the structure. In most cases, the major part of the light produced is trapped within the structure through total

internal reflection. As a result, the nonactive-region and active-region photon-recycling effect becomes relevant. This important physics has been incorporated into different physical models within Sentaurus Device. The nonactive photon-recycling (absorption of photons in nonactive regions) is switched on automatically by default. In most cases, the nonactive photon-recycling model is sufficient to capture the major physical effects because the volume of the active region is insignificant compared to the nonactive regions. Nonetheless, the active-region photon-recycling model can become important if there is a very high stimulated gain, which is usually not the case for GaN LEDs.

Important aspects of LED design are simulated easily by Sentaurus Device. These include current spreading flow, geometric design, and extraction efficiency.

LED Optics: Raytracing

Raytracing is used to compute the intensity of light inside an LED, as well as the rays that escape from the LED cavity to give the signature radiation pattern for the LED output. The basic theory of raytracing is presented in Raytracing on page 593.

Arbitrary boundary conditions can be defined. A detailed description of how to set up the boundary conditions for raytracing is discussed in Boundary Condition for Raytracing on page 605. This is particularly useful in 3D simulations where you can define reflecting planes to use symmetry for reducing the size of the simulation model.

In addition, you can use reflecting planes to take into account external components such as reflectors, an example of which is shown in Figure 61.

Figure 61   Using the reflecting boundary condition to define a reflector for LED raytracing

The raytracer needs to include the use of the `ComplexRefractiveIndex` model and to define the polarization vector. The syntax for this is:

```
Physics {...
   ComplexRefractiveIndex (...
      WavelengthDep ( real imag )
      CarrierDep( real imag )
      GainDep( real )                  # or real(log)
```

```
            TemperatureDep( real )
            CRImodel ( Name = "crimodelname" )
        )
        LED (...
            Optics (
                RayTrace(
                    PolarizationVector = Random    # or (x y z) vector
                    RetraceCRIchange = float       # fractional change to retrace rays
                    ...
                )
            )
        )
    }
```

When `PolarizationVector=Random` is chosen, random vectors that are perpendicular to
the starting ray directions are generated and assigned to be the polarization vector of each
starting ray. The direction of each starting ray is described in Isotropic Starting Rays From
Spontaneous Emission Sources and Anisotropic Starting Rays From Spontaneous Emission
Sources on page 934.

The keyword `RetraceCRIchange` specifies the fractional change of the complex refractive
index (either the real or imaginary part) from its previous state that will force a total
recomputation of raytracing.

Compact Memory Raytracing

A compact memory model has been built for LED raytracing. In the compact memory model,
the raytrees are no longer saved, and necessary quantities are computed as required and
extracted to compact storages of optical generation and optical intensity. As a result, the
memory use and footprint are significantly reduced, thereby enabling the raytracing simulation
of large LED structures. The syntax for activation is:

```
    Physics {...
        LED (...
            RayTrace(...
                CompactMemoryOption
            )
        )
    }
```

NOTE   The full active photon-recycling model does not work with the compact
memory model.

Isotropic Starting Rays From Spontaneous Emission Sources

The source of radiation from an LED is mainly from spontaneous emissions in the active region (this is further discussed in Spontaneous Emission Rate and Power on page 923). The spontaneous emission in the active region of the LED is assumed to be an isotropic source of radiation and can be conveniently represented by uniform rays emitting from each active vertex, as shown in Figure 62.

Figure 62   Uniform rays radiating isotropically from an active vertex source in (*left*) 2D space and (*right*) 3D space: only one-eighth of spherical space is shown for the 3D case

Isotropy requires that the surface area associated with each ray must be the same. The isotropy of the rays in 2D space is apparent. In 3D space, achieving isotropy is not as simple as dividing the angles uniformly. The elemental surface area of a sphere is $r^2 \sin\theta (d\theta)(d\phi)$, so uniformly angular-distributed rays are weighted by $\sin\theta$ and, therefore, do not signify isotropy.

To approximate this problem in 3D, a geodesic dome approximation is used (the geodesic dome is not strictly isotropic). Rays are directed at the vertices of the geodesic dome. The algorithm starts by constructing an octahedron and, then, recursively splits each triangular face of the octahedron into four smaller triangles.

The first stage of this splitting process is shown in Figure 62 (*right*), where rays are directed at the vertices of each triangle. The minimum number of rays is six, that is, one is directed along each positive and negative direction of the axes. If the first stage of recursive splitting is applied, a few more rays are constructed as shown in Figure 62, and the number of starting rays becomes 18. The second stage of recursive splitting gives 68 rays and so on. Therefore, you are constrained to selecting a fixed set of starting rays in the 3D case. Alternatively, you can input your own set of isotropic starting rays (see Reading Starting Rays From File on page 936).

Anisotropic Starting Rays From Spontaneous Emission Sources

In some LED designs, the geometry governs the polarization of the optical field in the device. The spontaneous gain is dependent on the direction of this polarization. Consequently, this leads to an anisotropic spontaneous-emission pattern at the source.

The anisotropic emission pattern is proposed to be described by the following parametric equations:

$$E_x = d1 \cdot \sin(\phi) + d4 \cdot \cos(\phi) \tag{1095}$$

$$E_y = d2 \cdot \sin(\phi) + d5 \cdot \cos(\phi) \tag{1096}$$

$$E_z = d3 \cdot \sin(\theta) + d6 \cdot \cos(\theta) \tag{1097}$$

where the intensity is given by:

$$I = E_x^2 + E_y^2 + E_z^2 \tag{1098}$$

The bases of sine and cosine are chosen based on the fact that the optical matrix element has such a functional form when polarization is considered (see Importing Gain and Spontaneous Emission Data With PMI on page 982). By changing the values of d1 to d6, different emission shapes can be orientated in different directions, and this feature allows you to modify the anisotropy of the spontaneous emission.

The syntax required to activate the anisotropic spontaneous emission feature is:

```
Physics {...
   LED (...
      Optics(...
         RayTrace(...
            EmissionType(
               #Isotropic          # default
               Anisotropic(
                  Sine(d1 d2 d3)
                  Cosine(d4 d5 d6)
               )
            )
         )
      )
   )
}
```

Randomizing Starting Rays

Spontaneous emission is a random process. To take into account the random nature of this process and still ensure that the emission of the starting rays from each active vertex source is isotropic, a randomized shift of the entire isotropic ray emission is introduced.

This is best illustrated in Figure 63 where only four starting rays are used for clarity. For each active vertex, a random angle is generated to determine the random shift of the distribution of the isotropic starting rays. The same concept is also used for the 3D case, and this gives a simple randomization strategy for using raytracing to model the spontaneous emissions.

Figure 63   Shifting the distribution of entire isotropic starting rays by an angle α

Pseudorandom Starting Rays

Randomization of the starting rays is activated by the keyword `RaysRandomOffset` in the following syntax:

```
Physics {...
   LED (...
      RayTrace (...
         RaysRandomOffset
#        RaysRandomOffset (RandomSeed = 123)    # seeding the generator
      )
   )
}
```

You also can fix the seed of the random number generator, and this will compute a pseudorandom set of starting rays, so that repeated runs of the same simulation will reproduce exactly the same raytracing results.

> **NOTE**   Without the keyword `RaysRandomOffset`, the default is a fixed angular shift that is determined by the active vertex number.

Reading Starting Rays From File

The geodesic ray distribution is not truly isotropic. As a result, some percentages of error are incurred when isotropy is really needed. To circumvent this issue, a new feature to allow you to read in a set of source isotropic starting rays has been implemented. The syntax is:

```
Physics {...
   LED (...
      Optics (...
         RayTrace (...
            RaysPerVertex = 1000
            SourceRaysFromFile("sourcerays.txt")
         )
      )
   )
}
```

It is important to note that `RaysPerVertex` specifies the number of direction vectors to read from the file. The file specified with `SourceRaysFromFile` contains 3D direction vectors for each starting ray; an example of which is `sourcerays.txt`:

```
-0.239117 0.788883 0.566115
0.776959 0.548552 -0.308911
-0.607096 -0.042603 0.793485
-0.158313 -0.276546 -0.947871
0.347036 -0.805488 0.480370
...
```

There are several methods for generating 3D isotropic rays, for example, the constrained centroid Voronoï tessellation (CCVT). On the other hand, you can also use this option to import experimentally measured ray distribution profiles.

Moving Starting Rays on Boundaries

Starting rays from active vertices on boundaries create the problem that half of those rays are propagated directly out of the device. To alleviate this problem, a new feature is implemented to allow you to shift the starting position of such rays inwards of the device. Typical values used are from 1 to 5 nm. The syntax is:

```
Physics {...
   LED (...
      Optics (...
         RayTrace (...
            MoveBoundaryStartRays(float)   # [nm]
         )
```

```
         )
      )
   }
```

Clustering Active Vertices

In 3D LED simulations, the number of active vertices can grow significantly when the electrical mesh is refined. This directly implies that the number of starting rays for raytracing increases significantly because that is a direct function of the number of active vertices.

Consequently, the resultant raytree is an exponential function of the number of starting rays, and this results in a very large raytracing problem, which can derail the simulation time and, in part, the memory usage (since the compact memory model declares storage arrays of the size of the number of active vertices).

The solution is to group the active vertices into clusters, with each cluster serving as a distributed source of starting rays for raytracing.

Three possible strategies of clustering the active vertices have been implemented.

Plane Area Cluster

Users select the total number of clusters to be generated. Then, this number is translated into equal area zones (also taking into account the aspect ratio) of the automatically detected QW plane. The active vertices are subsequently grouped into each of these zones such that each zone forms a cluster. The algorithm for plane area clustering is described as follows:

Assume you input the required cluster size, N_c. The aim is to fit as many *squarish* elements (of size $d \times d$) into the QW plane area (size XY) as possible, as shown in Figure 64.

Figure 64   Fitting as many squarish elements of size *d* x *d* into QW plane

The constraints of the problem are:

$$N_c = \frac{XY}{d^2} \tag{1099}$$

$$X = N_x d, \; N_x \text{ is an integer} \tag{1100}$$

$$Y = N_y d, \; N_y \text{ is an integer} \tag{1101}$$

Solving gives:

$$N_x = (\text{INTEGER})\sqrt{(X/Y)N_c} \tag{1102}$$

$$N_y = (\text{INTEGER})(Y/X)N_x \tag{1103}$$

Finally, the adjusted cluster size becomes:

$$N_c' = N_x \times N_y \tag{1104}$$

If no active vertices fall within a plane area segment, that segment is not added to the list of clusters. Therefore, you may see a smaller number of clusters than N_c'.

Nodal Clustering

A recursive algorithm is used to calculate how to group the active vertices for each cluster, such that each cluster receives, more or less, the same number of active vertices. The algorithm alternates the x- and y-coordinate partitioning of the list of active vertices, in an attempt to group a cluster of nearest neighboring active vertices. Unfortunately, this may not result in an even spatial distribution of clusters, which is a disadvantage of this method.

Optical Grid Element Clustering

The number of clusters cannot be set by users as it is defined by the number of optical grid elements. Active regions must be defined in both the electrical and optical grids. An effective bulk region in the optical grid is used to describe the active QW layers and can be meshed according to user requirements. Then, the electrical active vertices are grouped inside each of the optical grid active elements such that each optical-grid active element forms a cluster. In this way, you can control the distribution of the clusters for greater modeling flexibility.

> **NOTE** In all the above clustering methodologies, the center of each cluster is
> determined by the average of the active vertices that it encloses.

Using the Clustering Feature

The following keywords in the LED framework activate the clustering feature:

```
Physics {...
   LED ( ...
      Raytrace (...
         ClusterActive(
            ClusterQuantity = Nodes | PlaneArea | OpticalGridElement
            NumberOfClusters = <integer>      # for Nodes | PlaneArea
         )
      )
   )
}
```

Debugging Raytracing

Rays are assumed, by default, to irradiate isotropically from each active vertex. In the case of quantum wells, an artifact of this assumption may cause unrealistic spikes in the radiation pattern. Consider those source rays that are directed within the plane of the quantum wells. These rays will mostly transmit out of the device at the ending vertical edges of the quantum wells. Realistically, the rays would have a much higher probability of being absorbed and re-emitted into another direction than traversing the entire plane of the quantum well.

To circumvent this problem, use the anisotropic emission as described in Anisotropic Starting Rays From Spontaneous Emission Sources on page 934. Alternatively, one can try to exclude the source rays emitting within a certain angular range from the horizontal plane, that is, the plane of the quantum well. The power from these excluded rays will be distributed equally to the rest of the rays that are not within this angular range. This results in an approximate anisotropic emission shape at each active vertex. The syntax for this exclusion is:

```
Physics { ...
   LED ( ...
      Optics ( ...
         RayTrace ( ...
            ExcludeHorizontalSource(<float>)   # in degrees
         )
      )
   )
}
```

To add more flexibility to LED raytracing, debugging features are implemented. These include:

- Setting a fixed observation center for the LED radiation calculations.
- Fixing a constant wavelength for raytracing.

■ Allowing you to print and track the LED radiation rays (in a certain angular zone) back to its source active vertex.

These features are described in this syntax:

```
Physics { ...
   LED ( ...
      Optics ( ...
         RayTrace ( ...
            ObservationCenter = (<float> <float>)
                                       # in micrometers, 3 entries for 3D
            Wavelength = 888        # [nm] set fixed wavelength
            DebugLEDRadiation(<filename> <StartAngle> <EndAngle>
               <MinIntensity>)
         )
      )
   )
}
```

Print Options in Raytracing

The original `Print` feature of raytracing causes all ray paths to be printed. With multiple reflections or refractions and a large number of starting rays, the resultant image can become a black smudge. To reduce the number of ray paths that are printed, a `Skip` option is implemented within the `Print` feature. In addition, you can trace the ray paths originating from only a single active vertex. These features are described in this syntax:

```
Physics {
   LED (
      Optics (
         RayTrace (
            Print(Skip(<int>))          # skip printing every <int> ray paths
            Print(ActiveVertex(<int>))  # print only rays from active vertex
                                        # <int>
            PrintSourceVertices(<filename>)
            ProgressMarkers = <int>     # 1-100% intervals (integer)
         )
      )
   )
}
```

The option `PrintSourceVertices(<filename>)` outputs the list of active vertices, their global index numbering, and coordinates into the file specified by `<filename>`. If the number of source rays is large or the optical mesh is fine, raytracing takes some time to be completed. In this case, you can use the keyword `ProgressMarkers=<int>` to set the incremental completion meter.

The `Print` option only outputs rays as lines with no other information. To obtain a raytree that contains intensity and other information, you can plot the raytree using the keyword `RayTrees` in the `Plot` section of the command file:

```
Plot {...
   RayTrees
}
```

The resultant raytree is plotted in TDR format and can be visualized by Sentaurus Visual, where each branch of the raytree can be accessed individually.

Interfacing LED Starting Rays to LightTools®

To facilitate the rapid design of LED structures with its luminaire, the starting rays from active region vertices can be output directly to a ray file formatted for use in LightTools. Figure 65 shows a probable design flow.

Figure 65   LED design flow to optimize extraction efficiency by LightTools and coupled to Sentaurus Device LED device simulation

The set of rays is derived from the LED spontaneous emission power spectrum at each vertex of the device. This means that there is wavelength variability such that each starting ray carries a starting position, a direction, an intensity value, and a wavelength.

This feature is an extension of the `Disable` keyword, so that the internal Sentaurus Device raytracing engine will not be activated. The syntax is:

```
File {...
   Plot = "n99_des.tdr"
}

Physics {...
   LED (
      RayTrace(
         Disable(
            OutputLightToolsRays (
```

```
                    WavelengthDiscretization = <integer>    # spectrum discretization
                    RaysPerCluster = <integer>              # rays emitting from each
                                                            # active cluster
                    IsotropyType = InBuilt | Random | UserRays  # default is InBuilt
                    SaveType = Ascii | Binary       # choose ASCII or binary format
                )
            )
            ClusterActive()
            RaysPerVertex = <integer>               # used with SourceRaysFromFile()
            SourceRaysFromFile(string)
        )
    )
}

Solve {...
    Plot( Range=(0,1) Intervals=5 )
}
```

This feature can be used in conjunction with the `ClusterActive` section, so that the active vertices can be grouped into clusters to reduce the final number of rays. If the `ClusterActive` section is not present, every active vertex will be used as emission centers for the starting rays. It is also possible to import an isotropic distribution of point source rays from a file to be used for random-rotated distribution at different vertices. The span of the spectrum at each active cluster is computed automatically and divided into the numbers as specified by `WavelengthDiscretization`. The total number of starting rays is:

```
WavelengthDiscretization * RaysPerCluster * NumberOfActiveClusters
```

Two types of ray file format for LightTools can be chosen: ASCII or binary. The base name for the LightTools ray files is derived from the plot file name and is appended with either `_lighttools.txt` for the ASCII format or `_lighttools.ray` for the binary format.

For example, according to the above syntax, the following are the corresponding file names for the LightTools ray files:

```
n99_000000_des_lighttools.txt
n99_000001_des_lighttools.txt
...
n99_000000_des_lighttools.ray
n99_000001_des_lighttools.ray
...
```

These files can be read directly by LightTools as volume sources of rays (refer to the LightTools manual for more information).

Example: n99_000000_des_lighttools.txt

This example is an ASCII-formatted LightTools ray file (version 2.0 format):

```
# Synopsys Sentaurus Device to LightTools
# Ray Data Export File
LT_RDF_VERSION: 2.0
DATANAME: SentaurusDeviceRayData
LT_DATATYPE: radiant_power
LT_RADIANT_FLUX: 1.946806e-04
LT_FAR_FIELD_DATA: NO
LT_COLOR_INFO: wavelength
LT_LENGTH_UNITS: micrometers
LT_DATA_ORIGIN:                0             0              0
LT_STARTOFDATA
0.000000e+00 4.290000e-01 0.000000e+00 -0.163343 -0.986569 0.000000
5.451892e-05 470.395656
0.000000e+00 4.290000e-01 0.000000e+00 -0.163343 -0.986569 0.000000
1.817405e-04 459.664919
....
LT_ENDOFDATA
```

The first three columns denote the starting position (in micrometers) of the ray, the next three columns show the direction vector, and this is followed by the fractional power (as a fraction of `LT_RADIANT_FLUX`), and ends with the wavelength (in nanometers).

LED Radiation Pattern

Raytracing does not contain phase information, so it is not possible to compute the far-field pattern for an LED structure. Instead, the outgoing rays from the LED raytracing are used to produce the radiation pattern.

In 2D space, this is equivalent to moving a detector in a circle around the LED as shown in .

In 3D space, the detector is moved around on a sphere. The circle and sphere have centers that correspond to the center of the device. Sentaurus Device automatically determines the center of the device to be the midpoint of the device on each axis. Nonetheless, there is an option to allow you to set the center of observation (see and).

To examine the optical intensity inside the LED, use `RayTraceIntensity` in the `Plot` statement.

Figure 66   Measuring the radiation pattern in a circular path around LED at observation
radius, R

The syntax required to activate and plot the LED radiation pattern is located in the `File`,
`Physics-LED-Optics-RayTrace`, and `Solve-quasistationary` sections of the
command file:

```
File {...
   # ----- Activate LED radiation pattern and save -----
   LEDRadiation = "rad"

}
...
Physics {...
   LED (...
      Optics (...
         RayTrace(...
            LEDRadiationPara(1000.0,180) # (radius_micrometers, Npoints)
            ObservationCenter = (2.0 3.5 5.5)  # set center
         )
      )
   )
}
...
Solve {...

   # ----- Specify quasistationary -----
   quasistationary (...

      PlotLEDRadiation { range=(0,1) intervals=3 }

      Goal {name="p_Contact" voltage=1.8})
      {...}
}
```

The LED radiation plot syntax works in the same way as `GainPlot` (see Spontaneous Emission Power Spectrum on page 924) in the `Quasistationary` statement.

An explanation of this example is:

■ The base file name, `"rad"`, of the LED radiation pattern files is specified by `LEDRadiation` in the `File` section. The keyword `LEDRadiation` also activates the LED radiation plot.

■ The parameters for the LED radiation plot are specified by the keyword `LEDRadiationPara` in the `Physics-Optics-RayTrace` section. You must specify the observation radius (in micrometers) and the discretization of the observation circle (2D) or sphere (3D).

■ You can set the center of observation by including the keyword `ObservationCenter`. If this is not set, the center is automatically computed as the middle point of the span of the device on each axis.

■ The LED radiation pattern can only be computed and plotted within the `Quasistationary` statement. The keyword `PlotLEDRadiation` controls the number of LED radiation plots to produce.

■ The argument `range=(0,1)` in the `PlotLEDRadiation` keyword is mapped to the initial and final bias conditions. In this example, the initial and final (goal) `p_Contact` voltages are 0 V and 1.8 V, respectively. The number of `intervals=3`, which gives a total of four (= 3+1) LED radiation plots at 0 V, 0.6 V, 1.2 V, and 1.8 V. In general, specifying `intervals=n` produces (n+1) plots.

■ If the LED structure is symmetric, the LED radiation is only computed on a semicircle.

The following sections briefly describe the files that are produced in the LED radiation plot for the 2D and 3D cases.

Two-Dimensional LED Radiation Pattern and Output Files

Activating the LED radiation plot for a 2D LED simulation produces two different files (using the base name `"rad"`):

`rad_000000_LEDRad.plt`	The normalized radiation pattern versus observation angle, which can be viewed in Inspect.
`rad_000000_LEDRad_Polar0.tdr`	The normalized radiation pattern projected onto a grid file and can be viewed in Sentaurus Visual. The polar plot of the LED radiation pattern is then shown.

A sample output of the radiation plot of a 2D nonsymmetric LED structure is shown in Figure 67. The lower-left image corresponds to the file `rad_000000_LEDRad.plt` plotted by Inspect, and the right image is the product of the file `rad_000000_LEDRad_Polar.tdr` plotted by Sentaurus Visual.

Figure 67   (*Upper left*) LED internal optical intensity, (*lower left*) normalized radiation intensity versus observation angle, and (*right*) polar radiation plot computed by Sentaurus Device in 2D LED simulation

Three-Dimensional LED Radiation Pattern and Output Files

There are two output files for the radiation pattern in the case of a 3D LED simulation:

`rad_000000_des.tdr`	Data file containing the normalized radiation pattern. Use Sentaurus Visual for this file, and the spherical plot of the 3D LED radiation pattern is then shown. A sample of the radiation pattern of a 3D LED simulation is shown in Figure 68 on page 947.
`rad_000000_des_3Dslices.plt`	The 3D radiation pattern is extracted into polar plots on three planes that can be visualized using Inspect: – XYplane: $\theta = \pi/2$; plot far field for $\phi = 0$ to 2π. – XZplane: $\phi = 0, \pi$; plot far field for $\theta = 0$ to 2π. – YZplane: $\phi = \pi/2, 3\pi/2$; plot far field for $\theta = 0$ to 2π.

Figure 68   (*Left*) LED internal optical intensity and (*right*) normalized radiation intensity
projected on a sphere of 3D LED simulation

Staggered 3D Grid LED Radiation Pattern

In discretizing a 3D far-field collection sphere with regular longitudinal and latitude lines, the size of each surficial element critically depends on its location on the sphere. At the polar regions, the elements are very small compared to those along the equator. As the discretization increases, the disparity between the polar and equator surficial elements increases at the same rate.

The sampling rate for rays is constrained by the smallest collecting element, which, in this case, is the much smaller surficial element at the poles. In most cases, the polar regions are undersampled and the equator regions are oversampled due to the disparity in surficial element areas between the two regions. Undersampling at the poles also could lead to anomalous spikes in the far field since the far-field intensity is computed by the total ray power impinging that element and is divided by the elemental area. To adequately sample the polar regions, a significant number of rays must be used, resulting in a very large raytracing problem that may not be necessary.

To circumvent the abovementioned problems, the spherical collection space must be composed of more uniformly distributed elemental areas. The baseline requirement is that each elemental area on the surface of the collection sphere must be approximately the same size. The following simple approach is used:

1. Divide the sphere into concentric rings in the latitude planes. Each ring has a thickness of:

$$d_\theta = \int R d\theta = R\Delta\theta \tag{1105}$$

2. For each concentric ring, further subdivide the ring into elements with a width that is approximately $d\theta$.

Mathematically, assume that the sphere is divided into N_θ rings, so that the thickness of each ring is:

$$d_\theta = R\left(\frac{\pi}{N_\theta}\right) \tag{1106}$$

In each concentric ring (i) bound between θ_1 and θ_2, choose the order of θ such that:

$$\sin(\theta_2) > \sin(\theta_1) \tag{1107}$$

The circumference at θ_2 is $C_{\theta 2} = R\sin(\theta_2) \times 2\pi$. The constraint needed here is such that:

$$\frac{C_{\theta 2}}{N_\phi(i)} = d_\theta \tag{1108}$$

where $N_\phi(i)$ is the number of divisions for the concentric ring (i) and is an integer. Solving gives:

$$N_\phi(i) = (\text{INTEGER})[2\sin(\theta_2) \times N_\theta] \tag{1109}$$

At the poles of the sphere ($\theta = 0$ and $\theta = \pi$), the concentric rings collapse into a cap. The following constraint is imposed for these polar cap regions (essentially trying to match triangular area elements with squarish area elements):

$$0.5 \times \left(\frac{C_{\theta 2}}{N_\phi(i)}\right) \times d_\theta = d_\theta^2 \tag{1110}$$

Simplifying gives the number of divisions for the polar cap rings:

$$N_\phi(i) = (\text{INTEGER})[\sin(\theta_2) \times N_\theta] \tag{1111}$$

The total number of elemental areas is $\sum N_\phi(i)$.

Table 165 lists the total number of elements obtained from this simple approach.

Table 165 Total number of elements and area information as a function of N_θ

N_θ	Total number of surface elements	Smallest area (unit radius)	Largest area (unit radius)	Area skew = ratio of largest/smallest area
5	36	0.314159	0.399994	1.273
10	146	0.074372	0.097081	1.305
20	554	0.017705	0.024573	1.388
50	3296	0.002857	0.003945	1.381
100	12976	0.000715	0.000987	1.380

Table 165   Total number of elements and area information as a function of N_θ (Continued)

N_θ	Total number of surface elements	Smallest area (unit radius)	Largest area (unit radius)	Area skew = ratio of largest/smallest area
150	29013	0.000318	0.000439	1.381
200	51426	0.000179	0.000247	1.380

As N_θ increases, it is clear from Table 165 that the area skew (ratio of largest to smallest elemental area) stabilizes to a value of approximately 1.38.

To activate the new staggered 3D far-field grid, use the syntax:

```
Physics {
   LED (
      RayTrace(
         Staggered3DFarfieldGrid
      )
   )
}
```

If the keyword `Staggered3DFarfieldGrid` is not specified, the collection sphere reverts to the old (θ, ϕ) scheme to maintain backward compatibility.

Spectrum-Dependent LED Radiation Pattern

Unlike a laser beam with single-frequency emissions, rays emitting from an LED carry a spectrum of frequencies (or energies). Sentaurus Device monitors the spectrum of each ray as it undergoes the process of raytracing in and out of the device. The resultant spectrum of the LED radiation pattern can then be plotted.

To activate this feature, include the keyword `LEDSpectrum` in the command file:

```
Physics {...
   LED (...
      Optics (...
         RayTrace(...
            LEDSpectrum(<startenergy> <endenergy> <numpoints>)
         )
      )
   )
}
```

This feature must be used in conjunction with the `LEDRadiation` feature so that the file names of the LED radiation plots and the observation angles can be specified. Other notable aspects of the syntax are:

- `<startenergy>` and `<endenergy>` give the energy range of the spectrum to be monitored. These parameters are floating-point entries with units of eV.
- `<numpoints>` is an integer determining the number of discretized points in the specified energy range.

Tracing Source of Output Rays

Optimizing the extraction efficiency is critical in an LED design. Other than modifying the shape of the device, you can use the fact that the rays originating from certain zones in the active region have a higher escape or extraction rate. By designing the shape of the contact to channel higher currents into these zones, the extraction efficiency can effectively be increased.

To facilitate the identification of such zones, a feature that correlates the output rays to their source active vertices is implemented. The intensity of each output ray is added to an `LED_TraceSource` variable at each active vertex. At the end of the simulation, a profile of `LED_TraceSource` is obtained, which provides an indication of the best localized regions to which more current can be channeled.

The activation of this feature requires keywords to be inserted into two different statements of the command file:

```
Plot { ...
   LED_TraceSource
}

Physics { ...
   LED ( ...
      Optics(
         RayTrace ( ...
            TraceSource()
         )
      )
   )
}
```

NOTE   A far-field observation radius must be set for the `TraceSource` feature.

Interfacing Far-Field Rays to LightTools

LightTools is a robust raytracer that accepts a list of source rays as input, and it can optimize the packaging design for LEDs, that is, the luminaire. Such a design flow is shown in Figure 69.

Figure 69   Secondary LED design flow to optimize luminaire design by LightTools and coupled to Sentaurus Device LED device simulation

An interface has been built in Sentaurus Device to output farfield rays from an LED device simulation that can be input into LightTools as source rays. This feature requires the LED radiation plot to be activated simultaneously so that the rays can be output at various quasistationary and transient states. The syntax for activating this feature is:

```
Physics {
   LED (
      Optics (
         Raytracer (
            ExternalMaterialCRIFile = "string"
            OutputLightToolsFarfieldRays (
               Filename = "farfield"
               WavelengthDiscretization = <integer>
               SaveType = Ascii | Binary
            )
         )
      )
   )
}
```

The energy span of the spectrum is computed automatically, and you only need to input the wavelength discretization. The spectrum information is embedded inside the ray information as wavelength and relative intensity values. The relative intensity is a fraction of the total far-field power.

NOTE   In Sentaurus Device, raytracing and wavelength dependency of the refractive index can only be specified by using the complex refractive index model.

When the LED is embedded in another medium, the keyword `ExternalMaterialCRIFile` can be included to take wavelength-dependent complex refractive index changes into account (see External Material in Raytracer on page 615).

You have the option to output the ray information to either an ASCII file or a binary file. The ray information consists of the position vector (x,y,z), the direction cosine (x,y,z), the relative intensity, and the wavelength. Both file types contain identifying headers that are required by LightTools. The resultant name of the file is the user name with the suffix `_lighttools.txt` for the ASCII format or the suffix `_lighttools.ray` for the binary format. An example of an ASCII-formatted file is presented in Example: farfield_lighttools.txt.

Example: farfield_lighttools.txt

```
# Synopsys Sentaurus Device Farfield to LightTools
# Ray Data Export File
LT_RDF_VERSION: 2.0
DATANAME: SentaurusDeviceFarfieldRayData
LT_DATATYPE: radiant_power
LT_RADIANT_FLUX: 2.066459e-05
LT_FAR_FIELD_DATA: NO
LT_COLOR_INFO: wavelength
LT_LENGTH_UNITS: micrometers
LT_DATA_ORIGIN:             0             0             0
LT_STARTOFDATA
5.351638e+01 2.716777e+02 8.281585e+01 -0.198138 0.651751 0.732094
1.648189e-08 390.559610
3.000000e+02 7.388091e+01 4.290000e-01 0.637854 0.770158 0.000000
4.411254e-04 390.559610
1.001089e+02 3.000000e+02 4.290000e-01 -0.637854 0.770158 0.000000
2.585151e-05 390.559610
0.000000e+00 1.943600e+02 4.290000e-01 -0.637854 -0.770158 0.000000
2.783280e-06 390.559610
1.735878e+02 0.000000e+00 4.290000e-01 0.637854 -0.770158 0.000000
1.631101e-07 390.559610
```

Nonactive Region Absorption (Photon Recycling)

The default setting for LED simulations includes the contribution of absorbed photons in nonactive regions to the continuity equation as a generation rate. This is the basic concept of the nonactive-region photon recycling. In most cases, LEDs are designed with larger bandgap material in nonactive regions to eradicate intraband absorption.

As a result, it may not be necessary to include very small values of nonactive absorption in some situations. To allow for such flexibility, nonactive absorption can be switched off as an option. The syntax is:

```
Physics { ...
   LED ( ...
      Optics ( ...
         RayTrace ( ...
            NonActiveAbsorptionOff
            OptGenScaling = <float>
            BackgroundOptGen(<float>)    # [#/cm^3]
         )
      )
   )
}
```

If the keyword `NonActiveAbsorptionOff` is used, the plot variable `OpticalGeneration` still show values, but these values are not included in the continuity equation. A scaling factor, `OptGenScaling`, can be defined to scale the final value of optical generation. You also can set a background optical generation with the keyword `BackgroundOptGen`.

Device Physics and Tuning Parameters

Unlike a laser diode, an LED does not have a threshold current. Therefore, the carriers in the active region are not limited to any threshold value. This means that the spontaneous gain spectrum continues to grow as the bias current increases. The limiting factor for growth is when the QW active region is completely filled and leakage current increases significantly, or dark recombination processes start to dominate with increasing bias and temperature.

There are four main design concerns for an LED:

- Designing the basic layers to optimize the internal quantum efficiency. Polarization charge sheets are needed for AlGaN–GaN–InGaN interfaces, and junction tunneling models might be needed for thin electron-blocking layers. For mature QW technology such as InGaAsP systems, there can be predictive value in advanced $k \cdot p$ gain calculations for optical gain. However, for difficult-to-grow materials such as InGaN/AlGaN QWs, the uncertainties of

growth, mole fraction grading, interface clarity, and so on, make predictive modeling of optical gain almost impossible.

- Extraction efficiency. This is mainly a problem of the geometric shape of the LED structure and the complex refractive index profile of the structure. Temperature, wavelength, and carrier distribution can alter the complex refractive index profile, so the extraction efficiency changes with increasing current injection. Many LED structures have tapered sidewalls to help couple more light out of the device. The slope of the taper can be set as a parameter using Sentaurus Workbench, and the automatic parameter variation feature can be used to optimize the extraction efficiency of the LED geometry.

- Current spreading. It is desirable to spread the current uniformly across the entire active region so that total spontaneous emissions can be increased. In Sentaurus Device, there is an option to switch off raytracing in an LED simulation. Switching off raytracing only forgoes the extraction efficiency and radiation pattern computation; the total spontaneous emission power is still calculated. This can assist you in the faster optimization of an LED device for uniform current spreading.

- Thermal management, hot spots, how much heat is produced and how to cool the device. Temperature distribution also affects the mobility and complex refractive index profile and, therefore, impacts the current spreading profile and optical extraction efficiency.

Example of 3D GaN LED Simulation

An LED simulation is best run with a dual-grid approach. The electrical grid must be dense in vicinities where carrier transport details are important. On the other hand, a coarse grid is needed for raytracing. The following is a skeletal sample of command file syntax for a dual-grid 3D GaN LED simulation. Only highlights of the syntax that are important to LED simulations have been included.

The typical command file syntax is:

```
#########################
## Global declarations ##
#########################
File {...}

Math {
   Digits = 5
   NoAutomaticCircuitContact
   DirectCurrent
   Method = blocked
   # ILS should be chosen for big 3D simulations
   # For 2D, use Pardiso
   Submethod=ILS(set= 5)
     ILSrc= "
       set (5) {
```

```
            iterative(gmres(100), tolrel=1e-11, tolunprec=1e-4, tolabs=0,
               maxit=200);
            preconditioning(ilut(1e-9,-1), right);
            ordering(symmetric=nd, nonsymmetric=mpsilst);
            options(compact=yes, linscale=0, fit=5, refinebasis=1,
               refineresidual=30, verbose=5);
         }; "
      Derivatives
      Notdamped=20
      Iterations=15
      RelErrControl
      ErrRef(electron)=1e7
      ErrRef(hole)=1e7
      ElementEdgeCurrent
      ExtendedPrecision
      DualGridInterpolation ( Method=Simple )
      NumberOfThreads = maximum
      Extrapolate
   }

   #####################################
   ## Define the optical solver part ##
   #####################################
   OpticalDevice optDevice {
      File {
         Grid = "optic_msh.tdr"
         Parameters = "optparafile.par"
      }
      RaytraceBC {...}
      Physics {
         ComplexRefractiveIndex (
            WavelengthDep (real imag)
            TemperatureDep(real)
         )
      }
      Physics(Region="EffectiveQW") { Active }
   }

   ########################################
   ## Define the electronic solver part ##
   ########################################
   Device elDevice {
      Electrode {...}

      Thermode {...
         { Name="T_contact" Temperature=300.0 SurfaceResistance=0.05 }
      }

      File {
```

```
      Grid = "elec_msh.tdr"
      Parameters = "elecparafile.par"
      Current = "elsolver"
      Plot =    "elsolver"
      LEDRadiation = "farfield"
      Gain = "gainfilename"
   }

   # ----- Choose special LED related plot variables to output -----
   Plot {...
      RayTraceIntensity
      OpticalGeneration
      LED_TraceSource
      OpticalAbsorptionHeat
   #  RayTrees            # not for compact memory option
   }

   # ----- Specify gain plot parameters -----
   GainPlot { ... }

   Physics {
      Mobility ()
      EffectiveIntrinsicDensity (NoBandGapNarrowing)
      AreaFactor = 1
      IncompleteIonization
      Thermionic
      Fermi
      RecGenHeat

      OpticalAbsorptionHeat(
         Scaling = 1.0
         StepFunction( EffectiveBandgap )
      )

      # Complex refractive index model needed for raytracer
      ComplexRefractiveIndex (
         WavelengthDep (real imag)
         TemperatureDep (real)
      )

      LED (
         SponScaling = 1   * scale matrix element with this factor
         Optics (
            RayTrace(
   #         Disable      # this is for purely electrical investigation
               CompactMemoryOption         # use compact memory model
               Coordinates = Cartesian
               Staggered3DFarfieldGrid
```

```
            # ----- Set ray starting and terminating conditions -----
            PolarizationVector = Random
            RaysPerVertex = 20
            RaysRandomOffset (RandomSeed = 123)
            Depthlimit = 100
            MinIntensity = 1e-5

            # ---------- Set output options ---------
            TraceSource()
               LEDRadiationPara(10000,60)     # (<radius-microns>, Npoints)

            # Choose LED wavelength option
            # Fixed wavelength by entering a <float>, units in [nm]
            Wavelength=AutoPeak   # or Effective or AutoPeakPower or <float>
         )
      )
      # ----- Quantum well options -----
         QWTransport
         QWExtension = autodetect
         Strain
      Broadening = 0.04
      Lorentzian
   )

# Turn on tunneling for electron blocking layer if necessary
#  eBarrierTunneling "rline1" ()


}

# ----- Define recombination models for non-active regions -----
Physics (material = "AlGaN") { Recombination (SRH(TempDep) Radiative) }
Physics (material = "GaN") { Recombination (SRH(TempDep) Radiative) }

# ----- Set QWs as active regions ----
Physics (region="QW1") { Recombination(-Radiative SRH(TempDep)) Active }
...
Physics (region="QW6") { Recombination(-Radiative SRH(TempDep)) Active }

# ---- Include polarization sheet charges between interfaces ----
Physics (RegionInterface="Window/Cap") {
   Traps(FixedCharge Conc=-2.666746e+12)
}
Physics (RegionInterface="Barrier6/Buffer") {
   Traps(FixedCharge Conc=-1e+12)
}
Physics (RegionInterface="Barrier0/Window") {
   Traps(FixedCharge Conc=3.8e+12)
```

```
      }
      Physics(RegionInterface="Barrier0/QW1") {Traps((FixedCharge Conc=1e12))}
      Physics(RegionInterface="QW1/Barrier1") {Traps((FixedCharge Conc=-1e12))}
      ...

      Math {
         # ---- Define tunneling nonlocal line for electron blocking layer ----
         NonLocal "rline1" (
            Barrier(Region = "Window")
         )
         }
      }

   ##################################################################
   ## Define mixed-mode system section for dual grid simulation ##
   ##################################################################
   System {
      elDevice d1 ( anode=vdd cathode=gnd ) { Physics { OptSolver="opt" } }
      Vsource_pset drive(vdd gnd) { dc = 2.72 }
      Set ( gnd = 0.0 )
      optDevice opt ()
   }

   ##############################
   ## Define solving sequence ##
   ##############################
   Solve {
      Coupled (Iterations = 40) { Poisson }
      Coupled (Iterations = 40) { Poisson Electron Hole }
      Coupled { Poisson Electron Hole Contact Circuit }
      Coupled { Poisson Electron Hole Contact Circuit Temperature }
      Quasistationary (
         InitialStep = 0.05
         MaxStep = 0.05
         Minstep = 5e-3
         Plot { range=(0,1) intervals=5 }
         PlotGain { range=(0,1) intervals=5 }
         PlotLEDRadiation { range=(0,1) intervals=5 }
         Goal { Parameter=drive.dc Value=3.8 }
      ) {
         # Full self-consistent electrical+thermal+optics simulation
         Plugin(breakonfailure) {
            Coupled(Iterations = 20) {Electron Hole Poisson Contact Circuit
                                      Temperature}
            Optics
         }
      }
   }
```

Some comments about the command file syntax:

- Multithreading for the raytracer can be activated by specifying `NumberOfThreads` in the global `Math` section. A value of `maximum` has been chosen in this case so that Sentaurus Device will use the maximum number of threads available on the machine.

- The solver must be ILS for 3D simulations, due to the large matrix that needs to be solved. The parameters for ILS must be tuned for optimal convergence.

- `ExtendedPrecision` is recommended for use in GaN device simulations.

- Various special raytrace boundary conditions can be chosen and are set in the `RayTraceBC` section. For details about these special boundary contacts, see Boundary Condition for Raytracing on page 605.

- Polarization charges at AlGaN–GaN–InGaN interfaces are added using fixed trap charges.

- The wavelength used in raytracing is computed automatically to be the wavelength at the peak of the spontaneous emission spectrum. If a fixed wavelength is required, you have the option of setting it by using the `Wavelength` keyword.

- The QW regions must be labelled as `Active` in both the optical and electrical device declarations so that proper internal mapping can be performed. You also must include the keyword `Recombination(-Radiative)` in the QW active regions because the spontaneous emission computation in these regions uses the special LED model and, therefore, the default radiative recombination model should be switched off.

- The `ComplexRefractiveIndex` model must be used in conjunction with the raytracer. In addition, a `PolarizationVector` must be defined with the raytracer.

- When `CompactMemoryOption` is chosen, the raytrees are not saved internally, so plotting the `RayTrees` or using `Print(Skip(<integer>))` is disabled.

- Activating the nonlocal tunneling model requires the keyword `eBarrierTunneling` in the `Physics` section and the `NonLocal` line definition in the `Math` section (see Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722 for more details).

- The `Plugin` feature is used to create the full self-consistent simulation framework between the electrical, thermal, and optics. To disengage full self-consistency, remark off the `Plugin` and `Optics` statements, in which case, the `Optics` will only be solved once at each bias step.

- The dual-grid electrical and optical feature has been used. If you select a single-grid simulation, you only need to copy the `Physics-LED` section of this example and insert it into the `Physics` section of a typical single-grid command file.

> **NOTE** Raytracing can be disabled in an LED simulation by using the keyword `Disable` in the `RayTrace` statement if you do not require the computation of the extraction efficiency and radiation pattern.

Table 271 on page 1455 lists all the arguments for the LED `RayTrace` option.

References

[1]   W.-C. Ng and M. Pfeiffer, "Generalized Photon Recycling Theory for 2D and 3D LED Simulation in Sentaurus Device," in *6th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD-06)*, Singapore, pp. 127–128, September 2006.

[2]   W.-C. Ng and G. Létay, "A Generalized 2D and 3D White LED Device Simulator Integrating Photon Recycling and Luminescent Spectral Conversion Effects," in *Proceedings of SPIE, Light-Emitting Diodes: Research, Manufacturing, and Applications XI*, vol. 6486, February 2007.

CHAPTER 35 Modeling Quantum Wells

This chapter presents the physics of quantum wells, and methods of gain calculations for the quantum wells and bulk regions.

These gain methods include the simple rectangular well model, and gain physical model interface (PMI). Various gain-broadening mechanisms and strain effects are discussed. A localized quantum well (QW) model is presented together with a simplified InGaN/GaN QW gain model.

Overview

In this section, the focus is on two aspects of modeling the quantum well:

- Radiative recombination processes important in a quantum well
- Gain calculations

A few types of recombination processes are important in the quantum well:

- Auger and Shockley–Read–Hall (SRH) recombinations deplete the QW carriers, and they form the dark current.
- Radiative recombination contains the stimulated and spontaneous recombination processes, which are important processes in LEDs.

These recombinations must be added to the carrier continuity equations to ensure the conservation of particles.

The gain calculation is based on Fermi's golden rule and describes quantitatively the radiative emissions in the form of the stimulated and spontaneous emission coefficients. These coefficients contain the optical matrix element $|M_{ij}|^2$, which describes the probability of the radiative recombination processes. In the quantum well, computing the optical matrix element requires knowledge of the QW subbands and QW wavefunctions.

Sentaurus Device offers several options for computing the gain spectrum:

- A simple finite well model with analytic solutions. In addition, strain effects and polarization dependence of the optical matrix element are handled separately.
- A localized QW model that uses a trapezoidal QW model to take localized electric field effects into account.

- A simplified InGaN/GaN QW gain model that provides analytic forms to adjust the parameters of the effective masses, various band offsets, and so on. These are subsequently used in the gain calculations.

- A nonlocal QW model that uses the 1D Schrödinger solver on a nonlocal mesh to compute the QW subbands and QW wavefunctions (see Nonlocal Mesh for 1D Schrödinger on page 286). This model supports arbitrary potential wells.

- User-specified gain routines in C++ language can be coupled self-consistently with Sentaurus Device using the physical model interface (PMI).

Radiative Recombination and Gain Coefficients

After the carriers are captured in the active region, they experience either dark recombination processes (such as Auger and SRH) or radiative recombination processes (such as stimulated and spontaneous emissions), or escape from the active region. This section describes how stimulated and spontaneous emissions are computed in Sentaurus Device.

Stimulated and Spontaneous Emission Coefficients

In the active region of the LED, radiative recombination is treated locally at each active vertex. The stimulated and spontaneous emissions are computed using Fermi's golden rule.

At each active vertex of the quantum wells, the local stimulated emission coefficient is:

$$r^{\text{st}}(\hbar\omega) = \sum_{i,j} \int dE \, C_o \, k_{\text{st}} |M_{i,j}|^2 D(E) \times (f_i^C(E) + f_j^V(E) - 1) L(E)$$

(1112)

and the local spontaneous emission coefficient is:

$$r^{\text{sp}}(\hbar\omega) = \sum_{i,j} \int dE \, C_o \, k_{\text{sp}} |M_{i,j}|^2 D(E) f_i^C(E) f_j^V(E) L(E)$$

(1113)

where (for general III–V materials):

$$C_0 = \frac{\pi e^2}{n_g c \varepsilon_0 m_0^2 \omega}$$

(1114)

$$|M_{i,j}|^2 = P_{ij} |O_{i,j}|^2 \left(\frac{m_0}{m_e} - 1\right) \frac{m_0 E_g (E_g + \Delta)}{12 \left(E_g + \frac{2}{3}\Delta\right)}$$

(1115)

$$O_{i,j} = \int_{-\infty}^{\infty} dx \zeta_i(x) \zeta^*_j(x) \tag{1116}$$

$$f^C_{(i, \Phi_n, E)} = \left(1 + \exp\left(\frac{E_C + E_i + q\Phi_n + \frac{m_r}{m_e}E}{k_B T}\right)\right)^{-1} \tag{1117}$$

$$f^V_{(j, \Phi_p, E)} = \left(1 + \exp\left(\frac{E_V - E_j + q\Phi_p - \frac{m_r}{m_h}E}{k_B T}\right)\right)^{-1} \tag{1118}$$

$$D^r_{(E)} = \frac{m_r}{\pi \hbar^2 L_x} \tag{1119}$$

$$m_r = \left(\frac{1}{m_e} + \frac{1}{m_h}\right)^{-1} \tag{1120}$$

$L(E)$ is the gain-broadening function. The electron, light-hole, and heavy-hole subbands are denoted by the indices i and j. $f^C_{i(E)}$ and $f^V_{j(E)}$ are the local Fermi–Dirac distributions for the conduction and valence bands, $D^r_{(E)}$ is the reduced density-of-states, $|O_{i,j}|^2$ is the overlap integral of the quantum mechanical wavefunctions, and P_{ij} is the polarization-dependent factor of the momentum (optical) matrix element $|M_{i,j}|^2$. The spin-orbit split-off energy is Δ and E_g is the bandgap energy. The polarization-dependent factor P_{ij} in the optical matrix element is set to 1.0 for LED simulations. These emission coefficients determine the rate of production of photons when given the number of available quantum well carriers at the active vertex.

For materials of wurtzite crystal structure (InGaN), the optical matrix element $|M_{i,j}|^2$ and hole masses are different. These are explained in detail in Electronic Band Structure for Wurtzite Crystals on page 967.

k_{st} and k_{sp} are scaling factors for the optical matrix element $|M_{i,j}|^2$ of the stimulated and spontaneous emissions, respectively. They have been introduced to allow you to tune the stimulated and spontaneous gain curves. Consequently, these parameters can change the threshold current.

The activating keywords are `StimScaling` and `SponScaling` in the `Physics-LED` section of the command file:

```
Physics {...
    LED (...
```

```
            Optics (...)
            # ---- Scale stimulated & spontaneous gain ----
            StimScaling = 1.0   # default value is 1.0
            SponScaling = 1.0   # default value is 1.0
        )
    }
```

The differential gains for electrons and holes are given by the derivatives of the coefficient of stimulated emission $r^{st}(\hbar\omega)$ (see Eq. 1112) with regard to the respective carrier density. They can be plotted by including the keywords eDifferentialGain and hDifferentialGain in the Plot section of the command file.

Active Bulk Material Gain

The stimulated and spontaneous emission coefficients discussed are derived for the quantum well. However, these coefficients can apply to bulk materials with slight modifications. In bulk active materials, it is assumed that the optical matrix element is isotropic. The sum over the subbands is reduced to one electron, and one heavy-hole and one light-hole level, because there is no quantum-mechanical confinement in bulk material. In addition, the subband energies are set to $E_i = 0$, and the following coefficients are modified:

$$O_{i,j} = 1 \tag{1121}$$

$$D^r(E) = \frac{1}{2\pi^2}\left(\frac{2m_r}{\hbar^2}\right)^{3/2} E^{1/2} \tag{1122}$$

$$P_{i,j} = 1 \tag{1123}$$

All other expressions remain the same.

Stimulated Recombination Rate

The radiative emissions contribute to the production of photons but they also deplete the carrier population in the active region. At each active vertex, the stimulated recombination rate of the carriers must be equal to the sum of the photon production rate of every lasing mode so that conservation of particles is ensured. The stimulated recombination rate for each active vertex is:

$$R^{st}(x, y) = \sum_i r^{st}(\hbar\omega_i) S_i |\Psi_i(x, y)|^2 \tag{1124}$$

where the sum is taken over all lasing modes. The stimulated emission coefficient is computed locally at this active vertex and its value is taken at the lasing energy, $\hbar\omega_i$, of mode i. S_i is the photon rate of mode i, solved from the corresponding photon rate equation of mode i, and $|\Psi_i(x, y)|^2$ is the local optical field intensity of mode i at this active vertex. This stimulated recombination rate is entered in the continuity equations to account for the correct depletion of carriers by stimulated emissions.

The total stimulated recombination rates on active vertices can be plotted by including the keyword `StimulatedRecombination` in the `Plot` section of the command file.

Spontaneous Recombination Rate

The spontaneous emission rate and power are described in Spontaneous Emission Rate and Power on page 923. The total spontaneous recombination rates on active vertices can be plotted by including the keyword `SpontaneousRecombination` in the `Plot` section of the command file.

Fitting Stimulated and Spontaneous Emission Spectra

The stimulated and spontaneous emission spectra can be fine-tuned by scaling and shifting. The spectra can be scaled in magnitude by the keywords `StimScaling=<float>` and `SponScaling=<float>` in the `Physics-LED` section. It is also possible to shift the effective emission wavelength (and, therefore, the spectra) by an energy amount specified as `GainShift=<float>`.

Gain-Broadening Models

Three different line-shape broadening models are available: Lorentzian, Landsberg, and hyperbolic-cosine. These line-shape functions, $L(E)$, are embedded in the radiative emission coefficients in Eq. 1112 and Eq. 1113 to account for broadening of the gain spectrum.

Lorentzian Broadening

Lorentzian broadening assumes that the probability of finding an electron or a hole in a given state decays exponentially in time [1]. The line-shape function is:

$$L(E) = \frac{\Gamma/(2\pi)}{(E_g - \hbar\omega + E)^2 + (\Gamma/2)^2} \tag{1125}$$

Landsberg Broadening

The Landsberg model gives a narrower, asymmetric line-shape broadening, and its line-shape function is:

$$L(E) = \frac{(\Gamma(E))/(2\pi)}{(E_g - \hbar\omega + E)^2 + (\Gamma(E)/2)^2} \tag{1126}$$

where:

$$\Gamma(E) = \Gamma \sum_{k=0}^{3} a_k \left(\frac{E}{q\Psi_p - q\Psi_n}\right)^k \tag{1127}$$

and $q\Psi_p - q\Psi_n$ is the quasi-Fermi level separation. The coefficients a_k are:

$$
\begin{aligned}
a_0 &= 1 \\
a_1 &= -2.229 \\
a_2 &= 1.458 \\
a_3 &= -0.229
\end{aligned}
\tag{1128}
$$

Hyperbolic-Cosine Broadening

The hyperbolic-cosine function has a broader tail on the low-energy side compared to Lorentzian broadening, and the line-shape function is:

$$L(E) = \frac{1}{4\Gamma} \cdot \frac{1}{\cosh^2\left(\frac{E}{2\Gamma}\right)} \tag{1129}$$

Syntax to Activate Broadening

You can select only one line-shape function for gain broadening. This is activated by the keyword `Broadening` in the `Physics-LED` section of the command file:

```
Physics {...
   LED (...
      Optics (...)
      # --- Lineshape broadening functions, choose one only ----
      Broadening (Type=Lorentzian Gamma=0.01)
#     Broadening (Type=Landsberg Gamma=0.01)      # Gamma in [eV]
#     Broadening (Type=CosHyper Gamma=0.01)
```

```
        )
    }
```

`Gamma` is the line width Γ, which must be defined in units of eV. If no `Broadening` keyword is detected, Sentaurus Device assumes the gain is unbroadened and does not perform the energy integral in Eq. 1112 and Eq. 1113.

Electronic Band Structure for Wurtzite Crystals

To account for the strong coupling of the three valence bands (heavy holes (HH), light holes (LH), and crystal-field split-holes (CH)) in wurtzite crystals, the localized quantum-well model in Sentaurus Device supports a parabolic band approximation using effective masses at the Γ-point. It is derived from the three-band $\vec{k} \cdot \vec{\mathbf{p}}$ method and considers strain effects assuming a growth direction along the c-axis of the hexagonal lattice. Based on general band-structure parameters for wurtzite crystals and a given strain defined by the mismatch of lattice constants, the band offsets and effective masses parallel and perpendicular to the growth direction are computed.

Starting from the diagonal strain tensor defined as:

$$\varepsilon_{xx} = \varepsilon_{yy} = \frac{a_s - a_0}{a_0} \tag{1130}$$

$$\varepsilon_{zz} = -2\frac{C_{13}}{C_{33}}\varepsilon_{xx} \tag{1131}$$

$$\varepsilon_{xy} = \varepsilon_{yz} = \varepsilon_{zx} = 0 \tag{1132}$$

where a_s corresponds to the lattice constant of the substrate, and a_0 is the lattice constant of the unstrained layer. The energies of the valence band edge can be written as [2]:

$$E_{hh}^0 = E_v^0 + \Delta_1 + \Delta_2 + \theta_\varepsilon + \lambda_\varepsilon \tag{1133}$$

$$E_{lh}^0 = E_v^0 + \frac{\Delta_1 - \Delta_2 + \theta_\varepsilon}{2} + \lambda_\varepsilon + \sqrt{\left(\frac{\Delta_1 - \Delta_2 + \theta_\varepsilon}{2}\right)^2 + 2\Delta_3^2} \tag{1134}$$

$$E_{ch}^0 = E_v^0 + \frac{\Delta_1 - \Delta_2 + \theta_\varepsilon}{2} + \lambda_\varepsilon - \sqrt{\left(\frac{\Delta_1 - \Delta_2 + \theta_\varepsilon}{2}\right)^2 + 2\Delta_3^2} \tag{1135}$$

with θ_ε and λ_ε expressing their dependency on the shear deformation potentials D_1 to D_4:

$$\theta_\varepsilon = D_3 \varepsilon_{zz} + D_4 (\varepsilon_{xx} + \varepsilon_{yy}) \tag{1136}$$

$$\lambda_\varepsilon = D_1 \varepsilon_{zz} + D_2 (\varepsilon_{xx} + \varepsilon_{yy}) \tag{1137}$$

The strain-dependent conduction band edge is given by:

$$E_c^0 = E_v^0 + \Delta_1 + \Delta_2 + E_g + P_{c\varepsilon} \tag{1138}$$

where the energy shift $P_{c\varepsilon}$ is due to the hydrostatic deformation potentials parallel (a_{cz}) and perpendicular (a_{ct}) to the growth direction:

$$P_{c\varepsilon} = a_{cz} \varepsilon_{zz} + a_{ct} (\varepsilon_{xx} + \varepsilon_{yy}) \tag{1139}$$

In the above expressions for the band edges (Eq. 1133–Eq. 1135, and Eq. 1138), E_v^0 is used as the reference energy and stands for the CH band-edge energy in the absence of spin-orbit interaction. A summary of all band structure–related and strain-related parameters used in this section along with their specification in the Sentaurus Device parameter file is given in Table 166 and Table 167.

Table 166 Parameters defined in BandstructureParameters section of parameter file

Symbol	Parameter name	Unit	Description
A_1	A1	–	Hole effective mass parameter.
A_2	A2	–	Hole effective mass parameter.
A_3	A3	–	Hole effective mass parameter.
A_4	A4	–	Hole effective mass parameter.
Δ_{so}	so	eV	Spin-orbit split energy.
Δ_{cr}	cr	eV	Crystal-field split energy.
Δ_1		eV	Defined as $\Delta_{cr} = \Delta_1$.
Δ_2		eV	Defined as $\Delta_{so} = 3\Delta_2$.
Δ_3		eV	Defined as $\Delta_{so} = 3\Delta_3$.

Table 167 Parameters defined in QWStrain section of parameter file

Symbol	Parameter name	Unit	Description
a_0	a0	m	Lattice constant at T = 300 K.
α	alpha	m/K	Model parameters describing linear temperature dependency of lattice constant: $a_0(T) = a_0 + \alpha(T - T_0)$
T_0	Tpar	K	

Table 167   Parameters defined in QWStrain section of parameter file (Continued)

Symbol	Parameter name	Unit	Description
C_{33}	C_33	eV	Elastic constant.
C_{13}	C_13	eV	Elastic constant.
a_{cz}	a_c	eV	Hydrostatic deformation potential parallel to crystal growth direction[1].
a_{ct}	a_c	eV	Hydrostatic deformation potential perpendicular to crystal growth direction[1].
D_1	D1	eV	Shear deformation potential.
D_2	D2	eV	Shear deformation potential.
D_3	D3	eV	Shear deformation potential.
D_4	D4	eV	Shear deformation potential.

1. a_{cz} and a_{ct} are assumed to be equal.

Based on a three-band 6×6 Hamiltonian matrix needed to describe the strong coupling of the three valence bands, analytic solutions for the dispersion relations $E(\vec{k})$ can be derived [2][3][4]. Performing a series expansion of E at the Γ-point up to the second order in k yields the effective masses that are used with the localized quantum-well model:

$$m_{hh}^z = -m_0(A_1 + A_3)^{-1} \tag{1140}$$

$$m_{hh}^t = -m_0(A_2 + A_4)^{-1} \tag{1141}$$

$$m_{lh}^z = -m_0\left(A_1 + \left(\frac{E_{lh}^0 - \lambda_\varepsilon}{E_{lh}^0 - E_{ch}^0}\right)A_3\right)^{-1} \tag{1142}$$

$$m_{lh}^t = -m_0\left(A_2 + \left(\frac{E_{lh}^0 - \lambda_\varepsilon}{E_{lh}^0 - E_{ch}^0}\right)A_4\right)^{-1} \tag{1143}$$

$$m_{ch}^z = -m_0\left(A_1 + \left(\frac{E_{ch}^0 - \lambda_\varepsilon}{E_{ch}^0 - E_{lh}^0}\right)A_3\right)^{-1} \tag{1144}$$

$$m_{ch}^t = -m_0\left(A_2 + \left(\frac{E_{ch}^0 - \lambda_\varepsilon}{E_{ch}^0 - E_{lh}^0}\right)A_4\right)^{-1} \tag{1145}$$

where A_1 to A_4 are called the hole effective mass parameters, which must be specified by users as shown in Table 166 on page 968.

To activate the simplified model for the treatment of the band structure of wurtzite crystals, the crystal type must be indicated in the `Physics` section of the command file.

If strain is to be accounted for, the substrate lattice constant must be specified as a reference for the computation of the strain tensor in each layer as shown here:

```
Physics {
   LED (
      Bandstructure ( CrystalType = Wurtzite )
      Strain ( RefLatticeConst = 3.183e-10 )   #[m]
   )
}
```

Besides the computation of the band-edge energies and the effective masses using the formulas in Eq. 1133–Eq. 1135, Eq. 1138, and Eq. 1140–Eq. 1145, it is possible to define these quantities explicitly. Each valence band can be characterized by a ladder specification as described in Explicit Ladder Specification on page 288. For materials exhibiting the wurtzite crystal structure, the syntax of the explicit ladder specification is extended to classify the specific hole type (HH, LH, or CH). This is needed for labeling the corresponding results such as subband energies or overlapping integrals during visualization.

For example, to explicitly define the properties of the various valence bands considering arbitrary strain, that is, the amount of strain is not declared to the tool, the ladder specification in the `SchroedingerParameters` section reads as follows:

```
SchroedingerParameters {
   Formula = 0,4
   hLadder(0.4376, 1.349, 1, 0.002, HeavyHole)
   hLadder(0.4373, 0.4375, 1, 0.003, LightHole)
   hLadder(0.4376, 0.4378, 1, 0.004, CrystalFieldSplitHole)
}
```

where the first and second entry of `hLadder` correspond to the values for the parallel (m^z) and the perpendicular (m^t) effective mass. The third entry indicates the ladder degeneracy, which is set to 1 for GaN-based semiconductors, and the fourth entry is used to specify the band offset with respect to the valence band edge without strain in eV. To activate the explicit ladder specification, the value of `Formula` for holes must be set to 4.

> **NOTE** In this parameter file excerpt of the `SchroedingerParameters` section, the value of `Formula` for electrons is set to 0, which uses the isotropic density-of-states mass as both the quantization mass (m^z) and the mass (m^t) perpendicular to it.

The keyword `Formula` is used to select one of several options for defining effective masses and band offsets, which are summarized in Table 168 on page 971. You can specify a single value, which only affects the specification for holes and uses the default value of 0 for

electrons. Using a value pair allows the explicit specification of Formula for both electrons (first value) and holes (second value).

Table 168   Supported values of Formula for localized quantum-well model

Formula	Description	Limitations
0	Use isotropic density-of-states mass as m^z and m^t.	Only supported for electrons.
2	Use me, mh, and ml to specify relative effective mass for electrons, heavy holes, and light holes, respectively.	Only supported for electrons, light holes, and heavy holes. Cannot be used if NumberOfValenceBands is set to a value greater than 2 in the command file. No distinction between m^z and m^t. Band offsets due to strain cannot be specified explicitly.
4	Use eLadder(...) specification for electrons, and use hLadder(...) specification for holes.	
5	Effective masses and band offsets are computed based on parameters specified in BandstructureParameters and QWStrain sections using parabolic band approximation as described in Electronic Band Structure for Wurtzite Crystals on page 967.	Only supported for holes.

Optical Transition Matrix Element for Wurtzite Crystals

To compute the spontaneous emission spectrum, $r^{\mathrm{sp}}(E)$, in LED simulations as defined in Eq. 1113, p. 962, the optical transition matrix element must be evaluated. For quantum wells grown along the c-axis of the wurtzite crystal, the polarization-dependent transition matrix element for the different conduction band–to–valence band transitions can be written as [5]:

$$\left|M_{\mathrm{hh}}^{\mathrm{TE}}\right|^2 = \frac{3}{2}O_{ij}(M_b^{\mathrm{TE}})^2 \tag{1146}$$

$$\left|M_{\mathrm{lh}}^{\mathrm{TE}}\right|^2 = \frac{3}{2}\cos^2(\theta_e)O_{ij}(M_b^{\mathrm{TE}})^2 \tag{1147}$$

$$\left|M_{\mathrm{ch}}^{\mathrm{TE}}\right|^2 = 0 \tag{1148}$$

$$\left|M_{\mathrm{hh}}^{\mathrm{TM}}\right|^2 = 0 \tag{1149}$$

$$\left|M_{lh}^{\mathrm{TM}}\right|^2 = \frac{3}{2}\sin^2(\theta_e)O_{ij}(M_b^{\mathrm{TM}})^2 \tag{1150}$$

$$\left|M_{\mathrm{ch}}^{\mathrm{TM}}\right|^2 = \frac{3}{2}O_{ij}(M_b^{\mathrm{TM}})^2 \tag{1151}$$

where O_{ij} refers to the overlap integral between the envelope wavefunctions of the i-th electron subband and the j-th valence subband. The anisotropic bulk momentum matrix elements are given by:

$$(M_b^{\mathrm{TE}})^2 = \frac{m_0}{6}\left(\frac{1}{m_c^z}-1\right)\frac{(E_g+\Delta_1+\Delta_2)(E_g+2\Delta_2)-2\Delta_3^2}{E_g+2\Delta_2} \tag{1152}$$

$$(M_b^{\mathrm{TM}})^2 = \frac{m_0}{6}\left(\frac{1}{m_c^t}-1\right)\frac{E_g[(E_g+\Delta_1+\Delta_2)(E_g+2\Delta_2)-2\Delta_3^2]}{(E_g+\Delta_1+\Delta_2)(E_g+\Delta_2)-\Delta_3^2} \tag{1153}$$

where m_c^z and m_c^t denote the relative electron mass parallel and perpendicular to the quantization direction, respectively, and m_0 denotes the electron rest mass. The angle θ_e is defined as:

$$k_z = \left|\vec{k}\right|\cos(\theta_e) \tag{1154}$$

where $\vec{k}$ refers to the electron vector, and $\cos(\theta_e)=1$ at the Γ-point of the quantum-well subband.

Arbitrary polarization is modeled as a linear combination of TE and TM polarization according to:

$$\left|M_{i,j}\right|^2 = a\cdot\left|M_{i,j}^{\mathrm{TE}}\right|^2 + (1-a)\cdot\left|M_{i,j}^{\mathrm{TM}}\right|^2 \tag{1155}$$

where a is called the `PolarizationFactor`, which can be set in the `QWLocal` section as shown here. For purely TE or TM simulations, it is sufficient to set `Polarization` to the respective identifier:

```
Physics {
   QWLocal (
      Polarization = TE          # TM
      # or
      Polarization = Mixed
      PolarizationFactor = 0.4   # must be in interval [0 1]
   )
}
```

Simple Quantum-Well Subband Model

This section describes the solution of the Schrödinger equation for a simple finite quantum-well model. This is the default model in Sentaurus Device. This simple quantum-well (QW) subband model is combined with separate QW strain (see Strain Effects on page 976) to model most (III–V material) quantum-well systems.

In a quantum well, the carriers are confined in one direction. Of interest are the subband energies and wavefunctions of the bound states, which can be solved from the Schrödinger equation. In this simple QW subband model, it is assumed that the bands for the electron, heavy hole, and light hole are decoupled, and the subbands are solved independently by a 1D Schrödinger equation.

The time-independent 1D Schrödinger equation in the effective mass approximation is:

$$\left(-\frac{\hbar^2}{2} \frac{\partial}{\partial x} \frac{1}{m(x)} \frac{\partial}{\partial x} + V(x) - E^i \right) \zeta^i(x) = 0 \tag{1156}$$

where $\zeta^i(x)$ is the i-th quantum mechanical wavefunction, E^i is the i-th energy eigenvalue, and $V(x)$ is the finite well shape potential.

With the following ansatz for the even wavefunctions:

$$\zeta(x) = C_1 \begin{cases} \cos\left(\frac{\kappa l}{2}\right) e^{-\alpha(|x| - l/2)} &, \quad |x| > l/2 \\ \cos(\kappa x) &, \quad |x| \le l/2 \end{cases} \tag{1157}$$

and the odd wavefunctions:

$$\zeta(x) = C_2 \begin{cases} \pm\sin\left(\frac{\kappa l}{2}\right) e^{\mp(x \mp l/2)} &, |x| > l/2 \\ \sin(\kappa x) &, |x| \le l/2 \end{cases} \tag{1158}$$

Eq. 1156 becomes [1]:

$$\alpha\frac{l}{2} + \frac{m_b}{m_w} \kappa\frac{l}{2} \cot\left(\kappa\frac{l}{2}\right) = 0 \tag{1159}$$

$$\alpha\frac{l}{2} - \frac{m_b}{m_w} \kappa\frac{l}{2} \tan\left(\kappa\frac{l}{2}\right) = 0 \tag{1160}$$

with:

$$\kappa = \frac{\sqrt{2m_w E}}{\hbar} \tag{1161}$$

$$\alpha = \frac{\sqrt{2m_b(\Delta E_c - E)}}{\hbar} \tag{1162}$$

The first transcendental equation gives the even eigenvalues, and the second one gives the odd eigenvalues. The wavefunctions are immediately obtained with Eq. 1157 and Eq. 1158 after the subband energy E has been computed. Having obtained the wavefunctions and subband energies, the carrier densities of the 1D-confined system are also computed by:

$$n(x) = N_e^{2D} \sum_i |\zeta_i(x)|^2 F_0(\eta_n - E_i) \tag{1163}$$

$$p(x) = N_{hh}^{2D} \sum_j |\zeta_{j(x)}|^2 F_0(\eta_p - E_{hh}^j) + N_{lh}^{2D} \sum_m |\zeta_{m(x)}|^2 F_0(\eta_p - E_{lh}^m) \tag{1164}$$

where $F_0(x)$ is the Fermi integral of the order 0, and η_n, η_p denote the chemical potentials. The indices hh and lh denote the heavy and light holes, respectively.

The effective densities of states are:

$$N_e^{2D} = \frac{k_B T m_e}{\hbar^2 \pi L_x} \tag{1165}$$

$$N_{lh/hh}^{2D} = \frac{k_B T m_{lh/hh}}{\hbar^2 \pi L_x} \tag{1166}$$

where L_x is the thickness of the quantum well. The thickness of each quantum well is automatically detected in Sentaurus Device by scanning the material regions for the keyword `Active`.

The effective masses of the carriers in the quantum well can be changed inside the parameter file:

```
eDOSMass
{
 * For effective mass specification Formula1 (me approximation):
 * or Formula2 (Nc300) can be used :
        Formula = 2     # [1]
 * Formula2:
 * me/m0 = (Nc300/2.540e19)^2/3
 * Nc(T) = Nc300 * (T/300)^3/2
```

```
       Nc300    = 8.7200e+16    # [cm-3]
 * Mole fraction dependent model.
 * If just above parameters are specified, then its values will be
 * used for any mole fraction instead of an interpolation below.
 * The linear interpolation is used on interval [0,1].
       Nc300(1)        = 6.4200e+17    # [cm-3]
}
...
SchroedingerParameters:
{ * For the hole masses for Schroedinger equation you can
 * use different formulas.
 * formula=1 (for materials with Si-like hole band structure)
 *    m(k)/m0=1/(A+-sqrt(B+C*((xy)^2+(yz)^2+(zx)^2)))
 *    where k=(x,y,z) is unit normal vector in reciprocal
 *    space. '+' for light hole band, '-' for heavy hole band
 * formula=2: Heavy hole mass mh and light hole mass ml are
 *    specified explicitly.
 * Formula 2 parameters:
       Formula = 2     # [1]
       ml      = 0.027 # [1]
       mh      = 0.08  # [1]
 * Mole fraction dependent model.
 * If just above parameters are specified, then its values will be
 * used for any mole fraction instead of an interpolation below.
 * The linear interpolation is used on interval [0,1].
       ml(1)   = 0.094 # [1]
       mh(1)   = 0.08  # [1]
}
```

Syntax for Simple Quantum-Well Model

This simple QW subband model is the default model when the `QWTransport` model is activated:

```
Physics {...
   LED (...
      Optics (...)
      # ----- Specify QW model and physics -----
      QWTransport
      QWExtension = AutoDetect   # QW widths auto-detection
   )
}
```

Table 265 on page 1453 provides the keywords that are associated with this simple QW model.

Strain Effects

It is well known that strain of the quantum well modifies the stimulated and spontaneous emission gain spectra. Due to the deformation potentials in the crystal at the well–bulk interface and valence band mixing effects, band structure modifications occur mainly for the valence bands. They have an impact on the optical recombination and transport properties.

In the simple QW subband model discussed in the previous section, a simpler approach to the QW strain effects is adopted. The simple QW subband model does not include nonparabolicities of the band structure, arising from valence band mixing and strain, in a rigorous manner. However, by carefully selecting the effective masses in the well, a good approximation of the strained band structure can be obtained [6]. The effective masses can be changed in the parameter file as previously shown.

Basically, strain has two impacts on the band structure. Due to the deformation potentials, the effective band offsets of the conduction and valence bands are modified. This is included in the simple QW subband model by:

$$\delta E_C = 2a_c\left(1 - \frac{C_{12}}{C_{11}}\right)\varepsilon \tag{1167}$$

$$\delta E_V^{HH} = 2a_v\left(1 - \frac{C_{12}}{C_{11}}\right)\varepsilon + b\left(1 + 2\frac{C_{12}}{C_{11}}\right)\varepsilon \tag{1168}$$

$$\delta E_V^{LH} = 2a_v\left(1 - \frac{C_{12}}{C_{11}}\right)\varepsilon - b\left(1 + 2\frac{C_{12}}{C_{11}}\right)\varepsilon + \frac{\Delta}{2} - \left(-\frac{1}{2}\sqrt{\Delta^2 + 9\delta E_{sh}^2 - 2\delta E_{sh}\Delta}\right) \tag{1169}$$

where a_n and a_c are the hydrostatic deformation potential of the conduction and valence bands, respectively. The shear deformation potential is denoted with b and Δ is the spin-orbit split-off energy. The elastic stiffness constants are C_{11} and C_{12}, and ε is the relative lattice constant difference in the active region. The hydrostatic component of the strain shifts the conduction band offset by δE_C and shifts the valence band offset by $\delta E_V^0 = 2a_v(1 - C_{12}/C_{11})\varepsilon$.

The shear component of the strain decouples the light hole and heavy hole bands at the Γ point, and shifts the valence bands by an amount of $\delta E_{sh} = b(1 + 2C_{12}/C_{11})\varepsilon$ in opposite directions.

Syntax for Quantum-Well Strain

The strain shift can be activated by the keyword `Strain` in the `Physics-LED` section of the command file:

```
Physics {...
   LED (...
      Optics (...)
      # --- QW physics ---
      QWTransport
      QWExtension = AutoDetect
      # --- QW strain ---
      Strain
   )
}
```

The parameters a_n, a_c, and b can be entered as `a_nu`, `a_c`, and `b_shear`, respectively, in the `QWStrain` section of the parameter file:

```
QWStrain
{
 * Deformation Potentials (a_nu, a_c, b, C_12, C_11
 * and strainConstant eps :
 * Formula:
 * eps = (a_bulk - a_active)/a_active
 * dE_c = ...
 * dE_lh = ...
 * dE_hh = ...
      eps = -1.0000e-02      # [1]
      * a_nu = 1.27          # [1]
      * a_c = -5.0400e+00    # [1]
      * b_shear = -1.7000e+00  # [1]
      * C_11 = 10.11         # [1]
      * C_12 = 5.61          # [1]
}
```

The elastic stiffness constants C_{11} and C_{12} can be specified by `C_11` and `C_12`. Due to valence band mixing and strain, the valence bands can become nonparabolic. However, within a small range from the band edge, parabolicity can still be assumed. In the simulation, you can modify the effective heavy hole and light hole masses in the parameter file for the subband calculation to account for this effect.

The spin-orbit split-off energy can be specified in the `BandstructureParameters` section of the parameter file:

```
BandstructureParameters{
   ...
```

```
            so = 0.34   # [eV]
            ...
      }
```

Localized Quantum-Well Model

In GaN-based quantum-well systems, the polarization charge sheets at the interfaces of the quantum well or barrier induce a large field within the quantum well. These fields skew the energy bands and cause mismatches in the alignment of the electron and hole wavefunctions.

The localized quantum-well model takes into account field effects in a fully coupled methodology. The activation syntax is included in the `Physics` section of each active quantum well:

```
   Physics (region="QW1") {...
      Active(Type=QuantumWell)
      QWLocal (
         NumberOfElectronSubbands = 5
         NumberOfLightHoleSubbands = 2
         NumberOfHeavyHoleSubbands = 4
         NumberOfCrystalFieldSplitHoleSubbands = 3
         NumberOfValenceBands = 3
   #   -ElectricFieldDep
         WidthExtraction (
            # indicate side regions or materials of QW if sides
            # do not coincide with domain boundaries
            SideRegion = ("reg1", ..., "regn")
            SideMaterial = ("mat1", ..., "matn")
            MinAngle = (<float>, <float>)
            ChordWeight = <float>
         )
      )
   }
```

By default, the electric field dependency is activated in the localized quantum-well model. However, it can be deactivated by using the `-ElectricFieldDep` keyword. The maximum number of subbands for electrons, heavy holes (HH), light holes (LH), and crystal-field split-holes (CH) must be specified to enable Sentaurus Device to limit the scope of the computation. The actual number of subbands used is computed as the simulation progresses. By default, only the heavy-hole (HH) band and the light-hole (LH) band are considered. Changing the value of `NumberOfValenceBands` from 2 to 3 includes the crystal-field split-hole (CH) band in the computation and is the recommended setting for materials exhibiting the wurtzite crystal system.

A `WidthExtraction` section is included to enable you to specify how the quantum-well thickness can be extracted. This thickness is important to define the quantum-well width so as to compute the solution to the Schrödinger equation. `MinAngle` and `ChordWeight` are parameters used in a special method to compute the thickness of the quantum-well layer that is not aligned to one of the major axes (see Thickness Extraction on page 313).

If the `QWLocal` section is defined in the global `Physics` section, the parameters of the maximum number of bands in each band are applied to all the specified `Active(Type=QuantumWell)` regions.

By default, the localized quantum-well model does not account for the correction of the densities in the quantum well due to quantization. To take quantization into account, use the `eDensityCorrection` and `hDensityCorrection` options of `QWLocal`. For more details, see Quantum-Well Quantization Model on page 309.

> **NOTE** The variables in Table 169 also apply to the nonlocal quantum-well model.

Table 169   Variables for plotting when using the localized quantum-well model

Variable	Description
QW_chEigenEnergy	Eigenenergies of the crystal-field split-hole bound states [eV].
QW_chNumberOfBoundStates	Actual number of QW bound states for crystal-field split-holes.
QW_chRelativeEffectiveMass	Relative effective mass of crystal-field split-holes.
QW_chStrainBandShift	Shift in crystal-field split-hole band due to strain effects.
QW_eEigenEnergy	Eigenenergies of the electron bound states [eV].
QW_ElectricFieldProjection	Electric field in the QW [V/cm]. **NOTE** This variable does not apply to the nonlocal quantum-well model.
QW_eNumberOfBoundStates	Actual number of QW bound states for electrons.
QW_eRelativeEffectiveMass	Relative effective mass of electrons.
QW_eStrainBandShift	Shift in conduction band due to strain effects.
QW_hhEigenEnergy	Eigenenergies of the heavy-hole bound states [eV].
QW_hhNumberOfBoundStates	Actual number of QW bound states for heavy holes.
QW_hhRelativeEffectiveMass	Relative effective mass of heavy holes.
QW_hhStrainBandShift	Shift in heavy-hole band due to strain effects.
QW_lhEigenEnergy	Eigenenergies of the light-hole bound states [eV].
QW_lhNumberOfBoundStates	Actual number of QW bound states for light holes.
QW_lhRelativeEffectiveMass	Relative effective mass of light holes.

Table 169   Variables for plotting when using the localized quantum-well model (Continued)

Variable	Description
QW_lhStrainBandShift	Shift in light-hole band due to strain effects.
QW_OverlapIntegral	Overlap integrals between electron and hole wavefunctions.
QW_QuantizationDirection	Quantization direction of the QW.
QW_Width	Extracted width of the QW [μm].

You also can include any of the variables in Table 169 on page 979 in the `CurrentPlot` statement, for example:

```
CurrentPlot { ...
   QW_eEigenEnergy (
      Minimum (Region = "QW1")
      Maximum (Region = "QW1")
      Average (Region = "QW1")
   )
}
```

> **NOTE**   As this is an advanced model, if you are interested in using this model, contact TCAD Support for assistance in evaluating whether this model is suitable for use in your device (see Contacting Your Local TCAD Support Team Directly on page xliii).

Nonlocal Quantum-Well Model Using 1D Schrödinger Solver

The most rigorous model available in Sentaurus Device to model quantum wells is the 1D Schrödinger solver on a nonlocal mesh that covers the quantum-well structure (see Nonlocal Mesh for 1D Schrödinger on page 286). A nonlocal mesh consists of numerous cutlines parallel to the quantization direction on which the potential distribution and effective masses are extracted. On each nonlocal line, the 1D Schrödinger solver computes the eigenenergies and the wavefunctions. Then, the eigenenergies of the bound states and the overlap integrals of the wavefunctions for the various optical transitions are interpolated back to the device simulation mesh to calculate the radiative recombination.

This model also supports the simulation of mole fraction–graded quantum wells by defining the band-structure parameters and the effective masses as mole fraction dependent (see Mole-Fraction Specification on page 17 and Parameters for Composition-Dependent Materials on page 24).

To use the 1D Schrödinger solver for quantum wells:

1. Construct a special-purpose *nonlocal* mesh that covers the quantum-well structure (see Nonlocal Mesh for 1D Schrödinger on page 286). The nonlocal lines should extend beyond the well region into the barrier regions on either side by approximately the well width.

2. Activate the 1D Schrödinger solver on the nonlocal line mesh with appropriate parameters (see Using 1D Schrödinger on page 287, 1D Schrödinger Parameters on page 287, and Electronic Band Structure for Wurtzite Crystals on page 967).

3. Mark quantum-well regions as active by specifying `Active(Type=QuantumWell)` in the corresponding region-specific `Physics` sections.

For example, to use the 1D Schrödinger solver to simulate a quantum well that is 3 nm wide and whose plane is perpendicular to the z-axis, specify the following syntax in the command file:

```
Physics (Region="QW1") { Active(Type=QuantumWell) }

NonLocal "QW1" (
    RegionInterface="QW1/Barrier0"
    Length = 6e-7
    Permeation = 3e-7
    Direction = (0 0 1)
    MaxAngle = 5
    Discretization = 1e-8
    -Transparent(Region="Barrier0")
)

Physics {
    Schroedinger "QW1" (Electron Hole Polarization = TE -DensityCorrection)
}
```

By default, the nonlocal quantum-well model accounts for the correction of the densities in the quantum well due to quantization. However, at the beginning, it is recommended to disable the correction of the densities (`-DensityCorrection`) as it has an adverse effect on convergence as shown in this example. For details, see 1D Schrödinger Model on page 290.

The variables in Table 169 on page 979 can be plotted when using the nonlocal quantum-well model. These variables also can be specified in the `CurrentPlot` statement (see Tracking Additional Data in the Current File on page 110) and the `NonlocalPlot` statement (see Visualizing Schrödinger Solutions on page 290).

> **NOTE** As this is an advanced model, if you are interested in using this model, contact TCAD Support for assistance in evaluating whether this model is suitable for use in your device (see Contacting Your Local TCAD Support Team Directly on page xliii).

Importing Gain and Spontaneous Emission Data With PMI

Sentaurus Device can import external stimulated and spontaneous emission data through the physical model interface (PMI). The gain PMI concept is illustrated in Figure 70.

Sentaurus Device calls the user-written gain calculations through the PMI with the variables: electron density n, hole density p, electron temperature eT, hole temperature hT, and transition energy E. The user-written gain calculation then returns the gain g and the derivatives of gain with respect to n, p, eT, and hT to Sentaurus Device. The derivatives are required to ensure proper convergence of the Newton iterations. In this way, the user-import gain is made self-consistent within the simulation.

Figure 70   Concept of the gain PMI

Implementing Gain PMI

The PMI uses the object-orientation capability of the C++ language (see Chapter 38 on page 1043). A brief outline is given here of the gain PMI.

In the Sentaurus Device header file `PMIModels.h`, the following base class is defined for gain:

```
class PMI_StimEmissionCoeff : public PMI_Vertex_Interface {
public:
    PMI_StimEmissionCoeff (const PMI_Environment& env);
    virtual ~PMI_StimEmissionCoeff ();

    virtual void Compute_rstim
    (double E,
    double n,
    double p,
    double et,
```

```
    double ht,
    double& rstim) = 0;

    virtual void Compute_drstimdn
    (double E,
    double n,
    double p,
    double et,
    double ht,
    double& drstimdn) = 0;

    virtual void Compute_drstimdp
    (double E,
    double n,
    double p,
    double et,
    double ht,
    double& drstimdp) = 0;

    virtual void Compute_drstimdet
    (double E,
    double n,
    double p,
    double et,
    double ht,
    double& drstimdet) = 0;

    virtual void Compute_drstimdht
    (double E,
    double n,
    double p,
    double et,
    double ht,
    double& drstimdht) = 0;
};
```

To implement the PMI model for gain, you must declare a derived class in the user-written header file:

```
#include "PMIModels.h"

class StimEmissionCoeff : public PMI_StimEmissionCoeff {
// User-defined variables for his/her own routines
 private:
    double a, b, c, d;

 public:
    // Need a constructor and destructor for this class
    StimEmissionCoeff (const PMI_Environment& env);
```

```
        ~StimEmissionCoeff ();

        // --- User needs to write the following routines in the .C file ---
        // The value of the function is return as the last pointer argument

        // stimulated emission coeff value
        void Compute_rstim (double E,
                            double n,
                            double p,
                            double et,
                            double ht,
                            double& rstim);

        // derivative wrt n
        void Compute_drstimdn (double E,
                               double n,
                               double p,
                               double et,
                               double ht,
                               double& drstimdn);

        // derivative wrt p
        void Compute_drstimdp (double E,
                               double n,
                               double p,
                               double et,
                               double ht,
                               double& drstimdp);

        // derivative wrt eT
        void Compute_drstimdet (double E,
                                double n,
                                double p,
                                double et,
                                double ht,
                                double& drstimdet);

        // derivative wrt hT
        void Compute_drstimdht (double E,
                                double n,
                                double p,
                                double et,
                                double ht,
                                double& drstimdht);
    };
```

Next, you must write the functions `Compute_rstim`, `Compute_drstimdn`, `Compute_drstimdp`, `Compute_drstimdet`, and `Compute_drstimdht` to return the values of the stimulated emission coefficient and its derivatives to Sentaurus Device using this gain PMI. If you have, for example, a table of gain values, you must implement the above functions to interpolate the values of the gain and derivatives from the table.

The spontaneous emission coefficient can also be imported using the PMI. The implementation is exactly the same as the stimulated emission coefficient, and you only need to replace `StimEmissionCoeff` with `SponEmissionCoeff` in the above code example.

References

[1] L. A. Coldren and S. W. Corzine, *Diode Lasers and Photonic Integrated Circuits*, New York: John Wiley & Sons, 1995.

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[3] S. L. Chuang and C. S. Chang, "k.p method for strained wurtzite semiconductors," *Physical Review B*, vol. 54, no. 4, pp. 2491–2504, 1996.

[4] M. Kumagai, S. L. Chuang, and H. Ando, "Analytical solutions of the block-diagonalized Hamiltonian for strained wurtzite semiconductors," *Physical Review B*, vol. 57, no. 24, pp. 15303–15314, 1998.

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Part IV Mesh and Numeric Methods

This part of the *Sentaurus™ Device User Guide* contains the following chapters:

CHAPTER 36 Automatic Grid Generation and
Adaptation Module AGM

*This chapter describes the automatic generation and adaptation
module for quadtree-based simulation grids of physical devices in
stationary simulations.*

The approach is based on a local anisotropic grid adaptation technique for the stationary drift-diffusion model [1][2][3] and has been extended formally to thermodynamic and hydrodynamic simulations.

Overview

NOTE   In its current status, AGM is not designed to improve the speed of simulations but rather to support users in generating simulation grids in a semi-automatic fashion. In fact, using AGM slows down the simulation time considerably as the control of the grid sizes is difficult, and the recomputation of solutions on adaptively generated grids is, in the presence of strong nonlinearities, a time-consuming task. Therefore, it is not recommended to use AGM throughout large simulation projects in a fully automatic adaptation mode. The integration of AGM in Sentaurus Device is incomplete as incompatibilities occur with certain features of Sentaurus Device.

The accuracy of approximate solutions computed by many simulation tools depends strongly on the simulation grid used in the discretization of the underlying problem. The major aim of grid adaptation is to obtain numeric solutions with a controlled accuracy tolerance using a minimal amount of computer resources using *a posteriori* error indicators to construct appropriate simulation grids. The main building blocks of a local grid adaptation module for stationary problems are the adaptation criteria (local error indicators that somehow determine the quality of grid elements), the adaptation scheme (determining whether and how the grid will be modified on the basis of the adaptation criteria), and the recomputation procedure of the approximate solution on adaptively generated grids. In the framework of finite-element methods for linear, scalar, and elliptic boundary-value problems, grid adaptation has reached a mature status [4].

The semiconductor device problem consists of a nonlinearly coupled system of partial differential equations, and the true solution of the problem exhibits layer behavior and

singularities, posing additional difficulties for grid adaptation modules. Several adaptation criteria have been proposed in the literature [1]. For the overall robustness of adaptive simulations, the recomputation of the solution is a very serious (and, sometimes, very time-consuming) problem.

The adaptation procedure used in Sentaurus Device is based on the approach developed in [1], [2], and [3]. It uses the idea of equidistributing local dissipation rate errors and aims at accurate computations of the terminal currents of the device. A quadtree mesh structure is used to enable anisotropic grid adaptation on boundary Delaunay meshes required by the discretization used in Sentaurus Device. The recomputation procedure relies on local and global characterizations of dominating nonlinearities and includes relaxation techniques based on the solution of local boundary value problems and a global homotopy technique for large avalanche generation.

The intention of the AGM module in its current status is to support the generation of a simulation grid and to provide some flexibility for users to influence the adaptation process. This allows users to find, in a semi-automatic process, a compromise of accuracy requirements and mesh sizes. The module supports:

- Two-dimensional device structures
- Default quadtree refinement approach of Sentaurus Mesh
- Grid adaptation for stationary problems (adaptive `Coupled` and `Quasistationary`)

Coarsening during adaptation is not supported.

Grid adaptation of 3D devices also is formally supported using the octree approach of Sentaurus Mesh but, for realistic structures, the performance remains beyond acceptable limits.

General Adaptation Procedure

The general grid adaptation flow is outlined in the following example:

```
compute solution on actual grid

coupled adaptation loop {
   // adaptation decision
   for all adaptive devices {
      check if adaptation is required
   }
   check if coupled adaptation is required

   // adaptation strategy
   for all adaptive devices {
      generate new grid
      initialize data on new grid and perform local smoothing
   }
```

```
      // recompute solution
      solve fully coupled system on new grids
}
```

The core ingredients of the flow are the adaptation criteria, which decide whether and how the grid is modified, and the meshing engine, which performs the changes of the grid. Sentaurus Device makes use of the Sentaurus Mesh meshing engine.

Adaptation Scheme

The meshing engine builds a refinement tree, which consists of axis-aligned refinement boxes. The root refinement box covers the whole device structure. A refinement box in the tree is split into several finer refinement boxes according to refinement requests. The leaf elements of the tree cover the whole device by nonoverlapping refinement boxes.

Adaptation Decision

The decision as to whether a new mesh will be constructed is based on local and global adaptation criteria. The local adaptation criteria are, in general, applied to the leaf elements of the refinement tree.

Adaptation Criteria

The adaptation criteria determine whether and how the grid will be modified. In [1], adaptation criteria for the nonlinearly coupled system of equations for the drift-diffusion model have been proposed, aiming at accurate computations of the terminal currents of the device. They use the close relationship between the system dissipation rate and the terminal currents, and estimate the error of the dissipation rate. This is performed by either solving related local Dirichlet problems or using the residual error estimation technique. Both techniques are well known in the framework of finite-element discretizations for scalar and elliptic boundary-value problems [4].

In practice, these criteria are often computationally too expensive, lead to large grid sizes, and are hard to control by users. Sentaurus Device supports two types of refinement criterion. The first type supports refinement based on values of a scalar field. It is a heuristic refinement, does not provide error estimation, is easily controlled by users, and is useful if physically relevant fields are considered. The second type adopts the residual error estimator for the dissipation rate of [1].

Refinement on Local-Field Variation

These criteria control the variation of a scalar field on grid elements. For a user-specified field represented on vertices of the grid, elements are refined if differences of the vertex values exceed a user-supplied value. Using the doping concentration as a field, such criteria are typically used in mesh generation processes. In the adaptation module, you can use any scalar field defined on vertices known by the simulator, for example, `ConductionBandEnergy` or `DissipationRateDensity`.

Refinement on Residual Error Estimation

The residual adaptation criteria, so far applicable only to 2D structures, estimate the *error of the quantity F* per grid element T. In analogy to standard methods, they measure jumps of the density of interest across inter-element boundaries. The error for a 2D element T is given as:

$$\eta_T(F) = \frac{|T|}{|N_e(T)|} \sum_{T' \in N_e(T)} \left| \omega_F^h(T') - \omega_F^h(T) \right| \tag{1170}$$

where:

- $\omega_F^h(T)$ denotes the approximate element functional density (on element T and T', respectively).
- $N_e(T)$ is the set of (semiconductor) elements sharing an edge with T.
- $|N_e(T)|$ is the number of elements.
- $|T|$ is the volume of T.

So far, the residual refinement criterion is only available for the AGM dissipation rate `AGMDissipationRate`, which is defined as:

$$D_{\text{AGM}} = \hat{w}_n \int_\Omega \mu_n n \left| \vec{J}_n \right|^2 dx + \hat{w}_P \int_\Omega \mu_p p \left| \vec{J}_p \right|^2 dx + \hat{w}_r kT \int_\Omega R_{\text{abs}} \left| \ln\left(\frac{np}{n_{i,\text{eff}} p_{i,\text{eff}}} \right) \right| dx \tag{1171}$$

where $R_{\text{abs}} = \sum \hat{w}_{R_i} |R_i|$ is the weighted absolute sum of individual generation–recombination processes with their individual weights $\hat{w}_{R_i}$. You can modify all weights $\hat{w}_i$.

Solution Recomputation

For the recomputation of the solution, data is interpolated onto the new simulation grid, and iterative smoothing techniques are applied to improve the robustness of the procedure.

Device-Level Data Smoothing

In the first step, the electrostatic potential is adjusted to interpolated data by applying the so-called electrostatic potential correction (EPC), that is, a mixed linear and nonlinear Poisson equation is solved using a Newton algorithm. To achieve almost self-consistent solutions for the coupled equations of the device, local Dirichlet problems are solved approximately, resulting in the so-called nonlinear node block Jacobi iteration (NBJI). The node block iterations are performed only on a subset of all grid vertices.

For remarkable avalanche generation, a homotopy technique (or continuation technique), here called *avalanche homotopy*, is applied to improve the robustness of the recomputation procedure, that is, the true avalanche generation is decoupled globally from the equations and is integrated stepwise into the solution process. As the avalanche generation F_{ava} is an additive term, the equations to be solved $F(x) = F_b(x) + F_{ava}(x) = 0$ can be split into a basic part F_b and the avalanche generation term F_{ava}, where x represents the unknown solution variables. With the fixed avalanche generation $\widehat{F}_{ava}$ interpolated from the old grid, the avalanche homotopy now reads:

$$H_{ava}(x, t) = F_b(x) + (1 - t)\widehat{F}_{ava} + tF_{ava}(x) \tag{1172}$$

where $t \in [0;1]$ is the homotopy parameter ramped from 0 to 1. For $t = 0$, the homotopy is reduced to a simplified problem, while for $t = 1$ the fully coupled system is solved. Therefore, the avalanche homotopy is similar to a quasistationary simulation where the avalanche generation is ramped (instead of specified parameters).

System-Level Data Smoothing

On the system level, a self-consistent solution for the original fully coupled system of equations is computed by the Newton algorithm.

Specifying Grid Adaptations

If you want to perform simulations using the grid adaptation capability, you must specify which device instances should be adaptive by adding a `GridAdaptation` section into the device instance description. The device structure must be defined, for example, in the form of a Sentaurus Mesh boundary file and command file, by specifying `Boundary` in the corresponding `File` section.

Having the device instance adaptive, you must indicate which solve statements should invoke grid adaptation; otherwise, no adaptation occurs.

The following illustrates the basic components for a single-device simulation:

```
File { ...
   Boundary = "meshing_bnd.tdr"       * input boundary description
   Grid     = "./DIR-test/grid_des"   * reinterpreted as OUTPUT
}
GridAdaptation ( ... )                 * device adaptation parameters
Solve { ...
   Coupled ( ... GridAdaptation ( ... ) ) { ... }
   Quasistationary ( ... GridAdaptation ( ... ) ) { ... }
}
```

The relevant keywords are:

- `Boundary` in `File`: Specify the (common) base name for the Sentaurus Mesh boundary and command files, defining the device structure.

- `Grid` in `File`: In contrast to nonadaptive simulations, where `Grid` specifies the input device structure, here `Grid` is used to output files. As soon as you plot a device structure, the simulator creates additionally a file that contains the grid and all doping species, which can be used as fixed input device structures. These files are numbered automatically.

- `GridAdaptation` in `Device` section or global section: Specify the device-specific adaptation parameters as described in Adaptive Device Instances on page 994.

- `GridAdaptation` in `Coupled`/`Quasistationary`: Make the solve statement adaptive as described in Adaptive Solve Statements on page 1003.

Adaptive Device Instances

A device instance is adaptive if the keyword `GridAdaptation` is specified as a section of the instance description. Several parameters can be passed to the instance by specifying parameter entries for the keyword, that is:

```
GridAdaptation ( <agm-device-par-list> )
```

Device Structure Initialization

The device structure is defined by some geometric information (including contacts, regions, and material information) and some data fields defined in the regions (such as doping profiles).

You can initialize the device structure for the AGM module in two ways, either using the Sentaurus Mesh boundary and command file, or using an element grid file (in TDR format).

The initialization method is selected in the `Meshing` section of the `GridAdaptation` section:

```
GridAdaptation ( ...
   Meshing ( ...
      InitializationMethod = FromBoundaryAndCommand | FromElementGrid
   )
)
```

Initialization From Sentaurus Mesh Boundary and Command Files

For this initialization method, the AGM module requires a description of the device structure in the form of a Sentaurus Mesh boundary file and command file. From the boundary file, the geometric structure is taken; while in the command file, doping profiles and refinement information are defined. The boundary file is specified in the `File` section of the device by:

```
File { ... Boundary = "meshing_bnd.tdr" }
```

and the corresponding command file is read. All refinement statements in the Sentaurus Mesh command file are applied (or explicitly disabled by `-UseMeshCommandFileRefinement`).

Initialization From Element Grid File

You need to select `InitializationMethod = FromElementGrid`. In this case, the specified `BoundaryFile` of the `Math` section is assumed to be an element grid file. The grid given in this file is taken as the first simulation mesh of the device. Necessary doping profiles must be contained in the file.

The AGM module extracts from the grid itself some approximating refinement information, which is used if the first adaptive `Solve` statement evaluates whether grid adaptation will be performed.

Extracting Refinement Information

There are alternative approaches to extracting refinement information from the element grid: `ElementSize`, `Laplacian`, and `Gaussian`. They are selected by `Method` in `FromElementGrid`.

The `ElementSize` method tries to approximate the refinement by inspecting explicitly the size of the elements. The refinement stops if a direction-dependent resolution is reached.

The `Laplacian` and `Gaussian` methods try to approximate the point density extracted from the element grid but, in general, they do not approximate the elements directly. Therefore, the generated refinement information is more regular, and the generated grids have, in general, only some sparse similarity to the given grid, leading typically to a large number of vertices. For this reason, the `Laplacian` and `Gaussian` methods are not recommended.

Parameters Affecting Initialization From Element Grid

The parameters affecting the structure initialization from the element grid are specified in `FromElementGrid`:

■ `ElementSize`: Specifies the parameters for the `ElementSize` method:

•　`Resolution`: Specifies the size (in μm) per direction when refinement stops. This allows you to avoid refinement to artificially small elements in the approximated grid.

■ `Gaussian`: Specifies the parameters for the `Gaussian` method:

•　`Alpha`: Determines the density of the approximating grid (larger than or equal to `1.`). Small values lead to coarser grids.

■ `Method`: Selects the method approximating the given grid. The alternatives are `ElementSize`, `Laplacian`, and `Gaussian`.

> **NOTE**　The meshing parameters `AxisAligned2d` and `AxisAligned3d` have an explicit impact on refinement information (see Parameters Affecting Meshing Engine on page 998). The meshing parameters `Delaunizer2d` and `Delaunizer3d` do not affect refinement information directly, but they are taken into account when building the simulation grid.

Example

```
GridAdaptation ( ...
   Meshing ( ...
      InitializeMethod=FromElementGrid
      FromElementGrid (
         Method=ElementSize
         ElementSize ( Resolution = ( 1.e-4 1.e-4 1.e-4 ) )
         Gaussian ( Alpha=1. )
      )
   )
)
```

Device Adaptation Parameters

There are parameters that affect the grid generation process or the device-specific smoothing process.

Parameters Affecting Grid Generation

The following device parameters are supported:

- `MaxCLoops`: Determines the maximum number of adaptations of this instance within one coupled adaptation.
- `Weights`: Modifies the AGM dissipation rate (see Eq. 1171, p. 992) of the instance used in the adaptation criteria. The keywords `eCurrent`, `hCurrent`, and `Recombination` refer to the weights $\hat{w}_n$, $\hat{w}_p$, and $\hat{w}_r$, respectively; while `Avalanche`, for example, refers to the corresponding weight of the avalanche generation in R_{abs}. By default, all weights are 1.

Example

```
GridAdaptation ( ...
   MaxCLoops = 5
   Weights ( eCurrent=1.e-2 hCurrent=1.e-1 Recombination=1.e-3 Avalanche=1. )
)
```

Parameters Affecting Smoothing

The following parameters influence device-specific data smoothing:

- `Poisson`: Uses the electrostatic potential correction (EPC) procedure.
- `Smooth`: Uses the node block Jacobi iteration (NBJI) procedure.
- `AvaHomotopy`: Uses the avalanche homotopy procedure. You can change to some extent its behavior, as it takes the following parameters:

  - `Iterations`: Sets the number of iterations for the Newton algorithms used during its application (internally, this number is multiplied by 5).

  - `LinearParametrization`: Uses a linear parameterization of the homotopy parameter.

  - `Extrapolate`: Allows extrapolation during avalanche homotopy.

  - `Off`: Switches off avalanche homotopy.

Example

```
GridAdaptation ( ...
   * parameters affecting recomputation
   Poisson          * use electrostatic potential correction (EPC)
   Smooth           * use node block Jacobi iteration (NBJI)
   AvaHomotopy ( -Off Iterations=5 LinearParametrization Extrapolate )
)
```

Parameters Affecting Meshing Engine

Several parameters are passed to the meshing engine, which are collected in the `Meshing` section. Within this section, you have the following parameters:

- `AxisAligned2d`: Sets the parameters for the axis-aligned algorithm in two dimensions (quadtree approach). See Table 213 on page 1418 for valid options, and refer to the *Sentaurus™ Mesh User Guide* for their definitions.

- `AxisAligned3d`: Sets the parameters for the axis-aligned algorithm in three dimensions (octree approach). See Table 213 for valid options, and refer to the *Sentaurus™ Mesh User Guide* for their definitions.

- `Delaunizer2d`: Sets the parameters for the delaunizer of the meshing engine in two dimensions. See Table 219 on page 1420 for valid options, and refer to the *Sentaurus™ Mesh User Guide* for their definitions.

- `Delaunizer3d`: Sets the parameters for the delaunizer of the meshing engine in three dimensions. See Table 219 for valid options, and refer to the *Sentaurus™ Mesh User Guide* for their definitions.

- `InitializationMethod`: Selects the mode to initialize the AGM module, that is, either the default `FromBoundaryAndCommand` or `FromElementGrid`.

- `UseMeshCommandFileRefinement`: Uses the refinement specification in the mesh command file to generate the initial grid if `FromBoundaryAndCommand` is used. Default is true.

Example

```
GridAdaptation ( ...
   Meshing ( ...
      InitializationMethod=FromBoundaryAndCommand
      UseMeshCommandFileRefinement
      AxisAligned2d ( ... MaxNeighborRatio=1.e6 )
      AxisAligned3d ( Smoothing )
      Delaunizer2d ( MaxAngle=165. )
      Delaunizer3d ( MaxSolidAngle=360. )
   )
)
```

Adaptation Criteria

The adaptation criteria are listed in the device-specific `GridAdaptation` section (see Command File Example on page 1005 and Table 222 on page 1421). Several types of adaptation criteria are available. The adaptation criteria are applied to the leaf elements of the actual refinement tree and decide individually if the leaf element must be refined. A leaf

element is refined if one criterion decides to refine it, that is, the adaptation criteria are combined by the Boolean *OR* operation.

Global Adaptation Constraints

The adaptation of the mesh can be disabled, based on the number of leaf elements to be refined, using `ElementLimit`. Let N_{leaf} be the actual number of leaf elements of the refinement tree and N_{adapt} be the number of leaf elements marked for adaptation (based on the adaptation criteria), then adaptation is disabled if:

$$N_{\text{adapt}} \leq C_{\text{Fraction}} \cdot N_{\text{leaf}} + C_{\text{Ignore}} \tag{1173}$$

where C_{Fraction} and C_{Ignore} are user-defined parameters.

To prevent artefacts at low numbers of leaf elements and to avoid adaptation at large numbers of leaf elements, you can restrict the application of the element limit to a range for N_{leaf} by using the parameters `Minimum` and `Maximum`. For example:

```
GridAdaptation ( ...
   ElementLimit (  * trigger adaptation using number of marked leaf elements
      Fraction = 1.e-4   * fraction of number of (total) leaf elements
      Ignore = 0         * absolute number of leaf elements
      Minimum = 1.e3     * apply for number of leaf elements above bound
      Maximum = 1.e5     * apply for number of leaf elements below bound
   )
)
```

Parameters Common to All Refinement Criteria

The following parameters are common for all refinement criteria (see also Table 215 on page 1419). Observe that some of the parameters can be ramped in quasistationary simulations (see Rampable Adaptation Parameters on page 1005):

- `MaxElementSize`: The maximal-allowed edge length in axis directions.

- `MinElementSize`: The minimal-allowed edge length in axis directions.

- `MeshDomain`: This allows you to reference to a spatial domain where the criterion will be applied. The domains are defined in the `Math` section as described below.

- `RefinementScale`: Defines a real-valued value s that limits adaptation within one coupled adaptation iteration to refinement boxes that are large compared to the actual refinement tree. That is, axis-aligned refinement boxes (of size b_i in axis-direction i) are only refined if $s \cdot b_i$ is greater than the minimum size of overlapping leaf elements of the refinement tree. Larger values of s lead to more refinement per adaptation iteration.

Example

```
GridAdaptation ( ...
    Criterion "c1"( ... )
    Criterion "c2"( ... )
)
```

Criterion Type: Element

A given vertex-based scalar quantity must fulfill the condition:

$$|a_1 - a_2| < \varepsilon_R \varepsilon_A \tag{1174}$$

where a_1 and a_2 are the quantity values at the vertices of each element edge.

If the logarithmic scale is selected, the following condition must be fulfilled:

$$|\text{sign}(a_1)\ln(\max(|a_1|/\varepsilon_A, 1)) - \text{sign}(a_2)\ln(\max(|a_2|/\varepsilon_A, 1))| < \ln(\varepsilon_R) \tag{1175}$$

This condition simplifies for values larger than ε_A to $|\ln(a_1) - \ln(a_2)| < \ln(\varepsilon_R)$ and accounts for smaller values and even negative values in a suitable fashion.

Parameters

In addition to the general criterion parameters (see Table 215 on page 1419), the following options are supported (see also Table 216 on page 1419):

■ `DataName`: Selects the physical vertex-based quantity.

■ `AbsError`: The parameter ε_A in both the linear and logarithmic condition above.

■ `Logarithmic`: Uses the logarithmic condition.

■ `RelError`: The parameter ε_R in both the linear and logarithmic condition above.

Example

```
Criterion "c1" (
    Type = Element                      * criterion type
    DataName = "DopingConcentration"    * considered quantity
    Logarithmic                         * select logarithmic scale
    AbsError = 1.e14                    * ignore values below given value
    RelError=10.                        * error bound (10. means each decade)
    MaxElementSize = ( 0.1 0.2 )        * maximal edge length in axis direction
    MinElementSize = ( 1.e-2 1.e-3 )    * minimal edge length in axis direction
    MeshDomain = "md1"                  * "md1" defined in Math
)
```

Criterion Type: Integral0

This criterion type refines elements with large integral values of a user-defined density-like quantity. An axis-aligned refinement box B is not refined if:

$$B f_B^p < B_0 f_0^p \qquad (1176)$$

where:

- f_B is the maximal value of quantity f within refinement box B.
- B is the volume of the axis-aligned refinement box.
- B_0 is a user-definable reference volume.
- f_0 is the reference value of quantity f, computed from the integral average within a user-definable range.
- p is a positive number.

Some remarks:

- For nonpositive functions the absolute modulus is considered.
- The power p allows you to scale the element size according powers of the local value of quantity f.
- The refinement direction is given by (and restricted to) the gradient of the quantity f, leading to anisotropic refinement. You might choose some kind of scaled isotropic refinement (see the `IsotropicRefinement` parameter).

Parameters

The criterion has the following specific parameters (see Table 217 on page 1419):

- `DataName`: The considered vertex-based quantity f.
- `QuantityPower`: Defines the power value p for quantity f.
- `ReferenceElementSize`: Specifies for each axis-direction i a size d_i (in µm) that defines the reference volume $B_0 = d_1 \cdot \ldots \cdot d_d$.
- `ReferenceQuantityRange`: Defines a range for the reference value f_0 (in units of the quantity f).
- `IsotropicRefinement`: Refines the refinement box B isotropically. This means that the box is preferably refined in axis-direction i with the largest ratio b_i / d_i, where b_i is the box size in direction i, and d_i is the corresponding size given by `ReferenceElementSize`.

Example

```
Criterion "c1" (
   Type = Integral0
   DataName = "eDensity"
   QuantityPower = 0.5
   ReferenceElementSize = (0.1 0.2 0.1)
   ReferenceQuantityRange = ( 1.e15 1e17 )
)
```

Criterion Type: Residual

This criterion estimates an error for the integral of the AGM dissipation rate density over the specified mesh domain. The mesh is not refined if the condition:

$$\eta < \varepsilon_R (D + \varepsilon_A) \tag{1177}$$

is fulfilled, where η is the sum of the element error estimators of the AGM dissipation rate in the definition domain.

Parameters

Besides the general criterion parameters (see Table 215 on page 1419), the following parameters are supported (see also Table 218 on page 1420):

- `AbsError`: The parameter ε_A in the condition above.

- `RelError`: The parameter ε_R in the condition above.

Example

```
Criterion "c1" (
   Type = Residual          * criterion type
   AbsError = 1.e-5         * global lower bound (units of dissipation rate)
   RelError = 1.e-1         * global relative error
   MaxElementSize = (0.1 0.2)
   MinElementSize = (1.e-2 1.e-3)
   MeshDomain = "semi"      * restrict to mesh domain
)
```

Mesh Domains

Mesh domains describe a geometric location of the simulation domain and are specified in the `Math` section of the instance. They are given as the union or intersection of a list of some basic mesh domain descriptions or other mesh domains, and are used to describe the definition domain of the refinement criteria.

Parameters

The available parameters are (see also Table 225 on page 1423):

- `Type`: Specifies which operation is applied to the list of spatial domains. You can select either union or intersection by specifying `Cup` or `Cap`, respectively. Building the union is the default operation.

- `Region`: The spatial domain covered by the region.

- `Box`: Defines an axis-aligned box by specifying minimum and maximum coordinates.

- `MeshDomain`: Another mesh domain defined before.

Example

```
Math { ...
   * mesh domain "semi" is the union of specified regions
   MeshDomain "semi" ( Region="bulk" Region="R2" )
   * mesh domain "channel" is intersection of the mesh domain "semi"
   * and the specified box
   MeshDomain "channel" (
      Type=Cap MeshDomain="semi" Box((-5 1.e-5 0.) (5 1.e-3 1.)) )
}
```

Adaptive Solve Statements

Grid adaptation is only performed for explicitly adaptive solve statements using the keyword `GridAdaptation`. Only the highest level `Coupled` and `Quasistationary` solve statements can be adaptive.

General Adaptive Solve Statements

The following parameter entries are interpreted by all adaptive solve statements:

- `MaxCLoops`: Sets maximal number of adaptation iterations per adaptive coupled system (default is 100 000).

- `Plot`: Enables device plots for all intermediate device grids.

- `CurrentPlot`: Enables plotting to current file after each coupled adaptation.

Adaptive Coupled Solve Statements

A `Coupled` solve statement can be adaptive if it is the highest level solve statement, and it can look like:

```
Coupled ( ... GridAdaptation ( MaxCLoops = 5 ) )
   { Poisson Electron Hole }
```

Adaptive Quasistationary Solve Statements

In the current implementation, a `Quasistationary` can be adaptive only if (a) it is the highest level solve statement, and (b) its system consists of a `Coupled` solve statement, that is, `Plugin` statements are not yet supported.

In adaptive quasistationary simulations, it may be useful to restrict the adaptation to certain ranges of the ramped parameter. This can be achieved by specifying parameter ranges or iteration numbers in a similar fashion as in `Plot` in solve statements using the `Time`, `IterationStep`, and `Iterations` keywords, for example.

Parameters

Besides the parameters for all adaptive solve statements, you can provide:

- `Iterations`: Adapts at specific iterations of the ramping process.
- `IterationStep`: Adapts only after a specified number of iterations.
- `Time`: Adapts if the ramping parameter falls into given ranges.

Example

```
Quasistationary ( ...
   GridAdaptation ( ...
      IterationStep = 10
      Iterations = ( 2 ; 7 )
      Time = ( Range = ( 0.2 0.4 ) ; range = (0. 1.)
         intervals = 5 ; 0.1 ; 0.99 )
   )
) { ... }
```

The fixed times specified by `Time` do not force adaptation at these values (which can be achieved by other methods, for example, adding plot statements for the required parameter values).

Performing Adaptive Simulations

Rampable Adaptation Parameters

Some of the criteria parameters can be ramped in quasistationary `Goal` statements. So far, this set includes the values given by `MaxElementSize`, `MinElementSize`, `AbsError`, and `RelError`. You have to refer to these parameters by their full qualified name.

Example

```
GridAdaptation ( ...
   Criterion "c1" ( Type = Element MaxElementSize = ( 0.1 0.2 ) ... )
)
Solve { ...
   Quasistationary ( ...
      Goal ( ModelParameter="AGM/Criterion(c1)/AbsError" Value=1.e12 )
      Goal ( ModelParameter="AGM/Criterion(c1)/MaxElementSize[0]"
             Value=1.e-2 )
   ) { ... }
}
```

Command File Example

The following example excerpt of a command file illustrates the adaptation specification:

```
File { ...
   * device structure input
   * (and implicit corresponding mesh command file)
   Boundary = "meshing_bnd.tdr"        * input boundary file
   Grid     = "./DIR-n2/n2_grid_des"   * used as OUTPUT base name
}
Math { ...
   MeshDomain "semi" ( Region="R1" Region="R2" )
}
GridAdaptation (                   * device-specific adaptation parameters
   MaxCLoops = 5                   * max number of adaptations per adaptive Coupled

   * recomputation parameters
   Poisson                         * perform electrostatic potential correction
   Smooth                          * perform node block Jacobi iteration
   AvaHomotopy ( Iterations=5 )
```

```
      * refine on doping concentration
      Criterion "c1" ( Type=Element DataName="DopingConcentration"
        AbsError=1.e12 RelError=10. Logarithmic
        MaxElementSize=(0.1 0.1) MinElementSize=(1.e-2 1.e-2)
        MeshDomain="semi"
      )
  )
  Solve {
    Coupled { Poisson Electron Hole }   * compute solution on initial grid

    * ramp goals of interest with adaptation
    Quasistationary ( ...
      GridAdaptation                    * adaptive quasistationary
    ) { Coupled { Poisson Electron Hole } }
  }
  Plot { ...
    AGMDissipationRate AGMDissipationRateDensity
    GradAGMDissipationRateDensity/Vector
    AGMDissipationRateAbsJump          * error estimator of residual criterion
  }
```

Limitations and Recommendations

Limitations

The grid adaptation approach implemented in Sentaurus Device has been developed for the drift-diffusion model and 2D quadtree-based simulation grids. For convenience, the approach has been formally extended to support other transport models and features available in Sentaurus Device, that is, AGM is formally compatible with the drift-diffusion, thermodynamic, and hydrodynamic transport models.

Nevertheless, it must be noted that AGM has been applied, so far, only to the drift-diffusion model and silicon devices. Total incompatibility is to be expected with the Schrödinger equation solver, heterostructures, interface conditions, and LED equations. These incompatibilities are only partially checked after command file parsing.

Recommendations

Initial Grid Construction

Using the structure initialization from the boundary and command files, the very first initial grid is constructed applying the refinement information from the mesh command file (assuming `UseMeshCommandFileRefinement` is true).

If `UseMeshCommandFileRefinement` is disabled, the initial grid consists essentially only of boundary vertices. To construct in the later case a realistic initial grid, some artificial quasistationary may be necessary, which ramps the criteria parameters such that these become effective.

Accuracy of Terminal Currents as Adaptation Goal

The choice of appropriate adaptation criteria depends on the adaptation goal. In most adaptive simulation procedures, the local discretization errors are used as adaptation criteria. This approach is not practicable for device simulation as the criteria lead to overwhelmingly large grid sizes. The residual adaptation criterion for the functional `AGMDissipationRate` aims for accurate computations of the device terminal currents, a minimal requirement for all simulation cases, allowing in principle some unresolved solution layers, which do not contribute to the terminal current computation.

AGM Simulation Times

Each coupled adaptation iteration requires remarkable simulation time. In contrast to linear or easy-to-solve problems, for device simulation, most time is consumed in the recomputation procedure of the solution due to the extreme nonlinearities of the problem and not in the pure adaptation of the grid.

The most time-consuming parts in many AGM simulations are (in order of importance):

1. Avalanche homotopy if the computation for $t = 1$ fails to converge (can be very expensive).

2. NBJI smoothing step (for large grid sizes).

3. EPC smoothing step.

4. Grid generation.

Large Grid Sizes

The low convergence order of the discretization causes relatively large grid sizes even for low accuracy requirements. Especially in the vicinity of solution layers and singularities, the point density is difficult to control.

To avoid such problems, increase `MinElementSize` for the responsible criterion: Elements that reach the allowed minimal edge length are no longer refined, and their local error does not contribute to the global error used in the adaptation decision. Therefore, realistic minimal element sizes stop refinement in singularities and layers.

Convergence Problems After Adaptation

It has been observed that, for very coarse simulation grids, the recomputation procedure shows convergence problems. Such problems can be solved by using slightly refined initial grids or by refining the coarsest possible grid (reduce `MaxElementSize` in refinement criteria).

AGM and Extrapolation

After adaptation within a quasistationary, extrapolation is not possible and the parameter step size may decrease. Extrapolation is supported as soon as two consecutive solutions are computed on the same mesh.

3D Grid Adaptation

The 3D grid adaptation has been formally integrated and tested for very simple test structures. However, for realistic structures, the implementation has not yet been optimized or extensively tested. Therefore, practical 3D grid adaptation is still not possible.

References

[1] B. Schmithüsen, *Grid Adaptation for the Stationary Two-Dimensional Drift-Diffusion Model in Semiconductor Device Simulation*, Series in Microelectronics, vol. 126, Konstanz, Germany: Hartung-Gorre, 2002.

[2] B. Schmithüsen, K. Gärtner, and W. Fichtner, *A Grid Adaptation Procedure for the Stationary 2D Drift-Diffusion Model Based on Local Dissipation Rate Error Estimation: Part I - Background*, Technical Report 2001/02, Integrated Systems Laboratory, ETH, Zurich, Switzerland, December 2001.

[3]   B. Schmithüsen, K. Gärtner, and W. Fichtner, *A Grid Adaptation Procedure for the Stationary 2D Drift-Diffusion Model Based on Local Dissipation Rate Error Estimation: Part II - Examples*, Technical Report 2001/03, Integrated Systems Laboratory, ETH, Zurich, Switzerland, December 2001.

[4]   R. Verfürth, *A Review of A Posteriori Error Estimation and Adaptive Mesh-Refinement Techniques*, Chichester: Wiley Teubner, 1996.

CHAPTER 37 Numeric Methods

This chapter presents some of the numeric methods used in Sentaurus Device.

Discretization

The well-known 'box discretization' [1][2][3] is applied to discretize the partial differential equations (PDEs). This method integrates the PDEs over a test volume such as that shown in Figure 71, which applies the Gaussian theorem and discretizes the resulting terms to a first-order approximation.

Figure 71   Single box for a triangular mesh in two dimensions

In general, box discretization discretizes each PDE of the form:

$$\nabla \cdot \vec{J} + R = 0 \tag{1178}$$

into:

$$\sum_{j \neq i} \kappa_{ij} \cdot j_{ij} + \mu(\Omega_i) \cdot r_i = 0 \tag{1179}$$

with values listed in .

Table 170 Box method parameters: coefficients and control volumes

Dimension	κ_{ij}	$\mu(\Omega_i)$
1D	$1/l_{ij}$	Box length
2D	d_{ij}/l_{ij}	Box area
3D	D_{ij}/l_{ij}	Box volume

In this case, the physical parameters j_{ij} and r_i have the values listed in Table 171, where $B(x) = x/(e^x - 1)$ is the Bernoulli function.

Table 171 Equations

Equation	j_{ij}	r_i
Poisson	$\varepsilon(u_i - u_j)$	$-\rho_i$
Electron continuity	$\mu^n(n_i B(u_i - u_j) - n_j B(u_j - u_i))$	$R_i - G_i + \frac{d}{dt}n_i$
Hole continuity	$\mu^p(p_j B(u_j - u_i) - p_i B(u_i - u_j))$	$R_i - G_i + \frac{d}{dt}p_i$
Temperature	$\kappa(T_i - T_j)$	$H_i - \frac{d}{dt}T_i c_i$

One special feature of Sentaurus Device is that the actual assembly of the nonlinear equations is performed elementwise, that is:

$$\sum_{e \in \text{elements}(i)} \left\{ \left(\sum_{j \in \text{vertices}(e)} \kappa_{ij}^e \cdot j_{ij}^e \right) + \mu(\Omega_i^e) \cdot r_i^e \right\} = 0 \tag{1180}$$

This expression is equivalent to Eq. 1179 but has the advantage that some parameters (such as ε, μ_n, μ_p) can be handled elementwise, which is useful for numeric stability and physical exactness. In the 2D case, the box method coefficients have simple visual values: $\kappa_{ij}^e = d_{ij}^e/l_{ij}$ (see Figure 71 on page 1011). In the 3D case, these values are not trivial.

Extended Precision

Although the coordinates of vertices of a mesh are stored with "double" precision accuracy, Sentaurus Device computes box method coefficients and control volumes, by default, with "long double" extended-precision accuracy. This is especially important for the accurate calculation of box method parameters in meshes that contain sliver elements. The procedure is as follows:

1. Read "double" precision coordinates of the mesh vertices.

2. Convert these coordinates to "long double" extended precision.

3. Compute box method parameters with "long double" extended precision.

4. Convert coefficients and control volumes back to "double" precision.

The extended-precision calculation of box method parameters can be switched off by specifying `-BM_ExtendedPrecision` in the global `Math` section of the command file.

> **NOTE** Extended-precision box method calculations are switched off if the global `Math` section contains either `BoxCoefficientsFromFile`, or `BoxMeasureFromFile`, or `NaturalBoxMethod` (see Saving and Restoring Box Method Coefficients on page 1021).

Box Method Coefficients in 3D Case

This section describes the coefficients of the box method in the 3D case.

Basic Definitions

Delaunay Mesh
A mesh is a *Delaunay mesh* if the interior of the circumsphere (circumcircle for two dimensions) of each element contains no mesh vertices.

Obtuse Element
An element is called *obtuse* if the center of the circumsphere (circumcircle) is outside this element.

Obtuse Face
Let `Pf` be the plane that contains the face `f` of an element. Each plane splits 3D space into two half-spaces `Sf1` and `Sf2`. A face `f` is called *obtuse* if the center of the circumsphere of the element and the element itself lie in different half-spaces `Sf1`, `Sf2`.

> **NOTE** In the 2D case, an obtuse triangle has only one obtuse edge.

> **NOTE** In the 3D case:
>
> • An obtuse prism has only one obtuse face.
>
> • An obtuse tetrahedron has one or two obtuse faces.
>
> • An obtuse pyramid has one, two, or three obtuse faces.

Non-Delaunay Element

An obtuse element is called *non-Delaunay* if the interior of the circumsphere (circumcircle) around this element contains another mesh vertex.

Voronoï Element Center and Voronoï Face Center

Let T be a mesh element. The center circumsphere (circle for two dimensions) around the element T is called the *Voronoï element center V_T*. Let f be the face of the element T. The center circumcircle around the face f is called the *Voronoï face center V_f*.

Voronoï Box and Face of the Voronoï Box

Let v be a vertex of the mesh and let $ev^n (1 \leq n \leq N)$ be the set of edges connected to vertex v. Let P_{ev}^n be the mid-perpendicular plane for the edge ev^n. The plane P_{ev}^n splits 3D space into two half-spaces. Let S_{ev}^n be the half-space that contains the vertex v. The intersection of all half-spaces S_{ev}^n is called the *Voronoï box B_v* of vertex v. Therefore, the Voronoï box B_v is the convex polyhedron and any face of B_v is a convex polygon that lies in the mid-perpendicular plane P_{ev}^n. This face called the *face of the Voronoï box F_{ev}^n*.

In addition, let $T_v^m (1 \leq m \leq M)$ be the set of elements per vertex v and let $T_{ev}^k (1 \leq k \leq K)$ be the set of elements per edge ev. For the Delaunay mesh, the next two propositions hold:

1. The vertices of the Voronoï box B_v are Voronoï element centers $(V_{T_v^1}, V_{T_v^2}, ..., V_{T_v^M})$.

2. The vertices of the face of the Voronoï box F_{ev}^n are Voronoï element centers $(V_{T_{ev}^1}, V_{T_{ev}^2}, ..., V_{T_{ev}^K})$ (see Figure 72 – Figure 74).

Figure 72   Face of Voronoï box for Delaunay mesh without obtuse elements: view of mid-perpendicular plane at edge *e* with Voronoï element centers V_{T^i} and the Voronoï face center $V_{f^{i,i+1}}$ between elements T^i and T^{i+1}

Figure 73   Element 5 is an obtuse element; the face of the Voronoï box is a polygon $(V_{T^1}, V_{T^2}, V_{T^3}, V_{T^4}, V_{T^5}, V_{T^1})$, and all vertices are Voronoï element centers

Figure 74   Element 5 is a non-Delaunay element; the face of the Voronoï box is a polygon $(V_{T^1}, V_{T^2}, V_{T^3}, R, V_{T^1})$, and vertex R is not a Voronoï element center

Element Intersection Box Method Algorithm

Sentaurus Device uses the element intersection box method algorithm. Let $S_{ev}^{T^i}$ be the area of intersection $F_{ev} \cap T^i$. For example:

1. Not obtuse elements (see Figure 72) or elements T^1, T^2, T^3 in (see Figure 73 and Figure 74):

$$S_{ev}^{T^i} = \mathrm{Area}(m_e, V_{f^{i-1, i}}, V_{T^i}, V_{f^{i, i+1}}, m_e)$$

2. Obtuse elements (see Figure 73 on page 1015):

$$S_{ev}^{T^4} = \text{Area}(m_e, V_{f^{3,4}}, V_{T^4}, V_{T^5}, p, m_e) \text{ and } S_{ev}^{T^5} = \text{Area}(m_e, p, V_{f^{5,1}}, m_e)$$

3. Non-Delaunay elements (see Figure 74 on page 1015):

$$S_{ev}^{T^4} = \text{Area}(m_e, V_{f^{3,4}}, R, p, m_e) \text{ and } S_{ev}^{T^5} = \text{Area}(m_e, p, V_{f^{5,1}}, m_e)$$

Let edge e have vertices $v1$, $v2$. If all elements around this edge are Delaunay elements, then $S_{ev1}^{T^i} = S_{ev2}^{T^i}$. For non-Delaunay elements, $S_{ev1}^{T^i} \neq S_{ev2}^{T^i}$.

The parameters needed for discretization, $\mu(\Omega_i^e)$ and κ_{ij}^e from Eq. 1180, p. 1012, are 2D arrays $\mu(T^i, v)$ and $\kappa(T^i, e)$ ($v \in T^i$ is a vertex of the element, and $e = e(v1, v2)$ is the edge of the element).

The options for computing the box method coefficients are:

■ `AverageBoxMethod`

$$\kappa(T^i, e) = 0.5 \cdot (S_{ev1}^{T^i} + S_{ev2}^{T^i})/(\text{length}(e)) \tag{1181}$$

For non-Delaunay elements, you have the average coefficient value.

■ `NaturalBoxMethod`

$$\kappa(T^i, e) = (S_{ev1}^{T^i})/(\text{length}(e)) \tag{1182}$$

This algorithm has no averaging.

Both algorithms have the same coefficients for the Delaunay mesh. Only one box method algorithm can be activated. After computing the box method coefficients, Sentaurus Device uses these values for computation control volumes $\mu(T^i, v)$ using standard analytic formulas.

Truncated Obtuse Elements

If a mesh has no obtuse elements, you have element-volume conservation for `Measure` values (see Figure 75 on page 1017):

$$\text{Vol}(T^i) = \sum_{v \in T^i} \mu(T^i, v) \tag{1183}$$

Figure 75   Element-volume conservation for mesh without obtuse elements

For a Delaunay mesh, you have total-volume conservation (see Figure 76):

$$V \equiv \sum_i \text{Vol}(T^i) = \sum_i \sum_{v \in T^i} \mu(T^i, v) \equiv V_{\text{BM}} \tag{1184}$$

Figure 76   Total-volume conservation for Delaunay mesh

For a non-Delaunay mesh, you have no even total-volume conservation (see Figure 77 on page 1018):

$$\delta V = abs(V - V_{\text{BM}}) > 0 \tag{1185}$$

Figure 77   Violation of total-volume conservation for non-Delaunay mesh

There are problems for which element-volume conservation is very important (such as optical electronic or diffusion in Sentaurus Process). For these operations, Sentaurus Device has the special option `MixAverageBoxMethod`.

In this case, Sentaurus Device uses `AverageBoxMethod` to compute the coefficients and the algorithm *truncation obtuse elements* to compute the control volumes. Figure 78 shows the difference between the original and truncated Voronoï polygons in the 2D case.

Figure 78   Algorithm truncation obtuse element: (*a*) Voronoï polygons before truncation –
P1(v1,1,2,5,4,v1), P2(v2,1,2,3,v2), P3(v3,3,2,5,6,v3), P4(v4,4,5,6,v4);
(*b*) Voronoï polygons after truncation – P1(v1,1,2,8,6,5,v1), P2(v2,1,2,3,4,v2),
P3(v3,4,3,8,6,7,v3), P4(v4,5,6,7,v4)

For the 3D case, a similar algorithm of truncation is used.

Table 211 on page 1403 lists all the available options for computing box method parameters.

Weighted Box Method Coefficients

The main goal of any space discretization is the generation of a Delaunay mesh. In this case, the box method coefficients are positive and the finite volume scheme [1] (Eq. 1180, p. 1012) is monotone. For a non-Delaunay mesh, the `AverageBoxMethod` coefficients are positive but the order of the approximation of PDEs is less than one. Sentaurus Mesh can use special technology – Delaunay–Voronoï weights – for which the *weighted Voronoï diagram* has no overlap control volume for a non-Delaunay mesh. As a result, the finite volume scheme is monotone and the order of the approximation PDEs is equal to one.

Weighted Points

A weighted point $\tilde{p} = (p, P^2)$ is interpreted as a sphere (circle in two dimensions) with a center p and radius P. The weighted distance between $\tilde{p}$ and $\tilde{x} = (x, X)$ is defined as [4] [5][6]:

$$\|\tilde{p} - \tilde{x}\| = \sqrt{\|p - x\|^2 - P^2 - X^2} \tag{1186}$$

The weighted points $\tilde{p}$ and $\tilde{x}$ are orthogonal if the weighted distance vanishes: $\|\tilde{p} - \tilde{x}\| = 0$.

In the 3D case, any four weighted points have a common orthogonal sphere called an *orthosphere*. Unless the four centers lie in a common plane, the orthosphere is unique and has a finite radius.

In the 2D case, any three weighted points have a common circle called an *orthocircle*. Unless the three centers lie in a common line, the orthocircle is unique and has a finite radius (see Figure 79).

Figure 79   Since the radii of all weighted vertices are positive, their centers lie outside the orthocircle

Weighted Voronoï Diagram

The weighted generalization of the Voronoï diagram is obtained by substituting a weighted vertex for vertices and an orthosphere (orthocircle) for circumspheres (circumcircles).

The weighted bisector plane B_{ij} between $\tilde{p}_i$ and $\tilde{p}_j$ is the locus of points at an equal-weighted distance from $\tilde{p}_i$ and $\tilde{p}_j$. The center of the orthosphere x is the intersection of the bisector planes $x = \bigcap_{i \neq j} B_{ij}$. The weighted middle point m_{ij} between $\tilde{p}_i$ and $\tilde{p}_j$ is the intersection of the segment $[p_i, p_j]$ and the bisector plane B_{ij}. The value m_{ij} is equal to:

$$m_{ij} = \alpha_i p_i + \alpha_j p_j \tag{1187}$$

where:

$$\alpha_i = 0.5\left(1 - \frac{P_i^2 - P_j^2}{\|p_i - p_j\|^2}\right), \ \alpha_j = 1 - \alpha_i \tag{1188}$$

Therefore, the weighted bisector plane B_{ij} is orthogonal to the segment $[p_i, p_j]$ and contains the weighted middle point m_{ij}, which is sufficient to compute the weighted coefficients and control volumes. If the radius $P_i \neq P_j$, the middle point $m_{ij} \neq 0.5(p_i + p_j)$ and the weighted Voronoï diagram has no overlap control volume for non-Delaunay meshes (see Figure 80). This is the main property of the weighted Voronoï diagram.

Figure 80   Two-dimensional non-Delaunay mesh: (*left*) not weighted Voronoï diagram has overlap elements and (*right*) weighted Voronoï diagram has no overlap elements

Sentaurus Process computes the squared radii (P_i^2, plot name: `DelVorWeight` [μm^2]) of the weighted vertices and writes them to a TDR file (see Sentaurus™ Process User Guide, Table 88 on page 742; option `StoreDelaunayWeight`). If the keyword `WeightedVoronoiBox` is specified in the `Math` section of the command file, Sentaurus Device reads the corresponding arrays from a TDR file and computes the weighted coefficients and measure.

Saving and Restoring Box Method Coefficients

Usually, the coefficients needed for discretization are computed inside Sentaurus Device. For experimental purposes, it may be preferred to use externally provided data. `Measure` and `Coefficients` ($\mu^e(\Omega_i)$ and κ^e_{ij} from Eq. 1180, p. 1012) can be stored in, and loaded into and from the debug file. There are two options for element numbering in such files:

- Internal Sentaurus Device numbering with `MeasureCoefficientsDebug` as the debug file name.

- Mesh numbering (from grid file) with `MeasureCoefficients.debug` as the debug file name for this option.

If the keyword `BoxMeasureFromFile` or `BoxCoefficientsFromFile` is specified in the `Math` section and there is file `MeasureCoefficientsDebug` in the simulation directory, Sentaurus Device reads the corresponding arrays from this file.

If the keyword `BoxMeasureFromFile(GrdNumbering)` or the keyword `BoxCoefficientsFromFile(GrdNumbering)` is specified and there is the file `MeasureCoefficients.debug`, Sentaurus Device reads the corresponding arrays from this file. If there are no such debug files but these keywords are specified, Sentaurus Device computes `Measure` and `Coefficients` and writes them in the corresponding file.

The format of the `MeasureCoefficientsDebug` file is as follows. In line `k` of the `Measure` section, the control volume for each element-vertex `j` of element `k` is stored (that is, value `Measure[k][j]`). The numeration of elements and local numeration of vertices inside the element (see Figure 83 on page 1080) correspond to the internal Sentaurus Device numbering.

The `Coefficients` section in this file has a similar format. For example, the `Measure` section in the file can appear as follows:

```
Measure {
   8.719666833501378e-08 4.359833416750702e-08 4.359833416750729e-08
   8.719666833501378e-08 4.359833416750702e-08 4.359833416750729e-08
   ...
}
```

The format of the `MeasureCoefficients.debug` file is different. There are four section: `Info`, `Elem_type`, `Measure`, and `Coefficients`. In line `k` of the `Measure` section, the control volume for each element-vertex `j` of element `k` is stored (that is, value `Measure[k][j]`). The numeration of elements and local numeration of vertices inside the element correspond to the grid file. The `Coefficients` section in the debug file has similar format. For example, the file can look like:

```
Info {
dimension      = 2
```

```
nb_vertices     = 10
nb_grd_elements = 11
nb_des_elements = 7
}

Elem_type {
  point       = 0
  line        = 1
  triangle    = 2
  rectangle   = 3
  tetrahedron = 5
  pyramid     = 6
  prism       = 7
  cuboid      = 8
}


                            Measure { # unit = [um^2]
# grd_elem  des_elem  elem_type
  0  0  2  1.828427124999999e+00 9.142135625000004e-01 9.142135625000002e-01
  1  1  2  4.052251462735666e+00 4.052251462735666e+00 8.104502925471332e+00
  ...
  7    -1    1        # contact or interface
  8    -1    1        # contact or interface
  ...
}


                            Coefficients { # unit = [1]
# grd_elem  des_elem  elem_type
  0  0  2  1.093836321204215e+00 1.100111438811216e-16 2.285533906249999e-01
  1  1  2  0.000000000000000e+00 8.379715512271076e-01 8.379715512271076e-01
  ...
  7    -1    1        # contact or interface
  8    -1    1        # contact or interface
  ...
}
```

Statistics About Non-Delaunay Elements

Information about region non-Delaunay elements and interface non-Delaunay elements is contained in the log file. For more information, see Utilities User Guide, Chapter 4 on page 25.

Region Non-Delaunay Elements

A log file contains common data about the mesh and information about non-Delaunay elements per region (for Delaunay mesh `DeltaVolume=0` and `non-DelaunayVolume=0`):

```
/-------- Region non-Delaunay elements ------------------------------------------------------
 Region        Volume    BoxMethodVolume  DeltaVolume  Elements  non-Delaunay    non-DelaunayVolume
  name         [um2]        [um2]            [%]                   Elements       [um2]      [%]
--------------------------------------------------------------------------------------------
 Nitride   1.9500000e-04  2.2635574e-04    16.080        53        12 (22.64 %)   1.8215e-04 (1.1e-05)
    . . .
 Oxide     6.0618645e-03  8.0705629e-03    33.137        2500     818 (32.72 %)   2.3715e-04 (2.0e-04)
 Silicon   3.5548100e-02  4.9531996e-02    39.338       12656    5057 (39.96 %)   1.0715e-04 (1.0e-05)
 Total     4.6402113e-02  6.4934852e-02    39.939       16550    6383 (38.57 %)   2.9218e-04 (2.1e-05)
\-------------------------------------------------------------------------------------------
```

Interface Non-Delaunay Elements

An *interface element* is an element that has a face (or edge in two dimensions) lying on the interface. A non-Delaunay element is an *interface non-Delaunay element* only if its obtuse face lies on the surface of the interface (see Figure 81).

Figure 81   Blue (1, 2, 3) and green (4, 5, 6) elements are oxide and silicon interface elements, respectively. Elements 2 and 4 are non-Delaunay elements, not interface non-Delaunay elements. Only element 3 is an interface non-Delaunay element.

The following is an example of a log file for interface non-Delaunay elements:

```
   /-------- Interface non Delaunay elements ------------------------------------
    Region1         Elements  non Delaunay    Volume          non Delaunay
    Region2                   Elements         [um2]          DeltaVolume [um2]

    ---------------------------------------------------------------------------
    ...........................................................................
    silicon          3         0 ( 0.00 %)   1.5775139e-03   0.0000000e+00 ( 0.00 %)
    oxide            3         1 ( 33.0 %)   1.6776069e-03   0.1100000e-03 ( 0.10 %)
    ...........................................................................
    Total            6         1 ( 16.0 %)   3.6951838e-02   0.1100000e+00 ( 0.05 %)
   \---------------------------------------------------------------------------
```

Plot Section

Table 172 lists the plot variables that may be useful for visualizing box method statistics (see Scalar Data on page 1340). See Utilities User Guide, Chapter 4 on page 25 for the definitions of these variables.

Table 172   Plot variable for box method data

Plot variable	Location
`BM_AngleElements`	Element
`BM_CoeffIntersectionNonDelaunayElements`	Element
`BM_ElementsWithCommonObtuseFace`	Element
`BM_ElementsWithObtuseFaceOnBoundaryDevice`	Element
`BM_ElementVolume`	Element
`BM_IntersectionNonDelaunayElements`	Element
`BM_VolumeIntersectionNonDelaunayElements`	Element
`BM_wCoeffIntersectionNonDelaunayElements`	Element
`BM_wElementsWithCommonObtuseFace`	Element
`BM_wElementsWithObtuseFaceOnBoundaryDevice`	Element
`BM_wIntersectionNonDelaunayElements`	Element
`BM_wVolumeIntersectionNonDelaunayElements`	Element
`BM_AngleVertex`	Vertex
`BM_EdgesPerVertex`	Vertex
`BM_ElementsPerVertex`	Vertex
`BM_ShortestEdge`	Vertex

AC Simulation

AC simulation is based on small-signal AC analysis. The response of the device to 'small' sinusoidal signals superimposed upon an established DC bias is computed as a function of frequency and DC operating point. Steady-state solution is used to build up a linear algebraic system [7] whose solution provides the real and imaginary parts of the variation of the solution vector $(\phi, n, p, T_n, T_p, T)$ induced by small sinusoidal perturbation at the contacts.

AC Response

The AC response is obtained from the three basic semiconductor equations (see Eq. 37, p. 173 and Eq. 53, p. 181) and from up to three additional energy conservation equations to account for electron, hole, and lattice temperature responses. In the following description of the AC system, the temperatures have been omitted in the solution vector and Jacobian for simplicity, a complete description being formally obtained by adding the temperature responses to the solution vector and the corresponding lines to the system Jacobian.

After discretization, the simplified system of equations can be symbolically represented at the node i of the computation mesh as:

$$F_{\phi i}(\phi, n, p) = 0 \tag{1189}$$

$$F_{ni}(\phi, n, p) = \dot{G}_{ni}(n) \tag{1190}$$

$$F_{pi}(\phi, n, p) = \dot{G}_{pi}(p) \tag{1191}$$

where F and G are nonlinear functions of the vector arguments ϕ, n, p, and the dot denotes time differentiation.

By substituting the vector functions of the form $\xi_{\text{total}} = \xi_{\text{DC}} + \tilde{\xi}e^{i\omega t}$ into Eq. 1189, Eq. 1190, and Eq. 1191 where $\xi = \phi, n, p$, ξ_{DC} is the value of ξ at the DC operating point, and $\tilde{\xi}$ is the corresponding response (or the phasor uniquely identifying the complex perturbation) and then expanding the nonlinear functions F and G in the Taylor series around the DC operating point and keeping only the first-order terms (the small-signal approximation), the AC system of equations at the node i can be written as:

$$\sum_j \begin{bmatrix} \dfrac{\partial F_{\phi i}}{\partial \phi_j} & \dfrac{\partial F_{\phi i}}{\partial n_j} & \dfrac{\partial F_{\phi i}}{\partial p_j} \\[2ex] \dfrac{\partial F_{ni}}{\partial \phi_j} & \dfrac{\partial F_{ni}}{\partial n_j} - i\omega\dfrac{\partial G_{ni}}{\partial n_j} & \dfrac{\partial F_{ni}}{\partial p_j} \\[2ex] \dfrac{\partial F_{pi}}{\partial \phi_j} & \dfrac{\partial F_{pi}}{\partial n_j} & \dfrac{\partial F_{pi}}{\partial p_j} - i\omega\dfrac{\partial G_{pi}}{\partial p_j} \end{bmatrix}_{DC} \begin{bmatrix} \tilde{\phi}_j \\[2ex] \tilde{n}_j \\[2ex] \tilde{p}_j \end{bmatrix} = 0 \tag{1192}$$

where the solution vector is scaled with respect to terminal voltages (at the contact where the voltage is applied, $\tilde{\phi}$ is 1). Therefore, the unit of carrier density responses is $\text{cm}^{-3}\text{V}^{-1}$ and the potential response is unitless.

The matrix of Eq. 1192 differs from the Jacobian of the system of equations Eq. 1189, Eq. 1190, and Eq. 1191 only by pure imaginary additive terms involving derivatives of G with respect to carrier densities.

The global AC matrix system is obtained by imposing the corresponding AC boundary conditions and performing the summation (assembling the global matrix).

Common AC boundary conditions used in AC simulation are Neumann boundary and oxide–semiconductor jump conditions carried over directly from DC simulation; Dirichlet boundary conditions for carrier densities where n and p at Ohmic contacts are $\tilde{n} = \tilde{p} = 0$; and Dirichlet boundary conditions for AC potential at Ohmic contacts that are used to excite the system.

After assembling the global AC matrix and taking into account the boundary conditions, the AC system becomes:

$$[J + iD]\tilde{X} = B \tag{1193}$$

where J is the Jacobian matrix, D contains the contributions of the G functions to the matrix, B is a real vector dependent on the AC voltage drive, and $\tilde{X}$ is the AC solution vector.

By writing the solution vector as $\tilde{X} = X_R + iX_I$ with X_R and X_I the real and imaginary part of the solution vector respectively, the AC system can be rewritten using only real arithmetic as:

$$\begin{bmatrix} J & -D \\ D & J \end{bmatrix} \begin{bmatrix} X_R \\ X_I \end{bmatrix} = \begin{bmatrix} B \\ 0 \end{bmatrix} \tag{1194}$$

The AC response is actually computed by solving the system Eq. 1193 or Eq. 1194.

An `ACPlot` statement in the `ACCoupled` command is used to plot AC responses $(\tilde{\phi}, \tilde{n}, \tilde{p}, \tilde{T}_n, \tilde{T}_p, \tilde{T})$. The responses are plotted in the AC plot file of Sentaurus Device with a separate file for each frequency.

For details of the `ACPlot` statement, see Table 187 on page 1385. For details and examples of small-signal AC analysis, see Small-Signal AC Analysis on page 96.

AC Current Density Responses

When the AC system is solved, the AC current density responses $\vec{\tilde{J}}_D$, $\vec{\tilde{J}}_n$, and $\vec{\tilde{J}}_p$ are computed using:

$$\vec{\tilde{J}}_D = -i\omega\varepsilon\nabla\tilde{\phi} \tag{1195}$$

$$\vec{\tilde{J}}_n = \left.\frac{\partial\vec{J}_n}{\partial\phi}\right|_{DC}\tilde{\phi} + \left.\frac{\partial\vec{J}_n}{\partial n}\right|_{DC}\tilde{n} + \left.\frac{\partial\vec{J}_n}{\partial p}\right|_{DC}\tilde{p} \tag{1196}$$

$$\vec{\tilde{J}}_p = \left.\frac{\partial \vec{J}_p}{\partial \phi}\right|_{DC} \tilde{\phi} + \left.\frac{\partial \vec{J}_p}{\partial p}\right|_{DC} \tilde{p} + \left.\frac{\partial \vec{J}_p}{\partial n}\right|_{DC} \tilde{n} \tag{1197}$$

The unit of current density responses is $\mathrm{Acm}^{-2}\mathrm{V}^{-1}$.

The responses of the heat fluxes for the lattice ($\vec{\tilde{S}}_L$), electrons ($\vec{\tilde{S}}_n$), and holes ($\vec{\tilde{S}}_p$) are analogous. Their unit is $\mathrm{Wcm}^{-2}\mathrm{V}^{-1}$.

The `ACPlot` statement in the `System` section is used to plot the AC current density responses. The responses are added to the AC solution response in the AC plot files of Sentaurus Device.

Harmonic Balance Analysis

Harmonic balance (HB) analysis is a frequency domain method to solve periodic and quasi-periodic time-dependent problems for steady-state solutions [8][9]. It is a popular method for RF circuit design applications. While transient discretization schemes allow the simulation of arbitrary time-dependent problems, HB more efficiently models periodic and quasi-periodic problems for systems with time constants that vary by many orders of magnitude. The detailed command file syntax is given Harmonic Balance on page 101.

Harmonic Balance Equation

In general, the dynamic mixed-mode simulation problem takes the form:

$$\frac{d}{dt}q[r, u(t, r)] + f[r, u(t, r), w(t)] = 0 \tag{1198}$$

where f and q are nonlinear functions, w represents explicitly time-dependent devices (in particular, voltage or current sources), and the function u is the vector of all solution variables.

Let f_1, ..., f_K be a set of different frequencies with $f_k > 0$, then both the sources and the solution are approximated by a truncated Fourier series:

$$u(t) = U_0 + \sum_{1 \le k \le K} \{U_k \exp(i\omega_k t) + U_k^* \exp(-i\omega_k t)\} \tag{1199}$$

A formal Fourier transform of Eq. 1198 results in the HB equation for the problem:

$$L(U) = i\Omega Q(U) + F(U) = 0 \tag{1200}$$

where F and Q are the finite Fourier series of f and q, respectively, Ω is the frequency matrix, and U is the vector of all Fourier coefficients of u.

Multitone Harmonic Balance Analysis

The multitone harmonic balance (HB) analysis makes use of the multidimensional Fourier transformation (MDFT). This means that the problem is mapped onto a problem in a multidimensional frequency and multidimensional time domain, hereby exploiting the equivalence of Fourier spectra of quasi-periodic functions with their corresponding multidimensional functions.

Multidimensional Fourier Transformation

The multidimensional Fourier transformation (MDFT) maps multidimensional functions onto a multidimensional spectrum.

Let M be a positive integer, the number of tones, $\hat{f}_1, \ldots, \hat{f}_M$, be a finite set of different positive numbers, the base frequencies of tones, and $H_1, \ldots, H_M$ nonnegative integer numbers, the maximal number of harmonics for each tone.

Define for each tone m the m-th base period $T_m := 1/\hat{f}_m$, the m-th circular frequency $\omega_m := 2\pi\hat{f}_m$, the m-th (minimum) number of sampling points $S_m := 2H_m + 1$, and the m-th (maximum) sampling interval $\delta_m = T_m/S_m$.

Furthermore, let $\underline{x} = (x_1, \ldots, x_M)^T$ denote the M-dimensional vector, and let $D_{\underline{x}} = \text{diag}(x_1, \ldots, x_M)$ denote the $M \times M$-matrix composed of the values $x_1, \ldots, x_M$.

The set of multi-indices associated with $\underline{H}$ is given by:

$$K := \{\underline{h} \in \mathbf{Z}^M : -H_m \leq h_m \leq H_m \text{ for all } 1 \leq m \leq M\} \tag{1201}$$

Let u^M be a function on the M-dimensional space $\mathbf{C}^M$ given by:

$$u^M(t_1, \ldots, t_M) = \sum_{\underline{h} \in K} U_{\underline{h}}^M \exp(i\underline{h}D_{\underline{\omega}}\underline{t}) \tag{1202}$$

with given complex numbers $U_{\underline{h}}^M$, then:

$$U_{\underline{h}}^M = \frac{1}{T} \int_0^{T_1} \ldots \int_0^{T_M} u^M(t_1, \ldots, t_M) \exp(-i\underline{h}D_{\underline{\omega}}\underline{t}) dt_1 \ldots dt_M \tag{1203}$$

with $T := \Pi_{1 \leq m \leq M} T_m$. $U^M = (U_{\underline{h}}^M)_{\underline{h} \in K}$ is the multidimensional spectrum of u^M.

Sampling the function in all dimensions at the equidistant sampling points $t_{\underline{s}} = D_{\underline{\delta}}\underline{s}(\underline{0} \le \underline{s} < \underline{S})$, the discrete MDFT is written formally as:

$$U^M = \Gamma^M u^M \tag{1204}$$

that is, Γ^M is a linear map from $\boldsymbol{C}^S$ onto $\boldsymbol{C}^S$ where $S := \Pi_{1 \le m \le M} S_m$ is the total number of sampling points.

Quasi-Periodic Functions

The multidimensional function u^M can be projected onto a one-dimensional time space by:

$$u(t) := u^M(t, \ldots, t) = \sum_{\underline{h} \in K} U_{\underline{h}} \exp(i\underline{h}\underline{\omega}t) \tag{1205}$$

Functions satisfying this representation are called quasi-periodic. The set:

$$\Lambda := \{f_{\underline{h}} \in \boldsymbol{R} : f_{\underline{h}} = \underline{h} \cdot \hat{f} \text{ for all } \underline{h} \in K\} \tag{1206}$$

is the spectrum domain associated with f and K (or $\underline{H}$). The projection is invertible if, for two different multi-indices $\underline{h}_1$ and $\underline{h}_2$ in K, the resulting frequencies $f_{\underline{h}_1}$ and $f_{\underline{h}_2}$ are different. Note that the one-dimensional Fourier spectrum of u coincides with the multidimensional spectrum of u^M.

While for the multidimensional function u^M S sample points can be specified to compute the multidimensional spectrum, the one-dimensional sample points for u are not well defined (but are rather virtual in the multidimensional time domain).

Multidimensional Frequency Domain Problem

The multitone HB analysis is essentially a translation of (one-dimensional or multidimensional) time-domain problems in a multidimensional frequency domain. Though originally derived from a time-domain problem, the circuit equations are directly specified in a multidimensional frequency domain. This avoids sampling of (one-dimensional) time-dependent sources, which cannot be performed accurately on a sample set of size S. This is the reason why the compact circuit models must provide the CMI-HB-MDFT function set.

The Fourier transformation of quasi-periodic functions is the composition:

$$\Gamma = \Gamma^M \circ P^{-1} \tag{1207}$$

where Γ^M is the multidimensional Fourier transformation of Eq. 1204 and P^{-1} is the inverse of the projection Eq. 1205.

One-Tone Harmonic Balance Analysis

For one-tone HB analysis, the standard discrete Fourier transformation can be used, which includes that the sampling points are defined explicitly in a (one-dimensional) time domain. Therefore, the problem can be extracted directly from the time-domain formulation of the circuit.

Solving HB Equation

The HB equation (Eq. 1200) is a nonlinear equation in U and is solved by the Newton algorithm. In each Newton step, the linear equation:

$$\frac{\partial L}{\partial U}(U) \cdot \delta U = -L(U) \tag{1208}$$

must be solved.

The Jacobian $\partial L / \partial U$ in Fourier space is computed from the Jacobian in the time domain as follows: For a nonlinear scalar function $g : \boldsymbol{R} \to \boldsymbol{R}$ and a T-periodic scalar signal $u(t)$, the Fourier coefficients $G \in \boldsymbol{C}^S$ of $g(u(t))$ are approximated:

$$G(U) = \Gamma g(\hat{u}) = \Gamma g(\Gamma^{-1} U) \tag{1209}$$

where Γ and Γ^{-1} are the discrete Fourier transform operator and its inverse, $\hat{u}$ is the vector of the time samples $u(t_i)$, and $g(\hat{u})$ is the vector of values $g(u(t_i))$.

The derivatives of the k-th Fourier component G_k with respect to the j-th Fourier component U_j read:

$$\frac{\partial G_k}{\partial U_j}(U) = \sum_l \Gamma_{kl} \frac{\partial g}{\partial U_j}(\hat{u}_l) = \sum_l \Gamma_{kl} \frac{\partial g}{\partial u}(\hat{u}_l) \Gamma_{lj}^{-1} \tag{1210}$$

The corresponding Jacobian is written in the compact form:

$$\frac{\partial G}{\partial U} = \Gamma \hat{J}_u \Gamma^{-1} \text{ with } \hat{J}_u = \frac{\partial g}{\partial u}(\hat{u}) \tag{1211}$$

For scalar functions g and u, $\hat{J}_u$ is a diagonal matrix; for vector-valued functions g and u, $\hat{J}_u$ is a block-diagonal matrix.

Using the notation above, Eq. 1200 becomes:

$$L(U) = i\Omega \Gamma q(\hat{u}(U)) + \Gamma f(\hat{u}(U)) = 0 \tag{1212}$$

and Eq. 1208 for the Newton step takes the form:

$$(i\Omega\Gamma\hat{J}_q\Gamma^{-1} + \Gamma\hat{J}_f\Gamma^{-1})\delta U = -L(U) \tag{1213}$$

The Newton algorithm constructs a sequence U^k of the Fourier coefficients of the time-domain solution vector u. The sequence is regarded as converged if both the residual $|L(U^k)|$ and the update error are small.

Solving HB Newton Step Equation

The memory requirements for storing the HB Jacobian matrix typically become very large, as its size is increased by a factor of S^2 compared to the corresponding DC or transient matrix. For a very small number of harmonics and a moderately sized simulation grid, using a direct linear solver may be feasible. However, the use of the GMRES(m) iterative method is recommended for most applications.

Restarted GMRES Method

The HB module makes use of a preconditioned restarted generalized minimum residual GMRES(m) method [10], a Krylow subspace method, which does not need to store the Jacobian in memory, as only matrix-vector products have to be computed.

GMRES(m) requires a suitable preconditioner to achieve convergence. A (left) preconditioner P is a matrix that approximates a given matrix A, but is much easier to invert than A itself. Instead of solving the linear equation $Ax = b$ for given A and b, the (left) preconditioned problem $P^{-1}Ax = P^{-1}b$ is solved. The preconditioner used for HB [11] takes the form:

$$P = i\Omega\begin{bmatrix} \bar{J}_q & & 0 \\ & ... & \\ 0 & & \bar{J}_q \end{bmatrix} + \begin{bmatrix} \bar{J}_f & & 0 \\ & ... & \\ 0 & & \bar{J}_f \end{bmatrix} \tag{1214}$$

where the matrix $\bar{J}_f$, and similarly $\bar{J}_q$, is computed as:

$$\bar{J}_f = \frac{1}{S} \sum_{0 \le s \le S-1} J_f(t_s) \tag{1215}$$

and J_f denotes the Jacobian of f with respect to u. The preconditioner equals the HB Jacobian in the limit of small signals, where the coupling terms between the frequencies vanish. Therefore, each diagonal block of P corresponds to the AC matrix for the respective harmonic. This preconditioner is well suited to 'moderately large' signal applications.

The preconditioner can be computed without an explicit Fourier transform, and its inversion is more economical than for the full Jacobian. The inversion is performed by applying a complex direct solver for each harmonic component separately, thereby requiring the computational costs of solving $(S + 1)/2$ complex-valued linear systems. The computational complexity is of the order $O(S)$ for inverting the preconditioner, and $O(S\ln(S))$ for one complete iteration step of the iterative solver, while the number of iterations necessary to achieve convergence is unknown (but bounded).

Direct Solver Method

For the direct solver, the complex-valued $S \times S$ linear system (Eq. 1213) is transformed to a $S \times S$ real-valued problem, which is possible as only real-valued functions are involved. The resulting linear system is solved by the direct solver PARDISO. The direct solver requires the entire matrix stored in memory. Therefore, the memory capacity is easily exceeded for increasing S. Additionally, the computational complexity is of the order $O(S^3)$.

Transient Simulation

Transient equations used in semiconductor device models and circuit analysis can be formally written as a set of ordinary differential equations:

$$\frac{d}{dt}q(z(t)) + f(t, z(t)) \;=\; 0 \tag{1216}$$

which can be mapped to the DC and transient parts of the PDEs.

Sentaurus Device uses implicit discretization of transient equations (see Eq. 1216) and supports two discretization schemes: simple backward Euler (BE) and composite trapezoidal rule/backward differentiation formula (TRBDF), which is the default.

Backward Euler Method

Backward Euler is a very stable method, but it has only a first-order of approximation over time-step h_n. The discretization can be written as:

$$q(t_n + h_n) + h_n f(t_n + h_n) \;=\; q(t_n) \tag{1217}$$

The local truncation error (LTE) estimation is based on the comparison of the obtained solution $q(t_n + h_n)$ with the linear extrapolation from the previous time-step.

The extrapolated solution is written as:

$$q^{\mathrm{extr}} = q(t_n) - \frac{f(t_n) + f(t_n + h_n)}{2} h_n \qquad (1218)$$

Then, in every point, the relative error can be estimated as $(q(t_n + h_n) - q^{\mathrm{extr}})/q(t_n + h_n)$.

Using Eq. 1217 and Eq. 1218, and estimating the norm of relative error, Sentaurus Device computes the value:

$$r = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left(\frac{f(t_n + h_n) - f(t_n)}{\varepsilon_{\mathrm{R,tr}} |q_n(t_n + h_n)| + \varepsilon_{\mathrm{A,tr}}} h_n \right)^2} \qquad (1219)$$

where the sum is taken over all unknowns (that is, all free vertices of all equations), and $\varepsilon_{\mathrm{R,tr}}$ and $\varepsilon_{\mathrm{A,tr}}$ are the relative and absolute transient errors, respectively.

The next time-step is estimated as:

$$h_{\mathrm{est}} = h_n r^{-1/2} \qquad (1220)$$

The value of the estimated time-step is used for h_{n+1} computation (see Controlling Transient Simulations on page 1034).

TRBDF Composite Method

The transient scheme [12] for the approximation of Eq. 1216 is briefly reviewed in this section. From each time point t_n, the next time point $t_n + h_n$ (h_n is the current step size) is not directly reached. Instead, a step in between to $t_n + \gamma h_n$ is made. This improves the accuracy of the method. $\gamma = 2 - \sqrt{2}$ has been shown to be the optimal value. Using this, two nonlinear systems are reached.

For the trapezoidal rule (TR) step:

$$2q(t_n + \gamma h_n) + \gamma h_n f(t_n + \gamma h_n) = 2q(t_n) - \gamma h_n f(t_n) \qquad (1221)$$

and for the BDF2 step:

$$(2 - \gamma)q(t_n + h_n) + (1 - \gamma)h_n f(t_n + h_n) = (1/\gamma)(q(t_n + \gamma h_n) - (1 - \gamma)^2 q(t_n)) \qquad (1222)$$

The local truncation error (LTE) is estimated after such a double step as:

$$\tau = \left[\frac{f(t_n)}{\gamma} - \frac{f(t_n + \gamma h_n)}{\gamma(1-\gamma)} + \frac{f(t_n + h_n)}{1-\gamma} \right] \tag{1223}$$

$$C = \frac{-3\gamma^2 + 4\gamma - 2}{12(2-\gamma)} \tag{1224}$$

Sentaurus Device then computes the following value from this:

$$r = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left(\frac{\tau_i}{\varepsilon_{R,tr} |q_n(t_n + h_n)| + \varepsilon_{A,tr}} \right)^2} \tag{1225}$$

where the sum is taken over all unknowns (that is, all free vertices of all equations), and $\varepsilon_{R,tr}$ and $\varepsilon_{A,tr}$ are the relative and absolute transient errors, respectively. Since the TRBDF method has a second-order approximation over h_n, the next step can be estimated as:

$$h_{est} = h_n r^{-1/3} \tag{1226}$$

The value of the estimated time-step is used for h_{n+1} computation (see Controlling Transient Simulations on page 1034).

Controlling Transient Simulations

By default, Sentaurus Device uses the TRBDF method. To switch to backward Euler (BE), the statement `Transient=BE` must be specified in the `Math` section.

To evaluate whether a time-step was successful and to provide an estimate for the next step size, the following rules are applied:

- If one of the nonlinear systems cannot be solved, the step is refused and tried again with $h_n = 0.5 \cdot h_n$.
- Otherwise, the inequality $r < 2f_{rej}$ is tested. If it is fulfilled, the transient simulation proceeds with $h_{n+1} = h_{est}$. Otherwise, the step is re-tried with $h_n = 0.9 \cdot h_{est}$.
- The LTE is checked only if the `CheckTransientError` option is selected; otherwise, the selection of the next time-step is based only on convergence of nonlinear iterations.

To activate LTE evaluation and time-step control, `CheckTransientError` must be specified either globally (in the `Math` section) or locally as an option in the `Transient` statement. The keyword `NoCheckTransientError` disables time-step control. The value of the relative error is defined by the parameter `TransientDigits` according to Eq. 14, p. 88.

Absolute error is given by the keyword `TransientError` or recomputed from `TransientErrRef` ($x_{\mathrm{ref,tr}}$) using Eq. 15, p. 89 (if `RelErrControl` is switched on). Sentaurus Device provides the default values of $\varepsilon_{\mathrm{R,tr}}$, $\varepsilon_{\mathrm{A,tr}}$, and $x_{\mathrm{ref,tr}}$. The coefficient f_{rej} is equal to 1 by default. You can define the values of $\varepsilon_{\mathrm{R,tr}}$, $\varepsilon_{\mathrm{A,tr}}$, $x_{\mathrm{ref,tr}}$, and f_{rej} globally in the `Math` section, or specify them as options in the `Transient` statement. In the latter case, it overwrites the default and `Math` specifications for this command.

Floating Gates

During a transient time step, the charge Q of a floating gate is updated as a function of the injection current i:

$$\Delta Q = \int_{t_1}^{t_2} i(t)\,dt \tag{1227}$$

ΔQ represents the charge increase for the time step $[t_1, t_2]$.

Because the floating-gate charge is not updated self-consistently during a transient step, but only as a postprocessing operation, the numeric update is given by:

$$\Delta Q = i(t_1) \cdot \Delta t \tag{1228}$$

where $\Delta t = t_2 - t_1$. The error of this numeric approximation is estimated by:

$$\Delta Q_{\mathrm{error}} = \frac{|i(t_2) - i(t_1)|}{2} \Delta t \tag{1229}$$

With the option `CheckTransientError`, the error $\Delta Q_{\mathrm{error}}$ in the charge update is monitored as well. In the case of relative error control (`RelErrControl`), a transient step is only accepted if the following condition holds:

$$\frac{\Delta Q_{\mathrm{error}}}{10^{-\mathtt{Digits}}(|Q| + \mathtt{ErrRef})} < 1 \tag{1230}$$

The values of `Digits` and `ErrRef` can be specified in the `Math` section:

```
Math {
   TransientDigits = 3
   TransientErrRef (Charge) = 1.602192e-19
}
```

In the case of absolute error control (`-RelErrControl`), a transient step is only accepted if the following condition holds:

$$\frac{\dfrac{\Delta Q_{\text{error}}}{q}}{10^{-\texttt{Digits}}\dfrac{|Q|}{q} + \texttt{Error}} < 1 \tag{1231}$$

The electron charge $q = 1.602192 \cdot 10^{-19}\text{C}$ is used as a scaling factor. The values of `Digits` and `Error` can be specified in the `Math` section:

```
Math {
   TransientDigits = 3
   TransientError (Charge) = 1e-3
}
```

Note that the values of `ErrRef` and `Error` are related by the equation:

$$\texttt{ErrRef} = \frac{\texttt{Error}}{10^{-\texttt{Digits}}}q \tag{1232}$$

Nonlinear Solvers

In the next two sections, the `Digits` variable corresponds to the keyword `Digits`, which can be given in the `Math` section (see Convergence and Error Control on page 137), or in parentheses of each `Plugin` or `Coupled` statement.

Fully Coupled Solution

For the solution of nonlinear systems, the scheme developed by Bank and Rose [13] is applied. This scheme tries to solve the nonlinear system $g(z) = 0$ by the Newton method:

$$\vec{g} + \vec{g'}\vec{x} = 0 \tag{1233}$$

$$\vec{z}^{j} - \vec{z}^{j+1} = \lambda\vec{x} \tag{1234}$$

where λ is selected such that $\|g_{k+1}\| < \|g_k\|$, but is as close as possible to 1. Sentaurus Device handles the error by computing an error function that can be defined by two methods.

The Newton iterations stop if the convergence criteria are fulfilled. One convergence criterion is the norm of the right-hand side, that is, $\|g\|$ in Eq. 1233. Another natural criterion may be the relative error of the variables measured, such as $\left\|\dfrac{(\lambda x)}{z}\right\|$.

Figure 82   Newton iteration

Conversely, for very small z updates, λx must be measured with respect to some reference value of the variable z_{ref}. The formula used in Sentaurus Device as the second convergence criterion is:

$$\frac{1}{\varepsilon_R}\frac{1}{N}\sum_{e,\,i}\frac{|z(e,i,j) - z(e,i,j-1)|}{|z(e,i,j)| + z_{\text{ref}}(e)} < 1 \tag{1235}$$

where $z(e,i,j)$ is the solution of the equation e (Poisson, electron, hole, and so on) at node i after Newton iteration j. The constant N is given by the total number of nodes multiplied by the total number of equations. The parameter ε_R is the relative error criterion.

The value of $\varepsilon_R = 10^{-\texttt{Digits}}$ is set by specifying the following in the `Math` section:

```
Math{...
   Digits = 5
}
```

where 5 is the default for `Digits`. The reference values $z_{\text{ref}}(e)$ ensure numeric stability even for cases when $z(e,i,j)$ is zero or very small. This error condition ensures that the respective equations are solved to an accuracy of approximately $z_{\text{ref}}(e)\varepsilon_R$.

Eq. 1235 can be written in the symbolic form:

$$\frac{1}{\varepsilon_R}\left\|\frac{\lambda x}{z^j + z_{\text{ref}}}\right\| < 1 \tag{1236}$$

Eq. 1236 can also be rewritten in the equivalent form:

$$\left\| \frac{\lambda \bar{x}}{\varepsilon_R \bar{z}^j + \varepsilon_A} \right\| < 1 \tag{1237}$$

where $\bar{z}^j = z^j / z^*$ and $\bar{x} = x / z^*$.

z^* is the normalization factor (for example, it is the intrinsic carrier density $n_i = 1.48 \times 10^{10} \, \text{cm}^{-3}$ for electron and hole equations, and the thermal voltage $u_{T0} = 25.8 \, \text{mV}$ for the Poisson equation).

The absolute error is related to the relative error through:

$$\varepsilon_A = \varepsilon_R \frac{z_{ref}}{z^*} \tag{1238}$$

Sentaurus Device supports two schemes for controlling the error conditions. The default scheme is based on Eq. 1235. The default values for the parameters z_{ref} are listed in Table 191 on page 1388. They also are accessible in the `Math` section:

```
Math{...
   ErrRef( Electron ) = 1e10
   ErrRef( Hole )     = 1e10
}
```

The second scheme is activated with the keyword `-RelErrControl` in the `Math` section and is based on Eq. 1237. The default values for the parameters ε_A are listed in Table 191. They also are accessible in the `Math` section:

```
Math{...
   -RelErrControl
   Error( Electron ) = 1e-5
   Error( Hole )     = 1e-5
}
```

'Plugin' Iterations

This is the traditional scheme, which is also known as 'Gummel iterations' in most other device simulators. Consider that there are `n` sets of nonlinear systems $g_j(z_1 \ldots z_n) = 0$. (n can be, for example, 3 and the sets can be the Poisson equation and two continuity equations.) This method starts with values $z_1^{(1)}, \ldots, z_n^{(1)}$ and then solves each set $g_j = 0$ separately and consecutively.

One loop could be:

$$g_1(z_1 z_2^{(i)} \ldots z_n^{(i)}) = 0 \Rightarrow z_1^{(i+1)} \tag{1239}$$

$$\ldots$$

$$g_1(z_1^{(i+1)} \ldots z_{n-1}^{(i+1)} z_n) = 0 \Rightarrow z_n^{(i+1)}$$

If an update (λx) of the solution between two successive plugin iterations is defined as:

$$(\lambda x) = z_j^{(i+1)} - z_j^{(i)} \tag{1240}$$

Eq. 1236 or Eq. 1237 can be applied for convergence control in plugin iterations.

References

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Part V External Interfaces

This part of the *Sentaurus™ Device User Guide* contains the following chapters:

Physical Model Interface

This chapter discusses the flexible interface that is used to add new physical models to Sentaurus Device.

Overview

The physical model interface (PMI) provides direct access to certain models in the semiconductor transport equations. You can provide new C++ functions to compute these models, and Sentaurus Device loads the functions at runtime using the dynamic loader. No access to the Sentaurus Device source code is necessary. You can modify the following models:

- Generation–recombination rate R_{net}, see Eq. 53, p. 181
- Avalanche generation, that is, ionization coefficient α in Eq. 419, p. 406
- Electron and hole mobilities μ_n and μ_p, see Eq. 56 and Eq. 57, p. 183
- Band gap, see Chapter 12 on page 249
- Bandgap narrowing E_{bgn}, see Band Gap and Electron Affinity on page 249
- Complex refractive index, see Complex Refractive Index Model Interface on page 586
- Electron affinity, see Band Gap and Electron Affinity on page 249
- Apparent band-edge shift, see Density Gradient Quantization Model on page 294
- Multistate configuration–dependent apparent band-edge shift, see Apparent Band-Edge Shift on page 483
- Multistate configuration–dependent thermal conductivity, heat capacity, and mobility, see Thermal Conductivity, Heat Capacity, and Mobility on page 485
- Effective mass, see Effective Masses and Effective Density-of-States on page 261
- Energy relaxation times τ, see Eq. 84, p. 197 to Eq. 86, p. 197
- Lifetimes τ, as used in SRH recombination (see Eq. 275, p. 331) and CDL recombination (see Eq. 395, p. 398)
- Thermal conductivity κ, see Eq. 69, p. 193 and Eq. 78, p. 196
- Heat capacity c_L, see Eq. 69, p. 193 and Eq. 92, p. 198
- Optical quantum yield, see Quantum Yield Models on page 544 and Optical Quantum Yield on page 1183
- Stress, see Stress on page 1186

- Space factor, see Metal Workfunction on page 242, Energetic and Spatial Distribution of Traps on page 450, Using the Trap Degradation Model on page 495, Using the eNMP Model on page 516, and SFactor Dataset or PMI Model on page 876

- Mobility stress factor, see Mobility Stress Factor PMI Model on page 875

- Trap capture and emission rates, see Local Capture and Emission Rates From PMI on page 461

- Trap energy shift, see Trap Energy Shift on page 1205

- eNMP transition rates, see eNMP Transition Rates PMI Model on page 519

- Piezoelectric polarization, see Piezoelectric Polarization on page 883

- Incomplete ionization, see Chapter 13 on page 277

- Hot-carrier injection, see Chapter 25 on page 737

- Piezoresistive coefficients, see Piezoresistance Mobility Model on page 859

- Raytracing contact, see Boundary Condition for Raytracing on page 605

- Spatial distribution function, see Heavy Ions on page 668

- Metal resistivity, see Transport in Metals on page 239

- Heat generation rate, see Thermodynamic Model for Lattice Temperature on page 193

- Thermoelectric power, see Thermoelectric Power (TEP) on page 913

- Metal thermoelectric power, see Thermoelectric Power (TEP) on page 913

- Diffusivity, see Hydrogen Transport on page 500

- Gamma factor, see Density Gradient Model on page 294

- Schottky resistance, see Resistive Contacts on page 213 and Resistive Interfaces on page 219

- Ferromagnetism and spin transport, see Chapter 30 on page 805

A separate interface is provided to add new entries to the current plot file, see Current Plot File of Sentaurus Device on page 1239.

An interface is available that allows postprocessing of data during a transient simulation (see Postprocess for Transient Simulation on page 1244).

A separate interface is provided for preprocessing data during a Newton iteration process and Newton step control (see Preprocessing for Newton Iterations and Newton Step Control on page 1246).

For most models, Sentaurus Device provides two equivalent interfaces:

- The standard interface (see Standard C++ Interface on page 1045) is based on the data type `double`. Separate subroutines must be written to evaluate the model and its derivatives. This interface provides performance comparable to the built-in models in Sentaurus Device.

- The simplified interface (see Simplified C++ Interface on page 1049) is based on the data type `pmi_float`. Only a single subroutine must be implemented to evaluate the model. For local models, the derivatives of the model are obtained by automatic differentiation. Furthermore, this interface also supports extended precision floating-point arithmetic (see Extended Precision on page 168).

The following steps are needed to use a PMI model in a Sentaurus Device simulation:

- A C++ subroutine must be implemented to evaluate the PMI model. In the case of the standard interface, additional C++ subroutines must be written to evaluate the derivatives of the PMI model with respect to all input variables.

- The `cmi` script produces a shared object file that Sentaurus Device loads at runtime (see Shared Object Code on page 1065).

> **NOTE** The version of the C++ compiler used for a PMI model must be identical to the version of the C++ compiler used at Synopsys to compile Sentaurus Device. Use the command `cmi -a` to verify the compiler versions.

- The `PMIPath` variable must be defined in the `File` section of the command file. This defines the search path for the shared object files. A PMI model is activated in the `Physics` section of the command file by specifying its name (see Command File of Sentaurus Device on page 1065).

- Parameters for PMI models can appear in the parameter file (see Parameter File of Sentaurus Device on page 1088).

These steps are discussed further in the following sections. The source code for the examples is in the directory `$STROOT/tcad/$STRELEASE/lib/sdevice/src`.

Standard C++ Interface

For each PMI model, you must implement a C++ subroutine to evaluate the model. Additional subroutines are necessary to evaluate the derivatives of the model with respect to all the input variables. More specifically, you must implement a C++ class that is derived from a base class declared in the header file `PMIModels.h`. In addition, a so-called virtual constructor function must be provided, which allocates an instance of the derived class.

For example, consider the implementation of Auger recombination as a new PMI model. (The built-in Auger recombination model is discussed in Auger Recombination on page 408.)

In its simplest form, Auger recombination can be written as:

$$R_{\text{net}} = C \cdot (n + p) \cdot (np - n_{\text{i,eff}}^2) \tag{1241}$$

Sentaurus Device needs to evaluate the value of R_{net} and the derivatives:

$$\frac{\partial R_{\text{net}}}{\partial n} = C(np - n_{\text{i,eff}}^2 + (n+p)p)$$

$$\frac{\partial R_{\text{net}}}{\partial p} = C(np - n_{\text{i,eff}}^2 + (n+p)n) \tag{1242}$$

$$\frac{\partial R_{\text{net}}}{\partial n_{\text{i,eff}}} = -2C(n+p)n_{\text{i,eff}}$$

In the header file `PMIModels.h`, the following base class is defined for recombination models:

```
class PMI_Recombination : public PMI_Vertex_Interface {

public:
  PMI_Recombination (const PMI_Environment& env);
  virtual ~PMI_Recombination ();

  virtual void Compute_r
    (const double t, const double n, const double p,
     const double nie, const double f, double& r) = 0;

  virtual void Compute_drdt
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdt) = 0;

  virtual void Compute_drdn
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdn) = 0;

  virtual void Compute_drdp
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdp) = 0;

  virtual void Compute_drdnie
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdnie) = 0;

  virtual void Compute_drdf
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdf) = 0;
};
```

To implement a PMI model for Auger recombination, you must declare a derived class:

```
#include "PMIModels.h"

class Auger_Recombination : public PMI_Recombination {

  double C;

public:
  Auger_Recombination (const PMI_Environment& env);
  ~Auger_Recombination ();

  void Compute_r
    (const double t, const double n, const double p,
     const double nie, const double f, double& r);

  void Compute_drdt
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdt);

  void Compute_drdn
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdn);

  void Compute_drdp
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdp);

  void Compute_drdnie
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdnie);

  void Compute_drdf
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdf);
};
```

The constructor of the derived class is invoked for each region of the device. In this example, the variable C is initialized from the parameter file:

```
Auger_Recombination::
Auger_Recombination (const PMI_Environment& env) :
  PMI_Recombination (env)
{ C = InitParameter ("C", 1e-30);
}
```

If the parameter C is not found in the parameter file, a default value of 10^{-30} is used (see Parameter File of Sentaurus Device on page 1088). During a Newton iteration, Sentaurus Device evaluates a PMI model for each mesh vertex. The method Compute_r() computes the

recombination rate for a given vertex. According to the parameter list, the recombination rate can depend on the following variables:

`t`	Lattice temperature
`n`	Electron density
`p`	Hole density
`nie`	Effective intrinsic density
`f`	Absolute value of electric field

The result of the function is stored in the parameter `r`:

```
void Auger_Recombination::
Compute_r (const double t, const double n, const double p,
           const double nie, const double f, double& r)
{ r = C * (n + p) * (n*p - nie*nie);
  if (r < 0.0) {
    r = 0.0;
  }
}
```

Besides `Compute_r()`, you must implement other methods to compute the partial derivatives of the recombination rate with respect to the input variables `t`, `n`, `p`, `nie`, and `f`. The implementation of `Compute_drdn()` to compute the value of $\partial R / \partial n$ is:

```
void Auger_Recombination::
Compute_drdn (const double t, const double n, const double p,
const double nie, const double f, double& drdn)
{ double r = C * (n + p) * (n*p - nie*nie);
  if (r < 0.0) {
    drdn = 0.0;
  } else {
    drdn = C * ((n*p - nie*nie) + (n + p) * p);
  }
}
```

Finally, you must provide a so-called virtual constructor function, which allocates a variable of the new class:

```
extern "C"
PMI_Recombination* new_PMI_Recombination (const PMI_Environment& env)
{ return new Auger_Recombination (env);
}
```

> **NOTE** This function must have C linkage and exactly the same name as declared in the header file `PMIModels.h`.

Simplified C++ Interface

There are PMI models that utilize the simplified C++ interface. Such PMI models, referred to as *simplified PMI models*, need to implement essentially only one function that computes the numeric value of the quantity of interest at the actual vertex of the simulation mesh. Derivatives of the quantity with respect to input quantities can be extracted automatically.

There are three C++ types that provide the appropriate interface for users:

- The simplified PMI models utilize a special numeric data type `pmi_float` (see Numeric Data Type pmi_float on page 1049).

- The simplified PMI models are derived from the `PMI_Vertex_Common_Base` class, providing an interface at the scope of the PMI model (see Runtime Support at Model Scope on page 1068).

- The main function of a simplified PMI model is called `compute` and has the form:

  ```
  void compute ( const Input& input, Output& output )
  ```

  where `Input` is a class derived from the `PMI_Vertex_Input_Base` class, providing runtime support at the compute scope (see Runtime Support at Compute Scope on page 1070).

Numeric Data Type pmi_float

The simplified interface is based on the data type `pmi_float`. This data type behaves similar to a `double`, and it supports all the usual arithmetic operations:

- Assignment:

  ```
  pmi_float x = 2;
  pmi_float y (x);
  ```

- Unary operators:

  ```
  +x; -y;
  ```

- Binary operators:

  ```
  x + y; x - y; x * y; x / y;
  ```

- Comparisons:

  ```
  x == y; x != y; x < y; x <= y; x > y; x >= y;
  ```

- Mathematical functions:

  ```
  abs(x); acos(x); acosh(x); asin(x); asinh(x); atan(x); atanh(x);
  atan2(y,x); cos(x); cosh(x); erf(x); erfc(x); exp(x); expm1(x); hypot(x,y);
  ```

```
isinf(x); isnan(x); ldexp(x,exp); log(x); log1p(x); log10(x); pow(x,y);
pow_int(x,n); sin(x); sinh(x); sqrt(x); tan(x); tanh(x);
```

■ Output:

```
std::cout << x;
```

The static function:

```
pmi_e_precision pmi_float::get_precision ()
```

returns the accuracy of the floating-point arithmetic. The result is expressed as an enumeration type:

```
enum pmi_e_precision {
    pmi_c_np,  // normal precision (double): -ExtendedPrecision
    pmi_c_xp,  // extended precision (long double): ExtendedPrecision
    pmi_c_dd,  // double-double: ExtendedPrecision(128)
    pmi_c_qd,  // quad-double: ExtendedPrecision(256)
    pmi_c_mp   // arbitrary precision: ExtendedPrecision(Digits=...)
};
```

Because the class `pmi_float` supports automatic differentiation, it must store both the value of a variable and the gradient vector of the derivatives with respect to the independent variables. The following methods are available to read the value of a variable, the size of its gradient vector, and the components of the gradient vector:

```
template <class des_t_float> des_t_float get_value ();
size_t size_gradient ();
template <class des_t_float> des_t_float get_gradient (size_t i);
```

Additional methods are available to set the value of a variable or its gradient:

```
template <class des_t_float> void set_value (const des_t_float a);
template <class des_t_float> void set_gradient (size_t i,
                                                const des_t_float a);
```

NOTE These methods for reading and writing the value and the gradient of a variable are not necessary for most models. They may be useful in cases where automatic differentiation yields wrong results.

Pseudo-Implementation of a Simplified PMI Model

Compared to the standard interface, the simplified interface only requires the implementation of a single subroutine to evaluate the model. As in Standard C++ Interface on page 1045, the following discusses how Auger recombination can be implemented as a PMI model.

The header file `PMI.h` defines the following base class for recombination models:

```
class PMI_Recombination_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      pmi_float t;    // lattice temperature
      pmi_float n;    // electron density
      pmi_float p;    // hole density
      pmi_float nie;  // effective intrinsic density
      pmi_float f;    // absolute value of electric field
   };

   class Output {
   public:
      pmi_float r;  // recombination rate
   };

   PMI_Recombination_Base (const PMI_Environment& env);
   virtual ~PMI_Recombination_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
};
```

To implement a user model, you must first declare a derived class:

```
#include "PMI.h"

class Auger_Recombination : public PMI_Recombination_Base {

private:
   double C;

public:
   Auger_Recombination (const PMI_Environment& env);
   ~Auger_Recombination ();

   virtual void compute (const Input& input, Output& output);
};
```

In the constructor, the variable `C` is initialized from the parameter file:

```
Auger_Recombination::
Auger_Recombination (const PMI_Environment& env) :
   PMI_Recombination_Base (env)

{ C = InitParameter ("C", 1e-30);
}
```

The constructor is called for each region of the device to ensure that regionwise parameters are handled correctly.

Next, the actual `Compute` function must be implemented. It relies on the auxiliary classes `Input` and `Output` to read the input variables, and to store the recombination rate:

```
void Auger_Recombination::
compute (const Input& input, Output& output)

{ output.r = C * (input.n + input.p) *
                 (input.n*input.p - input.nie*input.nie);
   if (output.r < 0.0) {
      output.r = 0.0;
   }
}
```

Finally, a virtual constructor must be supplied to allocate instances of the class `Auger_Recombination`:

```
extern "C"
PMI_Recombination_Base* new_PMI_Recombination_Base
   (const PMI_Environment& env)

{ return new Auger_Recombination (env);
}
```

> **NOTE** This function must have C linkage and exactly the same name as declared in the header file `PMI.h`.

It is possible to implement a model using both the standard interface and the simplified interface within the same file. In this case, Sentaurus Device will select the version based on the floating-point precision:

- The standard interface is selected for normal precision (64 bits). This ensures a performance similar to built-in models.
- The simplified interface is selected for extended precision floating-point arithmetic. No loss of accuracy occurs when the PMI model is invoked.

> **NOTE** The simplified interface is ideally suited for prototyping a new model. No derivatives need to be implemented, which accelerates the development cycle. After a model has been validated, it can be converted easily into the standard interface for performance-critical applications.

As the simplified interface calculates the derivatives for you, it is easy to overlook cases where the expressions themselves are well defined, but their derivatives are not. Assume, for example,

that your model computes $\sqrt{n - n_0}$, and you have ensured that $n - n_0$ cannot become negative. This is not enough because, when $n = n_0$, the derivative $1/2\sqrt{n - n_0}$ becomes infinite.

> **NOTE** Ensure that not only the expressions you use, but also their derivatives are always valid.

Nonlocal Interface

With the nonlocal interface model, values can be computed based on nonlocal values of the input variables. For example, the generation–recombination rate in a vertex may depend on the carrier densities observed in a remote vertex.

A nonlocal interface provides more flexibility but, in turn, requires additional functionality in the user PMI code. You must implement separate C++ functions for the following purposes:

Dependencies:

The variables that the model depends on must be declared, for example, electrostatic potential or carrier densities.

Structure of the Jacobian matrices:

For each input variable, the structure (stencil) of the corresponding Jacobian matrix must be declared, for example:

```
model value in vertex 17 depends on:
  electrostatic potential in vertex 22
  electron density in vertex 55
model value in vertex 18 depends on:
  hole density in vertex 35
  lattice temperature in vertex 44
```

Model values and their derivatives:

The code must evaluate the model values and their derivatives with respect to all dependencies.

Update of Jacobian matrices:

Optionally, the PMI can require an update in the structure of the Jacobian matrices. This can be useful if the model does not have purely geometric dependencies, but depends on the values of the solution as well. In this case, Sentaurus Device calls the PMI to request the updated structures of the Jacobian matrices.

Nonlocal PMIs are available with both the data type `double` (see Standard C++ Interface on page 1045) and the data type `pmi_float` (see Simplified C++ Interface on page 1049). However, the data type `pmi_float` is used only to support extended-precision floating-point arithmetic. It is not used for the purpose of automatic differentiation.

Jacobian Matrix

Sentaurus Device provides the classes `des_jacobian` (standard C++ interface) and `sdevice_jacobian` (simplified C++ interface) to represent Jacobian matrices. These classes are used to:

■ Define the structure of the Jacobian matrices, that is, the dependencies of the model values on the input variables.

■ Store the derivatives of the model values with respect to the input variables.

The size of a Jacobian matrix depends on the location of the model and the location of the input variable. The number of rows is determined by the location of the model. For example, the number of rows for a vertex-based model is given by the number of mesh vertices.

The supported locations are given by the type `des_data::des_location` (for the standard C++ interface):

```
typedef
   enum { vertex, edge, element, rivertex, element_vertex } des_location;
```

and by the type `sdevice_data::sdevice_location` (for the simplified C++ interface):

```
typedef
   enum { vertex, edge, element, rivertex, element_vertex } sdevice_location;
```

Similarly, the number of columns of a Jacobian matrix is determined by the location of the input variable. For example, the number of columns for an edge-based input variable is given by the number of mesh edges.

For a scalar model depending on a scalar input variable, each Jacobian entry is also a simple scalar. However, Sentaurus Device also supports the general case where the model value, or the input variable, or both are vector quantities. In this case, each entry in the Jacobian matrix becomes a small dense matrix of size number-of-inner-rows multiplied by number-of-inner-columns. The number of inner rows is given by the number of model values (1 for a scalar or the mesh dimension for vectors). Similarly, the number of inner columns is determined by the number of variable values (1 for a scalar or the mesh dimension for vectors).

The class `des_jacobian` provides the following methods:

```
des_jacobian (int rows, int cols, int inner_rows, int inner_cols);

int size_rows () const;
int size_cols () const;
int size_inner_rows () const;
int size_inner_cols () const;
int size_matrix () const;

void define_element (int row, int col);
double* element (int row, int col);

des_jacobian_iterator begin ();
des_jacobian_iterator end ();
des_jacobian_iterator lower_bound (int row, int col);
des_jacobian_iterator upper_bound (int row, int col);

void set (double value);
```

> **NOTE** The class `sdevice_jacobian` from the simplified C++ interface provides the same methods, except that the data type `pmi_float` is used instead of `double`.

The constructor creates a new empty Jacobian matrix with the given dimensions.

The methods `size_rows()` and `size_cols()` return the number of rows and columns, respectively. Similarly, the methods `size_inner_rows()` and `size_inner_cols()` return the number of inner rows and inner columns, respectively. The method `size_matrix()` returns the number of nonzero elements in the Jacobian.

Use the method `define_element()` to define the location of a nonzero matrix element. The value of the nonzero entry remains unspecified at this point. However, the required storage is allocated.

The method `element()` returns a pointer to an entry of the Jacobian matrix. A `NULL` pointer is returned for a nonexistent entry. The pointer defines the beginning of a dense matrix of size number-of-inner-rows multiplied by number-of-inner-columns. The entries in this matrix are stored in row-major order (C style). This means that the derivative of the i-th component of the result with respect to the j-th component of the input variable is stored in the location:

```
element() + i * size_inner_cols() + j
```

The two functions `begin()` and `end()` return iterators to traverse the nonzero elements of the Jacobian matrix. A typical loop would be:

```
des_jacobian J;
for (des_jacobian_iterator it = J.begin(); it != J.end(); it++) {
```

```
        int row = it.row();
        int col = it.col();
        double* value = it.val();
        // process element (row,col)
    }
```

The functions `lower_bound()` and `upper_bound()` provide a way to quickly find a range of nonzero elements. The function `lower_bound()` returns an iterator to the first nonzero element not less than (row,col) in row-major order. Similarly, `upper_bound()` returns an iterator to the first nonzero element greater than (row,col) in row-major order. Both functions can return `end()` to indicate a nonexistent element.

The following code fragment visits all nonzero elements in row 25:

```
des_jacobian J;
des_jacobian_iterator it_begin = J.lower_bound (25, 0);
des_jacobian_iterator it_end = J.lower_bound (26, 0);
for (des_jacobian_iterator it = it_begin; it != it_end; it++) {
    int row = it.row();
    int col = it.col();
    double* value = it.val();
    // process element (row,col)
}
```

The method `set()` can be used to initialize all matrix elements with a given value.

Example: Point-to-Point Tunneling Model

As an example, for a nonlocal generation–recombination model, consider a simple point-to-point tunneling model between two vertices v_1 and v_2. The model compares the electron and hole quasi-Fermi potentials in these two vertices. If $\Phi_{n,1} < \Phi_{p,2}$, the tunneling rate r is computed as:

$$r = Ae^{-B(E_{V,2} - E_{C,1})^2}\frac{\Delta}{1 + \Delta} \tag{1243}$$

where E_C is the conduction band energy, E_V is the valence band energy, and $\Delta = \Phi_{p,2} - \Phi_{n,1}$. The nonlocal transport is modeled by using the tunneling rate r as an electron recombination rate in vertex 1 and a hole recombination rate in vertex 2.

Similarly, if $\Phi_{p,1} > \Phi_{n,2}$, the tunneling rate r is computed as:

$$r = Ae^{-B(E_{C,2} - E_{V,1})^2}\frac{\Delta}{1 + \Delta} \tag{1244}$$

where $\Delta = \Phi_{p,1} - \Phi_{n,2}$. In this case, r is used as a hole recombination rate in vertex 1 and as an electron recombination rate in vertex 2.

In the header file `PMIModels.h`, the following base class is defined for nonlocal generation–recombination models:

```
class PMI_NonLocal_Recombination : public PMI_Device_Interface {

public:
   class Input {
   public:
      const des_region* region;          // all vertices belong to this region
      const std::vector<int>& vertices;  // list of vertices
   };

   class Output {
   public:
      std::vector<double>& elec;    // nonlocal recombination rates (electrons)
      std::vector<double>& hole;    // nonlocal recombination rates (holes)
      des_id_to_jacobian_map& J_elec;  // derivatives (electrons)
      des_id_to_jacobian_map& J_hole;  // derivatives (holes)
   };

   PMI_NonLocal_Recombination (const PMI_Device_Environment& env);
   virtual ~PMI_NonLocal_Recombination ();

   virtual void
      DefineDependencies (std::vector<des_data::des_id>& dependencies) = 0;

   virtual void DefineJacobians (des_id_to_jacobian_map& J_elec,
                                 des_id_to_jacobian_map& J_hole) = 0;

   virtual void Compute_parallel (const Input& input, Output& output) = 0;

   virtual bool NeedNewEdges () { return false; }
};
```

To implement the point-to-point tunneling model, you must declare a derived class:

```
#include "PMIModels.h"

class P2P_Recombination : public PMI_NonLocal_Recombination {

private:
   double A, B;                // model parameters
   int v1, v2;                 // vertex 1, vertex 2
   double measure1, measure2;  // semiconductor node measures for vertex 1 and 2

public:
   P2P_Recombination (const PMI_Device_Environment& env);
```

```
      void DefineDependencies (std::vector<des_data::des_id>& dependencies);
      void DefineJacobians (des_id_to_jacobian_map& J_elec,
                            des_id_to_jacobian_map& J_hole);
      void Compute_parallel (const PMI_NonLocal_Recombination::Input& input,
                             PMI_NonLocal_Recombination::Output& output);
      bool NeedNewEdges ();
   };
```

The constructor of the derived class reads the model parameters and computes the semiconductor node measures for the two vertices v_1 and v_2:

```
   P2P_Recombination::
   P2P_Recombination (const PMI_Device_Environment& env) :
     PMI_NonLocal_Recombination (env)
   {  A = InitParameter ("A", 1e25);
      B = InitParameter ("B", 50);
      v1 = InitParameter ("v1", 0);
      v2 = InitParameter ("v2", 1);

      const des_mesh* mesh = Mesh ();
      des_data* data = Data ();
      const double*const* measure = data->ReadMeasure ();

      // semiconductor node measure for vertex 1
      measure1 = 0;
      des_vertex* vertex1 = mesh->vertex (v1);
      for (size_t eli = 0; eli < vertex1->size_element (); eli++) {
         des_element* el = vertex1->element (eli);
         if (el->bulk ()->material () == "Silicon") {
            for (size_t vi = 0; vi < el->size_vertex (); vi++) {
               des_vertex* v = el->vertex (vi);
               if (v == vertex1) {
                  measure1 += measure [el->index()][vi];
               }
            }
         }
      }

      // semiconductor node measure for vertex 2
      measure2 = 0;
      des_vertex* vertex2 = mesh->vertex (v2);
      for (size_t eli = 0; eli < vertex2->size_element (); eli++) {
         des_element* el = vertex2->element (eli);
         if (el->bulk ()->material () == "Silicon") {
            for (size_t vi = 0; vi < el->size_vertex (); vi++) {
               des_vertex* v = el->vertex (vi);
               if (v == vertex2) {
                  measure2 += measure [el->index()][vi];
```

```
              }
            }
          }
        }
      }
```

The `InitParameter()` method for reading a parameter is documented in Runtime Support for Vertex-Based PMI Models on page 1067. Similarly, the functions for accessing the device mesh are discussed in Mesh-Based Runtime Support on page 1076.

The semiconductor node measures are used later in the `Compute_parallel()` method. They are necessary to ensure current conservation for arbitrary meshes.

The method `DefineDependencies()` defines the variables that will be read later when `Compute_parallel()` is invoked:

```
void P2P_Recombination::
DefineDependencies (std::vector<des_data::des_id>& dependencies)
{ dependencies.push_back (des_data::des_id (des_data::scalar,
                                            des_data::vertex,
                                            "eQuasiFermiPotential"));
  dependencies.push_back (des_data::des_id (des_data::scalar,
                                            des_data::vertex,
                                            "hQuasiFermiPotential"));
  dependencies.push_back (des_data::des_id (des_data::scalar,
                                            des_data::vertex,
                                            "ConductionBandEnergy"));
  dependencies.push_back (des_data::des_id (des_data::scalar,
                                            des_data::vertex,
                                            "ValenceBandEnergy"));
}
```

The tables in Appendix F on page 1339 show the variables that are available to all mesh-based PMIs. However, the following restrictions must be observed with regard to nonlocal models:

- Constant fields such as doping concentration, mole fraction concentrations, stress fields, or PMI user fields can be used without restrictions. No dependencies need to be defined in `DefineDependencies()`, and no derivatives need to be computed.

- Nonlocal PMIs can only use certain solution-dependent fields. Table 173 lists the subset of variables that are supported.

Table 173   Solution-dependent data available to nonlocal PMI models

Data name	Type	Location	Description
BandGap	scalar	vertex	Intrinsic band gap E_g
BandgapNarrowing	scalar	vertex	Bandgap narrowing E_{bgn}

Table 173   Solution-dependent data available to nonlocal PMI models (Continued)

Data name	Type	Location	Description
ConductionBandEnergy	scalar	element_vertex	Conduction band energy E_C
		vertex	
eDensity	scalar	vertex	Electron density n
eEffectiveStateDensity	scalar	vertex	Conduction band density-of-states (DOS) N_C
EffectiveIntrinsicDensity	scalar	vertex	Effective intrinsic density $n_{i,\,\mathrm{eff}}$
ElectricField	scalar	element	Electric field F
		vertex	
	vector	element	
		vertex	
ElectronAffinity	scalar	vertex	Electron affinity χ
ElectrostaticPotential	scalar	vertex	Electrostatic potential ϕ
eQuasiFermiPotential	scalar	vertex	Electron quasi-Fermi potential Φ_n
eRelativeEffectiveMass	scalar	vertex	Electron DOS mass m_n
eTemperature	scalar	vertex	Electron temperature T_n
hDensity	scalar	vertex	Hole density p
hEffectiveStateDensity	scalar	vertex	Valence band DOS N_V
hQuasiFermiPotential	scalar	vertex	Hole quasi-Fermi potential Φ_p
hRelativeEffectiveMass	scalar	vertex	Hole DOS mass m_p
hTemperature	scalar	vertex	Hole temperature T_p
InsulatorElectricField	scalar	vertex	Electric field F on insulator
	vector		
IntrinsicDensity	scalar	vertex	Intrinsic density n_i
LatticeTemperature	scalar	vertex	Lattice temperature T
SemiconductorElectricField	scalar	vertex	Electric field F on semiconductor
	vector		
SemiconductorGradValencebandEnergy	scalar	element	Gradient of valence band energy ∇E_V
	vector		

Table 173   Solution-dependent data available to nonlocal PMI models (Continued)

Data name	Type	Location	Description
ValenceBandEnergy	scalar	element_vertex	Valence band energy E_V
		vertex	

The method `DefineJacobians()` must perform two operations:

- Allocate all Jacobian matrices with the correct dimensions (see Jacobian Matrix on page 1054).

- Define the nonzero elements in all the Jacobian matrices. All the nonzero derivatives that will be computed later in the method `Compute_parallel()` must be defined at this point. The method `Compute_parallel()` cannot allocate additional nonzero entries.

For the point-to-point tunneling model, the method `DefineJacobians()` would be:

```
void P2P_Recombination::
DefineJacobians (des_id_to_jacobian_map& J_elec,
                 des_id_to_jacobian_map& J_hole)
{ const des_mesh* mesh = Mesh ();
  const int n_vertices = mesh->size_vertex ();

  // allocate Jacobians
  des_jacobian*& J_elec_eQF = J_elec [des_data::des_id
     (des_data::scalar, des_data::vertex, "eQuasiFermiPotential")];
  des_jacobian*& J_elec_hQF = J_elec [des_data::des_id
     (des_data::scalar, des_data::vertex, "hQuasiFermiPotential")];
  des_jacobian*& J_elec_EC = J_elec [des_data::des_id
     (des_data::scalar, des_data::vertex, "ConductionBandEnergy")];
  des_jacobian*& J_elec_EV = J_elec [des_data::des_id
     (des_data::scalar, des_data::vertex, "ValenceBandEnergy")];

  des_jacobian*& J_hole_eQF = J_hole [des_data::des_id
     (des_data::scalar, des_data::vertex, "eQuasiFermiPotential")];
  des_jacobian*& J_hole_hQF = J_hole [des_data::des_id
     (des_data::scalar, des_data::vertex, "hQuasiFermiPotential")];
  des_jacobian*& J_hole_EC = J_hole [des_data::des_id
     (des_data::scalar, des_data::vertex, "ConductionBandEnergy")];
  des_jacobian*& J_hole_EV = J_hole [des_data::des_id
     (des_data::scalar, des_data::vertex, "ValenceBandEnergy")];

  J_elec_eQF = new des_jacobian (n_vertices, n_vertices, 1, 1);
  J_elec_hQF = new des_jacobian (n_vertices, n_vertices, 1, 1);
  J_elec_EC = new des_jacobian (n_vertices, n_vertices, 1, 1);
  J_elec_EV = new des_jacobian (n_vertices, n_vertices, 1, 1);

  J_hole_eQF = new des_jacobian (n_vertices, n_vertices, 1, 1);
  J_hole_hQF = new des_jacobian (n_vertices, n_vertices, 1, 1);
```

```
            J_hole_EC = new des_jacobian (n_vertices, n_vertices, 1, 1);
            J_hole_EV = new des_jacobian (n_vertices, n_vertices, 1, 1);

            // define nonzero entries in Jacobians
            J_elec_eQF->define_element (v1, v1);
            J_elec_eQF->define_element (v2, v2);

            J_elec_hQF->define_element (v1, v2);
            J_elec_hQF->define_element (v2, v1);

            J_elec_EC->define_element (v1, v1);
            J_elec_EC->define_element (v2, v2);

            J_elec_EV->define_element (v1, v2);
            J_elec_EV->define_element (v2, v1);

            J_hole_eQF->define_element (v1, v2);
            J_hole_eQF->define_element (v2, v1);

            J_hole_hQF->define_element (v1, v1);
            J_hole_hQF->define_element (v2, v2);

            J_hole_EC->define_element (v1, v2);
            J_hole_EC->define_element (v2, v1);

            J_hole_EV->define_element (v1, v1);
            J_hole_EV->define_element (v2, v2);
        }
```

The method `Compute_parallel()` computes the electron and hole recombination rates and their derivatives. It may be called during the parallel assembly in Sentaurus Device. Therefore, it must be implemented in a thread-safe manner. During each call, only the model values and their derivatives for the vertices appearing in the vector `Input::vertices` must be computed.

The recombination rates are multiplied by the semiconductor node measure of the source vertex. This ensures current conservation for arbitrary meshes.

```
    void P2P_Recombination::
    Compute_parallel (const PMI_NonLocal_Recombination::Input& input,
    PMI_NonLocal_Recombination::Output& output)
    { des_data* data = Data ();

        const double* eQF =
           data->ReadScalar (des_data::vertex, "eQuasiFermiPotential");
        const double* hQF =
           data->ReadScalar (des_data::vertex, "hQuasiFermiPotential");
        const double* EC =
```

```
        data->ReadScalar (des_data::vertex, "ConductionBandEnergy");
const double* EV =
        data->ReadScalar (des_data::vertex, "ValenceBandEnergy");

des_jacobian* J_elec_eQF = output.J_elec [des_data::des_id
        (des_data::scalar, des_data::vertex, "eQuasiFermiPotential")];
des_jacobian* J_elec_hQF = output.J_elec [des_data::des_id
        (des_data::scalar, des_data::vertex, "hQuasiFermiPotential")];
des_jacobian* J_elec_EC = output.J_elec [des_data::des_id
        (des_data::scalar, des_data::vertex, "ConductionBandEnergy")];
des_jacobian* J_elec_EV = output.J_elec [des_data::des_id
        (des_data::scalar, des_data::vertex, "ValenceBandEnergy")];

des_jacobian* J_hole_eQF = output.J_hole [des_data::des_id
        (des_data::scalar, des_data::vertex, "eQuasiFermiPotential")];
des_jacobian* J_hole_hQF = output.J_hole [des_data::des_id
        (des_data::scalar, des_data::vertex, "hQuasiFermiPotential")];
des_jacobian* J_hole_EC = output.J_hole [des_data::des_id
        (des_data::scalar, des_data::vertex, "ConductionBandEnergy")];
des_jacobian* J_hole_EV = output.J_hole [des_data::des_id
        (des_data::scalar, des_data::vertex, "ValenceBandEnergy")];

// compute electron and hole recombination for vertices in input domain
for (size_t vi = 0; vi < input.vertices.size (); vi++) {
    const int v = input.vertices [vi];
    if (v == v1 || v == v2) {
        const int v_other = (v == v1) ? v2 : v1;
        const double weight = (v == v1) ? measure2 : measure1;

        if (eQF [v] < hQF [v_other]) {
            double delta = hQF [v_other] - eQF [v];  // delta > 0
            double rate = A * exp (-B * (EV [v_other] - EC [v]) *
                                        (EV [v_other] - EC [v])) *
                            delta / (1 + delta);
            double elec = weight * rate;

            // electron recombination
            output.elec [v] += elec;

            // derivatives
            double deriv_QF = elec / (delta * (1 + delta));
            double deriv_ECEV = 2 * elec * B * (EV [v_other] - EC [v]);
            *J_elec_eQF->element (v, v) -= deriv_QF;
            *J_elec_hQF->element (v, v_other) += deriv_QF;
            *J_elec_EC->element (v, v) += deriv_ECEV;
            *J_elec_EV->element (v, v_other) -= deriv_ECEV;
        }
```

```
            if (hQF [v] > eQF [v_other]) {
                double delta = hQF [v] - eQF [v_other];  // delta > 0
                double rate = A * exp (-B * (EC [v_other] - EV [v]) *
                                            (EC [v_other] - EV [v])) *
                              delta / (1 + delta);
                double hole = weight * rate;

                // hole recombination
                output.hole [v] += hole;

                // derivatives
                double deriv_QF = hole / (delta * (1 + delta));
                double deriv_ECEV = 2 * hole * B * (EC [v_other] - EV [v]);
                *J_hole_eQF->element (v, v_other) -= deriv_QF;
                *J_hole_hQF->element (v, v) += deriv_QF;
                *J_hole_EC->element (v, v_other) -= deriv_ECEV;
                *J_hole_EV->element (v, v) += deriv_ECEV;
            }
        }
    }
}
```

In this example, the dependencies of the model do not change as a function of the solution.
Therefore, the method `NeedNewEdges()` simply returns false:

```
bool P2P_Recombination::
NeedNewEdges ()
{ return false;   // nonlocal edges do not depend on solution
}
```

Finally, you must provide a so-called virtual constructor function, which allocates a variable of
the new class:

```
extern "C"
PMI_NonLocal_Recombination*
   new_PMI_NonLocal_Recombination (const PMI_Device_Environment& env)
{ return new P2P_Recombination (env);
}
```

> **NOTE** This function must have C linkage and exactly the same name as
> declared in the header file `PMIModels.h`.

The example presented in this section uses the data type `double` according to the standard C++
interface defined in the header file `PMIModels.h`. Alternatively, the simplified C++ interface
defined in the header file `PMI.h` uses the data type `pmi_float` to support extended-precision
floating-point arithmetic.

It is possible to implement a nonlocal model using both the standard interface and the simplified interface within the same file. In this case, Sentaurus Device selects the version based on the floating-point precision:

- The standard interface is selected for normal precision (64-bits). This ensures a performance similar to built-in models.

- The simplified interface is selected for extended-precision floating-point arithmetic. No loss of accuracy occurs when the PMI model is invoked.

Shared Object Code

Sentaurus Device assumes that the shared object code corresponding to a PMI model can be found in the file `modelname.so.arch`. The base name of this file must be identical to the name of the PMI model. The extension `.arch` depends on the hardware architecture. The script `cmi`, which is also a part of the CMI, can be used to produce the shared object files (see Compact Models User Guide, Runtime Support on page 150).

Command File of Sentaurus Device

To load PMI models into Sentaurus Device, the `PMIPath` search path must be defined in the `File` section of the command file. The value of `PMIPath` consists of a sequence of directories, for example:

```
File {
    PMIPath = ". /home/joe/lib /home/mary/sdevice/lib"
}
```

For each PMI model, which appears in the `Physics` section, the given directories are searched for a corresponding shared object file `modelname.so.arch`.

The PMI in Sentaurus Device provides access to mesh-based scalar fields specified by you. These fields must be defined on the device grid in a separate TDR (extension `.tdr`) data file. Up to 300 datasets (`PMIUserField0, ..., PMIUserField299`) can be defined. Sentaurus Device reads the user-defined fields if the corresponding file name is given in the command file:

```
File {
    PMIUserFields = "fields"
}
```

A PMI model can be activated in the `Physics` section of the command file by specifying the name of the PMI model in the appropriate part of the `Physics` section. Examples for different types of PMI models are:

- Generation–recombination models:

```
Physics {
   Recombination (pmi_model_name ...)
}
```

- Avalanche generation:

```
Physics {
   Recombination (Avalanche (pmi_model_name ...))
}
```

- Mobility models:

```
Physics {
   Mobility (
      DopingDependence (pmi_model_name)
      Enormal (pmi_model_name)
      ToCurrentEnormal (pmi_model_name)
      HighFieldSaturation (pmi_model_name driving_force)
   )
}
```

A PMI model name can only consist of alphanumeric characters and underscores (_). The first character must be either a letter or an underscore. A PMI model name can also be quoted as `"model_name"` to avoid conflicts with Sentaurus Device keywords.

All the PMI models can be specified regionwise or materialwise:

```
Physics (region = "Region.1") {
...
}
Physics (material = "AlGaAs") {
...
}
```

PMI models also recognize parameters in the command file. Usually, command file parameters are listed in parentheses after the model name, for example:

```
Physics {
  Recombination (pmi_model_name (a = 1
                                 b = "string"
                                 c = (1.2 3.4 5.6 7.8)
                                 d = ("red" "blue" "green")))
}
```

For certain models, the syntax differs from the above example, and this will be noted in the documentation (see Appendix G on page 1377).

> **NOTE** PMI model parameters also can be specified in the parameter file (see Parameter File of Sentaurus Device on page 1088). Parameters in the command file take precedence over parameters in the parameter file.

Certain values of PMI models can be plotted in the `Plot` section of the command file. The following identifiers are recognized:

- Generation–recombination models:

  ```
  Plot {
     PMIRecombination
     PMIeNonLocalRecombination  PMIhNonLocalRecombination
  }
  ```

- User-defined fields:

  ```
  Plot {
     PMIUserField0 PMIUserField1 ... PMIUserField299
  }
  ```

- Piezoelectric polarization:

  ```
  Plot {
     PE_Polarization/vector  PE_Charge
  }
  ```

- Metal conductivity (see Metal Resistivity on page 1260):

  ```
  Plot {
     MetalConductivity
  }
  ```

The current plot PMI can be used to add entries to the current plot file:

```
CurrentPlot {
   pmi_CurrentPlot
}
```

Runtime Support for Vertex-Based PMI Models

Inside vertex-based PMI models, you can access several functions described here. Essentially, they are split into two groups, namely, functions that are valid at the scope of the PMI model and functions that are valid only within the scope of `compute` functions.

Runtime Support at Model Scope

A standard vertex-based PMI is derived from the base class `PMI_Vertex_Interface`; whereas, a simplified vertex-based PMI is derived from the base class `PMI_Vertex_Base`. Both base classes are derived from the `PMI_Vertex_Common_Base` class and provide the following shared functionality:

```
const char* Name () const;
const char* Filename () const;
const char* ReadRegionName () const;
const char* ReadRegionMaterial () const;
des_materialgroup ReadRegionMaterialGroup () const;

const char* ReadDeviceName () const;

const PMIBaseParam* ReadParameter (const char* name
                                   [, const char* modelName]) const;
double InitParameter (const char* name, double defaultvalue
                      [, const char* modelName]) const;
void InitParameter (const char* name, std::vector<double>& value
                    [, const char* modelName]) const;
const char* InitStringParameter (const char* name,
                                 const char* defaultvalue
                                 [, const char* modelName]) const;
void InitStringParameter (const char* name,
                          std::vector<const char*>& value
                          [, const char* modelName]) const;
void double InitModelParameter (const char* name,
                          const char* modelName,
                          double defaultvalue);
void double InitOptoModelParameter(const char* name, double defaultvalue);

int ReadDimension () const;
void ReadReferenceCoordinates (double ref [3][3]) const;

size_t NumberOfMSConfigStates (const std::string& msconfig_name) const;
const std::string& MSConfigStateName (const std::string& msconfig_name,
                                      size_t state_index) const;
```

The method `Name()` returns the name of the PMI model as specified in the command file. Similarly, `Filename()` returns the name of the corresponding shared object file.

For the current region, you can call `ReadRegionName()` to determine its name, `ReadRegionMaterial()` to return the name of the region material, and `ReadRegionMaterialGroup()` to find the material group.

The possible values for the material group are:

```
PMI_Vertex_Common_Base::conductor
PMI_Vertex_Common_Base::insulator
PMI_Vertex_Common_Base::semiconductor
PMI_Vertex_Common_Base::unknown
```

`ReadDeviceName()` returns the name of the device.

The methods `ReadParameter()`, `InitParameter()`, and `InitStringParameter()` read the value of a parameter from the parameter file or command file (see Parameter File of Sentaurus Device on page 1088 and Command File of Sentaurus Device on page 1065). In these methods, `modelName` is an optional argument that allows the value of a parameter to be read from a different PMI model. The method `InitModelParameter()` allows PMI access to any built-in Sentaurus Device mole-fraction or constant parameters. `modelName` specifies the built-in model and `name` is the parameter within the specified model. When no valid model name or parameter name is found, the provided `defaultvalue` is returned instead. `InitModelParameter` is available only in the `Compute` function not in the PMI constructor. Similarly, the `InitOptoModelParameter()` method gives the PMI access to built-in numeric optoelectronic parameters. In this case, `name` is the full path to the parameter. `ReadDimension()` returns the dimension of the problem. The method `ReadReferenceCoordinates()` provides access to the reference coordinate system. It will return the identity matrix:

$$\mathrm{ref} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{1245}$$

in the case of the unified coordinate system (UCS). Otherwise, another coordinate system matrix is returned.

Multistate configuration–dependent models can call the two methods `NumberOfMSConfigStates()` and `MSConfigStateName()`. They return the number of states and the name of a state, respectively.

Reaction–Diffusion Species Interface (Model Scope)

The interface to reaction–diffusion (RD) species is the same for both standard and simplified PMI models, as it is provided in the common base class `PMI_Vertex_Common_Base`. The interface provides the following functions:

- `size_t RDSpecies_size ()`
  Returns the number of RD species defined for the actual device. Note that not all of these species need to be defined in the actual device region.

- `void get_RDSpecies_name (size_t isp, std::string& spname)`
  Returns the name of the species with device index `isp`.

- `bool RDSpecies_is_defined (size_t isp)`
  Returns true if the species with device index `isp` is defined in the actual region.

For simplified PMI models, the values for RD species concentrations can be extracted in the `compute` function from the `Input` interface (see Reaction–Diffusion Species Interface (Compute Scope) on page 1074). Note that standard PMI models do not have such an interface, that is, accessing RD species concentrations is not supported in this interface. However, within all PMI models, you can read such values using the `ReadScalar(const char*)` function.

Runtime Support at Compute Scope

The following interface functions depend on the local vertex where a model is evaluated. They are not available in the constructor of the PMI, but should only be called in the `Compute` function. In the case of the standard interface, these functions are a part of the base class `PMI_Vertex_Interface`; whereas, the simplified interface provides them through the base class `PMI_Vertex_Input_Base`:

```
void ReadCoordinate (double& x, double& y, double& z) const;
void ReadNearestInterfaceNormal (double& nx, double& ny, double& nz) const;
double ReadDistanceFromSemiconductorInsulatorInterface() const;
double ReadDistanceFromHighkInsulator() const;
int ReadNearestInterfaceOrientation() const;

double ReadLayerThickness () const;
double ReadLayerThicknessField () const;

double ReadTime () const;
double ReadTransientStepSize () const;
PMI_StepType ReadTransientStepType () const;

double ReadxMoleFraction () const;
double ReadyMoleFraction () const;

double ReadDoping (PMI_DopingSpecies species) const;
double ReadDoping (const char* SpeciesName) const;

double ReadDielectricConstant() const;
double ReadSemiconductorDielectricConstant() const;

int ReadDopingWell () const;

int IsUserFieldDefined (PMI_UserFieldIndex index) const;
double ReadUserField (PMI_UserFieldIndex index) const;
```

```
void WriteUserField (PMI_UserFieldIndex index, double value) const;

double ReadStress (PMI_StressIndex index) const;

bool ReadMSCOccupations (const std::string& msc_name, double* values) const;

double ReadeSHEDistribution (double energy) const;
double ReadhSHEDistribution (double energy) const;
double ReadeSHETotalDOS (double energy) const;
double ReadhSHETotalDOS (double energy) const;
double ReadeSHETotalGSV (double energy) const;
double ReadhSHETotalGSV (double energy) const;
```

> **NOTE** The support functions for the simplified interface use the data type `pmi_float`; whereas, the support functions for the standard interface use the data type `double`. However, their functionality is identical, and only the `double` version is documented.

The function `ReadCoordinate()` provides the coordinates of the current vertex [μm].

The function `ReadNearestInterfaceNormal()` provides the components of a unit vector in the direction of the nearest interface normal.

`ReadDistanceFromSemiconductorInsulatorInterface()` returns the distance of the current vertex to the nearest semiconductor–insulator interface (in μm) if the current vertex is in a semiconductor region; otherwise, the function returns minus that distance.

`ReadDistanceFromHighkInsulator()` returns the distance of the current vertex to the nearest high-k insulator (in μm). If no high-k insulator is found in the structure, the function returns a value < 0.

`ReadNearestInterfaceOrientation()` returns the auto-orientation framework orientation (as a three-digit integer) that is closest to the actual orientation at the nearest interface vertex (see Auto-Orientation Framework on page 37).

`ReadLayerThickness()` returns the value of the `LayerThickness` array [μm] for the current vertex (see LayerThickness Command on page 310).

`ReadLayerThicknessField()` returns the value of the `LayerThicknessField` array [μm] for the current vertex (see LayerThickness Command on page 310).

The functions `ReadTime()` and `ReadTransientStepSize()` return the simulation time and the current step size during a transient simulation [s]. `ReadTransientStepType()` provides access to the actual transient step type.

The enumeration type `PMI_StepType` is defined for identification:

```
enum PMI_StepType {
   PMI_UndefinedStepType = 0,
   PMI_TR = 1,
   PMI_BDF = 2,
   PMI_BE = 3
}
```

The methods `ReadxMoleFraction()` and `ReadyMoleFraction()` return the x and y mole fractions, respectively.

The methods `ReadDoping(species)` and `ReadDoping(SpeciesName)` return the doping profiles for the current vertex $[\text{cm}^{-3}]$. The string `SpeciesName` is the same as in the file `datexcodes.txt` (see Doping Specification on page 11). The enumeration type `PMI_DopingSpecies` is used to select the doping species, the incomplete ionization doping species, and their derivatives:

```
enum PMI_DopingSpecies {
  // Acceptors
  PMI_BoronActive,      // active Boron concentration
  PMI_BoronChemical,    // chemical Boron concentration
  PMI_AluminumActive,   // active Aluminum concentration
  PMI_AluminumChemical, // chemical Aluminum concentration
  PMI_IndiumActive,     // active Indium concentration
  PMI_IndiumChemical,   // chemical Indium concentration
  PMI_PDopantActive,    // active PDopant concentration
  PMI_PDopantChemical,  // chemical PDopant concentration
  PMI_Acceptor,         // total acceptor concentration

  // incomplete ionization entries
  PMI_AcceptorMinus,    // total incomplete ionization acceptor concentration
  PMI_AcceptorMinusPer_hDensity,
  PMI_AcceptorMinusPerT,

  // Donors
  PMI_PhosphorusActive,   // active Phosphorus concentration
  PMI_PhosphorusChemical, // chemical Phosphorus concentration
  PMI_ArsenicActive,      // active Arsenic concentration
  PMI_ArsenicChemical,    // chemical Arsenic concentration
  PMI_AntimonyActive,     // active Antimony concentration
  PMI_AntimonyChemical,   // chemical Antimony concentration
  PMI_NitrogenActive,     // active Nitrogen concentration
  PMI_NitrogenChemical,   // chemical Nitrogen concentration
  PMI_NDopantActive,      // active NDopant concentration
  PMI_NDopantChemical,    // chemical NDopant concentration
  PMI_Donor,              // total donor concentration
```

```
   // incomplete ionization entries
   PMI_DonorPlus,           // total incomplete ionization donor concentration
   PMI_DonorPlusPer_eDensity,
   PMI_DonorPlusPerT

   // additional species
   PMI_Carbon,
   PMI_CarbonChemical       // chemical Carbon concentration
};
```

> **NOTE** The species `PMI_Acceptor` and `PMI_Donor` are always defined. The
> remaining entries are only defined if they occur in the simulated device.
> The incomplete ionization entries are only accessible if the option
> `IncompleteIonization` is activated (see Chapter 13 on page 277).

The `ReadDielectricConstant` and `ReadSemiconductorDielectricConstant`
methods return the dielectric constant for the current vertex. The second method accounts for
only the dielectric constant in semiconductor.

The `ReadDopingWell()` method returns the index of the doping well for the current vertex
(see Initial Guess for Electrostatic Potential and Quasi-Fermi Potentials in Doping Wells on
page 178).

The method `IsUserFieldDefined()` checks if a user-defined field has been specified. The
enumeration type `PMI_UserFieldIndex` selects the desired field:

```
enum PMI_UserFieldIndex {
    PMI_UserField0, PMI_UserField1, ..., PMI_UserField99
};
```

If a specific user-field is defined, the method `ReadUserField()` reads its value for the current
vertex. For time-dependent user-fields, this is the value written in the last successful time step.
`WriteUserField()` allows the modification of the value of a specific user-field for the
current vertex. It writes to an auxiliary field. After a transient time step is finished, this
auxiliary field becomes the field accessible with `ReadUserField()`.

The method `ReadStress()` returns the value of one of the following stress components:

```
enum PMI_StressIndex {
   PMI_StressXX, PMI_StressYY, PMI_StressZZ,
   PMI_StressYZ, PMI_StressXZ, PMI_StressXY
};
```

Reaction–Diffusion Species Interface (Compute Scope)

For simplified PMI models, the class `PMI_Vertex_Input_Base` provides an interface for the extraction of RD species concentrations. Accessing the species concentrations through this interface supports the automatic derivative computations of the model quantity with respect to the species concentrations. For standard PMI models, such an interface is not supported. If the interface is enabled for the actual PMI model, the following function is available:

- `bool RDSpecies_supported ()`
  Accesses the actual `Input` class support to RD species and their concentrations. If there is no support, the other functions cannot be used. Most of the models do not support this interface.

If the `RDSpecies_supported()` function returns `true`, additional functions can be used:

- `size_t RDSpecies_size ()`
  Returns the number of RD species defined for the actual device. Note that not all of these species can be defined in the actual region.

- `void get_RDSpecies_name (size_t isp, std::string& spname)`
  Returns the name of the species with device index `isp`.

- `bool RDSpecies_is_defined (size_t isp)`
  Returns true if the species with device index `isp` is defined in the actual region.

- `pmi_float RDSpecies_concentration (size_t isp)`
  Returns the value of the concentration of the RD species with device index `isp`.

Experimental Runtime Support Functions

Vertex-based PMI models also have access to the following runtime functions:

```
double ReadScalar (const char* name) const;
void ReadVector (const char* name, double vector [3]) const;
```

These functions can be called in `Compute`, and they provide access to scalar and vector data of Sentaurus Device. See Table 178 on page 1340 and Table 179 on page 1372 for an overview of available data.

> **NOTE** This is an experimental feature, and it is provided 'as is', without warranty of any kind. In particular, you should be aware of the following limitations:
>
> - Whenever you access additional data in Sentaurus Device, you introduce new model dependencies. However, Sentaurus Device is unable to take into account the corresponding derivatives. Therefore, the convergence of the Newton solver may be affected.

- It is possible to introduce cyclic dependencies, which will result in an infinite loop.

Vertex-Based Runtime Support for Multistate Configuration–Dependent Models

The base class `PMI_MSC_Vertex_Interface` provides the same support as `PMI_Vertex_Interface`, plus additional functions needed by models that depend on a multistate configuration (see Chapter 18 on page 473):

```
class PMI_MSC_Vertex_Interface : public PMI_Vertex_Interface
{
public:
  PMI_MSC_Vertex_Interface(const PMI_Environment&,
    const std::string& msconfig_name,
    int model_index,
    const std::string& model_string);

  const std::string& msconfig_name () const;
  size_t nb_states () const;
  std::string& state ( size_t index ) const;
  int model_index () const;
  const std::string& model_string () const;
  virtual void init_parameter (){};
};
```

> **NOTE** In the case of the simplified interface, the base class `PMI_MSC_Vertex_Base` is used instead. However, it provides the same functionality as the base class `PMI_MSC_Vertex_Interface` and, therefore, it is not documented separately.

The constructor argument `msconfig_name` determines the name of the multistate configuration on which the model depends, and the constructor arguments `model_index` and `model_string` are an integer and a string that you can evaluate in your model. You call the constructor `PMI_MSC_Vertex_Interface` only indirectly using constructors of base classes of multistate configuration–dependent PMIs.

The function `nb_states` returns the number of states in the selected multistate configuration, `state` returns the name of a particular state, and `msconfig_name`, `model_index`, and `model_string` return the arguments of the constructor of the same name.

The function `init_parameter` is always called before the parameters are changed. It allows you to keep model-internal data up-to-date in cases such as ramping of parameters.

Mesh-Based Runtime Support

A standard mesh-based PMI is derived from the base class `PMI_Device_Interface`; whereas, a simplified mesh-based PMI is derived from the base class `PMI_Device_Base`. Both base classes provide the following shared functionality:

```
const char* Name () const;

const PMIBaseParam* ReadParameter (const char* name
                                   [, const char* modelName]) const;
double InitParameter (const char* name, double defaultvalue
                      [, const char* modelName]) const;
void InitParameter (const char* name, std::vector<double>& value
                    [, const char* modelName]) const;
const char* InitStringParameter (const char* name,
                                 const char* defaultvalue
                                 [, const char* modelName]) const;
void InitStringParameter (const char* name,
                          std::vector<const char*>& value
                          [, const char* modelName]) const;

const des_mesh* Mesh () const;
des_data* Data () const;
```

The method `Name()` returns the name of the PMI model as specified in the command file. The methods `ReadParameter()`, `InitParameter()`, and `InitStringParameter()` read the value of a parameter from the parameter file or command file (see Parameter File of Sentaurus Device on page 1088 and Command File of Sentaurus Device on page 1065). In these methods, `modelName` is an optional argument that allows the value of a parameter to be read from a different PMI model.

> **NOTE** Parameters for a mesh-based PMI must appear in the global parameter section in the parameter file. Regionwise or materialwise parameters are not supported.

The methods `Mesh()` and `Data()` provide access to the mesh and data of Sentaurus Device (see Device Mesh on page 1077 and Device Data on page 1084).

> **NOTE** In the case of the standard interface, the method `Data()` returns a variable of type `des_data`; whereas, in the case of the simplified interface, it returns a variable of type `device_data`. The type `des_data` is based on the data type `double`, and `sdevice_data` uses the data type `pmi_float`. Otherwise, their functionality is identical.

The following interface functions should only be called in the `Compute` function, but not in the constructor. The standard interface provides them as members of the base class `PMI_Device_Interface`; whereas, the simplified interface provides them as members of the base class `PMI_Device_Input_Base`:

```
double ReadTime () const;
double ReadTransientStepSize () const;
PMI_StepType ReadTransientStepType () const;
double ReadLayerThickness (int vertex) const;
double ReadLayerThicknessField (int vertex) const;
```

> **NOTE** The support functions for the simplified interface use the data type `pmi_float`; whereas, the support functions for the standard interface use the data type `double`. However, their functionality is identical, and only the `double` version is documented.

The functions `ReadTime()` and `ReadTransientStepSize()` return the simulation time and the current step size during a transient simulation [s]. `ReadTransientStepType()` provides access to the actual transient step type. The enumeration type `PMI_StepType` is defined for identification:

```
enum PMI_StepType {
   PMI_UndefinedStepType = 0,
   PMI_TR = 1,
   PMI_BDF = 2,
   PMI_BE = 3
}
```

The functions `ReadLayerThickness()` and `ReadLayerThicknessField()` return the corresponding values `LayerThickness` and `LayerThicknessField` (see LayerThickness Command on page 310).

Device Mesh

A device mesh of Sentaurus Device consists of a number of regions. A region is either a contact region consisting of a list of contact vertices or a bulk region consisting of a list of elements. An element is described by a list of vertices.

Vertex

In the file `PMIModels.h`, the class `des_vertex` is declared as follows:

```
class des_vertex {

public:
```

```
        size_t index () const;
        size_t element_vertex_index (const des_element* element) const;

        const double* coord () const;
        double coord (size_t i) const;

        bool equal_coord (des_vertex* v) const;

        size_t size_edge () const;
        des_edge* edge (size_t i) const;

        size_t size_element () const;
        des_element* element (size_t i) const;

        size_t size_region () const;
        des_region* region (size_t i) const;

        size_t size_regioninterface () const;
        des_regioninterface* regioninterface (size_t i) const;
    };
```

The value of `index()` can be used as an index for vertex-based data (see Device Data on page 1084). Similarly, the value of `element_vertex_index()` can be used as an index for element-vertex-based data.

The location of a vertex [μm] is given by its coordinates `coord()`. The two versions of the `coord()` function return the coordinates either as a vector or as individual components. The function `equal_coord()` should be used to check if two vertices have the same coordinates. For example, Sentaurus Device duplicates vertices along heterointerfaces. Consequently, two vertices with different indices can share the same coordinates.

`size_edge()` returns the number of edges connected to a vertex. The method `edge()` can be used to retrieve the i-th edge.

`size_region()` returns the number of regions containing a vertex. The method `region()` can be used to retrieve the i-th region.

`size_regioninterface()` reports how many region interfaces a vertex belongs to. The i-th region interface is returned by the method `regioninterface()`.

Edge

In the file `PMIModels.h`, the class `des_edge` is declared as follows:

```
class des_edge {

public:
   size_t index () const;

   des_vertex* start () const;
   des_vertex* end () const;

   size_t size_element () const;
   des_element* element (size_t i) const;

   size_t size_region () const;
   des_region* region (size_t i) const;
};
```

The value of `index()` can be used as an index for edge-based data (see Device Data on page 1084).

`start()` and `end()` return the first and second vertex connected to the edge, respectively.

`size_element()` returns the number of elements connected to an edge. The method `element()` can be used to retrieve the i-th element.

`size_region()` returns the number of regions containing an edge. The method `region()` can be used to retrieve the i-th region.

Element

In the file `PMIModels.h`, the class `des_element` is declared as follows:

```
class des_element {

public:
   typedef enum { point, line, triangle, rectangle, tetrahedron,
                  pyramid, prism, cuboid, tetrabrick } des_type;

   size_t index () const;

   des_type type () const;

   size_t size_vertex () const;
   des_vertex* vertex (size_t i) const;
```

```
        size_t size_edge () const;
        des_edge* edge (size_t i) const;

        des_bulk* bulk () const;

        size_t element_vertex_offset () const;
};
```

Figure 83 shows the numbering of vertices and edges for all element types.

Figure 83   Vertex and edge numbering

The value of index() can be used as an index for element-based data (see Device Data on page 1084). Similarly, element_vertex_offset() returns the start index for element-vertex-based data in this element.

`type()` returns the type of an element (point, line, triangle, rectangle, tetrahedron, pyramid, prism, cuboid, or tetrabrick). An element is mainly described by its vertices. `size_vertex()` returns the number of vertices in an element, and the method `vertex()` can be used to retrieve the i-th vertex. `size_edge()` returns the number of edges of an element. The method `edge()` can be used to retrieve the i-th edge. The method `bulk()` returns the bulk region containing the element.

Region

In the file `PMIModels.h`, the base class `des_region` is declared as follows:

```
class des_region {

public:
   typedef enum { bulk, contact } des_type;

   virtual des_type type () const = 0;

   std::string name () const;

   size_t size_vertex () const;
   des_vertex* vertex (size_t i) const;

   size_t size_edge () const;
   des_edge* edge (size_t i) const;
};
```

A mesh of Sentaurus Device consists of two types of region: bulk regions and contacts. The virtual method `type()` returns the type of a region. The name of a region is returned by `name()`. `size_vertex()` returns the number of vertices in a region. The method `vertex()` can be used to retrieve the i-th vertex. `size_edge()` returns the number of edges in a region. The method `edge()` can be used to retrieve the i-th edge.

The class `des_bulk` is derived from `des_region`:

```
class des_bulk : public des_region {

public:
   des_type type () const;

   std::string material () const;

   size_t size_element () const;
   des_element* element (size_t i) const;

   size_t size_regioninterface () const;
   des_regioninterface* regioninterface (size_t i) const;
};
```

material() returns the name of the material in a bulk region. size_element() returns the number of elements in a region. The method element() can be used to retrieve the i-th element. size_regioninterface() reports how many region interfaces are connected to this bulk region. The i-th region interface can then be retrieved by the method regioninterface().

Similarly, the class des_contact is also derived from des_region:

```
class des_contact : public des_region {

public:
   des_type type () const;
};
```

Region Interface

A region interface separates two bulk regions. It is described by the following class:

```
class des_regioninterface {

public:
   size_t index () const;

   des_bulk* bulk1 () const;
   des_bulk* bulk2 () const;

   bool is_heterointerface () const;

   size_t size_vertex () const;
   des_vertex* vertex (size_t i) const;
   size_t index (size_t local_vertex_index) const;
};
```

The value of index() is used to access the surface measure array (see Device Data on page 1084).

The two bulk regions connected to a region interface are returned by bulk1() and bulk2().

Use is_heterointerface() to determine if double points exist for this interface. For a heterointerface, each vertex belongs to either region 1 or region 2, but not both. For a regular interface, each vertex belongs to both region 1 and region 2.

The number of vertices contained in a region interface is returned by the method size_vertex(). The i-th vertex can be obtained by invoking vertex(). The method index(size_t local_vertex_index) is used to obtain the correct index for interface-based data (see Device Data on page 1084).

Mesh

In the file `PMIModels.h`, the class `des_mesh` is declared as follows:

```
class des_mesh {

public:
   int dim () const;
   void ref_coordinates (double ref [3][3]) const;
   double ref_coordinates (int i, int j) const;

   size_t size_vertex () const;
   size_t size_element_vertex () const;
   des_vertex* vertex (size_t i) const;

   size_t size_edge () const;
   des_edge* edge (size_t i) const;

   size_t size_element () const;
   des_element* element (size_t i) const;
   void find_elements (double x, double y, double z,
                        std::vector<des_element*>& elements) const;

   size_t size_region () const;
   des_region* region (size_t i) const;

   size_t size_regioninterface () const;
   des_regioninterface* regioninterface (size_t i) const;
};
```

The dimension of the mesh is given by `dim()`. The possible values are 1, 2, and 3. The two `ref_coordinates()` methods provide access to the reference coordinate system, either to the entire matrix or individual components of the matrix. They will return the identity matrix:

$$\text{ref} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{1246}$$

in the case of the unified coordinate system. Otherwise, another coordinate system matrix will be returned.

`size_vertex()` returns the number of vertices in the mesh. Similarly, the function `size_element_vertex()` returns the total number of element vertices in the mesh. The method `vertex()` can be used to retrieve the i-th vertex. `size_edge()` returns the number of edges in the mesh. The method `edge()` can be used to retrieve the i-th edge. `size_element()` returns the number of elements in the mesh. The method `element()` can

be used to retrieve the i-th element. For a given point with coordinates (x, y, z) in units of [µm], the method `find_elements()` computes a list of elements that contain this point.

`size_region()` returns the number of regions in the mesh. The method `region()` can be used to retrieve the i-th region. There are `size_regioninterface()` region interfaces in the mesh, and the i-th interface is returned by invoking `regioninterface()`.

Device Data

The class `des_data` provides the following functionality:

```
typedef enum { vertex, edge, element, rivertex, element_vertex } des_location;

const double*const* ReadCoefficient ();
const double*const* ReadMeasure ();
const double*const* ReadSurfaceMeasure ();
const double*const* ReadContactMeasure ();

const double* ReadScalar (des_location location, std::string name,
                          bool update=false);
const double*const* ReadVector (des_location location, std::string name,
                                bool update=false);
void WriteScalar (des_location location, std::string name,
                  const double* newvalue);

const double*const* ReadGradient (des_location location, std::string name,
                                  bool update=false);
const double* ReadFlux (des_location location, std::string name,
                        bool update=false);

size_t NumberOfMSCStates (const std::string& msc_name) const;
bool ReadMSCStateName (const std::string& msc_name, size_t state_index,
                       std::string& state_name) const;
bool ReadMSCOccupations (const std::string& msc_name,
                         const des_region* region,
                         double*const* values) const;

double ReadeSHEDistribution (des_bulk* r, des_vertex* v, double energy) const;
double ReadhSHEDistribution (des_bulk* r, des_vertex* v, double energy) const;
double ReadeSHETotalDOS (des_bulk* r, double energy) const;
double ReadhSHETotalDOS (des_bulk* r, double energy) const;
double ReadeSHETotalGSV (des_bulk* r, double energy) const;
double ReadhSHETotalGSV (des_bulk* r, double energy) const;

double interpolate (des_element* element,
                    const std::vector<double>& vertex_values,
                    double x, double y, double z,
                    des_interpolation interpolation = linear,
                    double arsinhfactor = 1) const;
```

NOTE   In the case of the simplified interface, the class `sdevice_data` provides the same methods, but uses the data type `pmi_float` instead of `double`. Otherwise, the functionality is identical.

The methods `ReadCoefficient()` and `ReadMeasure()` return the box method coefficients κ_{ij} and measure μ_{ij} used in Sentaurus Device (see Discretization on page 1011).

The `ReadCoefficient()` method returns a two-dimensional array. The two indices are the element index and the local edge number. The units are μm^{-1} in one dimension, 1 in two dimensions, and μm in three dimensions.

The following code fragment reads the coefficients for all element edges:

```
const des_mesh* mesh = Mesh();
des_data* data = Data();
const double*const* coeff = data->ReadCoefficient();
for (size_t eli = 0; eli < mesh->size_element(); eli++) {
  des_element* el = mesh->element(eli);
  for (size_t ei = 0; ei < el->size_edge(); ei++) {
    des_edge* e = el->edge(ei);
    const double c = coeff[el->index()][ei];
  }
}
```

NOTE   The values κ_{ij} returned by `ReadCoefficient()` are element–edge coefficients. The edge coefficients κ_i can be obtained by adding the contributions from all elements connected to an edge i.

The `ReadMeasure()` method returns a two-dimensional array. The two indices are the element index and the local vertex number. The units are μm in one dimension, μm^2 in two dimensions, and μm^3 in three dimensions.

The following code fragment reads the measures for all element vertices:

```
const des_mesh* mesh = Mesh();
des_data* data = Data();
const double*const* measure = data->ReadMeasure();
for (size_t eli = 0; eli < mesh->size_element(); eli++) {
  des_element* el = mesh->element(eli);
  for (size_t vi = 0; vi < el->size_vertex(); vi++) {
    des_vertex* v = el->vertex(vi);
    const double m = measure[el->index()][vi];
  }
}
```

NOTE   The values μ_{ij} returned by `ReadMeasure()` are element–vertex measures. The node measures μ_i can be obtained by adding the contributions from all elements connected to a vertex i.

The method `ReadSurfaceMeasure()` provides the surface measure associated with region interface vertices (edge length [μm] in two dimensions and surface area [μm^2] in three dimensions). The two indices are the region interface index and the local vertex number.

The method `ReadContactMeasure()` provides the contact measure associated with contact vertices (edge length [cm] in two dimensions and contact area [cm^2] in three dimensions). The two indices are the contact index and the local vertex number.

By default, the PMI *read* functions use a caching mechanism to access internal data entries (for performance reasons). The cache is updated after computing the initial values for the Newton process and after convergence of Newton iterations. This means that, during Newton iterations, the read functions return unchanged arrays. The `ReadScalar()`, `ReadVector()`, `ReadGradient()`, and `ReadFlux()` methods have an additional parameter `update` (default is `false`). If `update=true`, these methods will update array values for each call to that function. The standard call of these methods (`update=false`) is a good solution for postprocessing PMI functions (see Current Plot File of Sentaurus Device on page 1239). The `update=false` call of these methods is necessary for PMI models that are used during the Newton process (see Preprocessing for Newton Iterations and Newton Step Control on page 1246).

The methods `ReadScalar()`, `ReadVector()`, and `WriteScalar()` provide access to the data of Sentaurus Device. The values can be located on vertices, edges, elements, or region interfaces. See Table 178 on page 1340 and Table 179 on page 1372 for an overview of available scalar and vector data.

`ReadScalar()` returns a read-only one-dimensional array. Use the `index()` method in the classes `des_vertex`, `des_edge`, or `des_element` to access the array elements. The proper addressing of region interface datasets is shown in the code fragment below.

`ReadVector()` returns a read-only two-dimensional array. The first index selects the dimension (0, 1, 2) and the second index is used in the same way as for scalar data.

`WriteScalar()` writes back a one-dimensional array. The organization of the array is the same as for the arrays obtained with `ReadScalar()`. You must ensure that the size of the array is sufficient to hold all required entries.

`ReadGradient()` returns a 2D array that contains, for each vertex, the gradient of a chosen variable. Thereby, the first index selects the partial derivative:

$$[0] = \left(\frac{\partial}{\partial x}\right), [1] = \left(\frac{\partial}{\partial y}\right), [2] = \left(\frac{\partial}{\partial z}\right) \tag{1247}$$

The second index identifies the vertex. The actual implementation of `ReadGradient()` works for vertex-based datasets only.

`ReadFlux()` returns an array that contains, for each vertex, the surface integral of the gradient of a chosen variable taken over the boundary of the box divided by the box volume. The actual implementation of `ReadFlux()` works for vertex-based datasets only.

The following code fragment traverses all region interfaces and reads the surface measure and a dataset for each region interface vertex:

```
const des_mesh* mesh = Mesh();
des_data* data = Data();
const double*const* surface = data->ReadSurfaceMeasure();
const double* hot_elec = data->ReadScalar(des_data::rivertex,
                                          "HotElectronInj");
for (size_t rii = 0; rii < mesh->size_regioninterface(); rii++) {
   des_regioninterface* ri = mesh->regioninterface(rii);
   for (size_t vi = 0; vi < ri->size_vertex(); vi++) {
      des_vertex* v = ri->vertex(vi);
      const double sm = surface[ri->index()][vi];
      const double he = hot_elec[ri->index(vi)];
   }
}
```

The following code fragment traverses all contacts and reads the contact measure for each contact vertex:

```
const des_mesh* mesh = Mesh();
des_data* data = Data();
const double*const* contact_measure = data->ReadContactMeasure();
for (size_t ri = 0; ri < mesh->size_region(); ri++) {
   des_region* r = mesh->region(ri);
   if (r->type() == des_region::contact) {
      for (size_t vi = 0; vi < r->size_vertex(); vi++) {
         const double m = contact_measure[ri][vi];
      }
   }
}
```

The method `interpolate()` can be called to interpolate a vertex-based field within an element. The location of the interpolation is given by the coordinates (x, y, z) in units of $[\mu m]$. The field values v_i on the element vertices must be supplied in the vector `vertex_values`.

The following code fragment shows the proper usage:

```
std::vector<double> vertex_values;
double x = 1.0;  // interpolation location
double y = 1.0;
```

```
      double z = 1.0;

      for (size_t vi = 0; vi < element->size_vertex (); vi++) {
        des_vertex* v = element->vertex (vi);
        double vertex_value = 1.0;  // value of field on vertex v
        vertex_values.push_back (vertex_value);
      }
      double result = data->interpolate (element, vertex_values, x, y, z,
                                          des_data::arsinh, 10.0);
```

The following interpolation modes are supported:

```
des_data::linear
des_data::logarithmic
des_data::arsinh
```

Depending on the interpolation scheme (linear, logarithmic, or arsinh), the interpolated value *v* is given by:

$$v = \sum_i w_i v_i \tag{1248}$$

$$v = e^{\sum_i w_i \log v_i} \tag{1249}$$

$$v = \frac{1}{f}\sinh\left(\sum_i w_i \, \mathrm{asinh}(fv_i)\right) \tag{1250}$$

Sentaurus Device determines the weights w_i based on the distance of the point (x, y, z) from the vertices of the element. The weights are nonnegative and add up to 1.

Parameter File of Sentaurus Device

For each PMI model, a corresponding section with the same name can appear in the parameter file:

```
PMI_model_name {
   par₁ = value
   par₂ = value
   ...
}
```

NOTE   Parameter names can only consist of alphanumeric characters and underscores (_). The first character must be either a letter or an underscore.

Parameters can be numbers, or strings, or arrays of numbers or strings:

```
PMI_model_name {
  a = 1
  b = "string"
  c = (1.2 3.4 5.6 7.8)
  d = ("red" "blue" "green")
}
```

NOTE   Arrays must consist of either numbers or strings only. Mixed arrays containing both numbers and strings are not supported. An empty array, such as `c=()`, is considered a numeric array of size 0.

The parameters can be specified regionwise and materialwise:

```
Region = "Region.1" {
  PMI_model_name {
  ...
  }
}
Material = "AlGaAs" {
  PMI_model_name {
  ...
  }
}
```

The method `ReadParameter()` can be used to obtain the value of a parameter given its name. `ReadParameter()` returns a pointer to a variable of type `PMIBaseParam`:

```
const PMIBaseParam* p = ReadParameter ("name of parameter");
```

A `NULL` pointer indicates that the parameter has not been defined in the parameter file. Otherwise, the method:

```
PMIBaseParam::ValueType()
```

returns the value type (`PMIBaseParam::real` or `PMIBaseParam::string`) of the parameter. Similarly, the method:

```
PMIBaseParam::DataType()
```

returns the data type (`PMIBaseParam::scalar` or `PMIBaseParam::vector`) of the parameter. In the case of an array parameter, the size of the array can be obtained by:

```
PMIBaseParam::size()
```

The size of scalar parameters is always 1.

Depending on the type of a parameter, its value can be accessed through an assignment statement:

```
double a = *p;                  // real, scalar
double b = (*p)[index];         // real, vector
const char* c= *p;              // string, scalar
const char* d = (*p)[index];    // string, vector
```

An error occurs if the type of a parameter is incompatible with the left-hand side in the assignment statement.

In the case of a real scalar parameter, the method `InitParameter()` checks if the parameter has been specified in the parameter file:

```
double value = InitParameter ("pi", 3.14159);
```

If the parameter has been specified, the given value is taken. Otherwise, the default value is used.

An alternative version of `InitParameter()` is available for vector-valued parameters:

```
std::vector<double> v;
v.push_back (-1);               // default value
v.push_back (-2);               // default value
InitParameter ("vec", v);
```

If the parameter `vec` is found in the parameter file, the vector `v` is redefined with the new values. Otherwise, the existing default values in `v` are left unchanged.

Variants of these two methods are also available for string parameters:

```
const char* value = InitStringParameter ("scalar string", "default value");
std::vector<const char*> s;
InitStringParameter ("vector string parameter", s);
```

> **NOTE** PMI model parameters also can be specified in the command file (see Command File of Sentaurus Device on page 1065). Parameters in the command file take precedence over parameters in the parameter file.

Parallelization

During a parallel simulation, Sentaurus Device may invoke a PMI model concurrently from different threads. Therefore the computational functions must be implemented in a thread-safe manner. The following rules guarantee a thread-safe PMI:

- Do not use global variables.

- Class variables are only modified in the constructor and destructor. Class variables may be read in the computational functions, but they must not be modified.

- Within the computational functions, all temporary variables are allocated as either automatic variables or dynamic variables with the help of the `new` and `delete` operators.

Thread-Local Storage

The thread-local storage template class `PMI_TLS` provides a mechanism to store data per thread. This can be useful to optimize the runtime performance of a PMI. Consider an example where a large data structure is allocated and deallocated with each `compute` call:

```
class Recombination : public PMI_Recombination_Base {
public:
   ...
   void compute (const Input& input, Output& output)
   {
      BigData data;
      data.initialize ();
      // compute output
   }
};
```

With the help of the template class `PMI_TLS`, a copy of `BigData` is allocated for each thread on demand:

```
class Recombination : public PMI_Recombination_Base {
private:
   PMI_TLS<BigData> Data;

public:
   ...
   void compute (const Input& input, Output& output)
   {
      bool exists;
      BigData& data = Data.local (exists);
      if (!exists) {
         data.initialize ();
```

```
        }
        // compute output
    }
};
```

The function call `Data.local(exists)` creates a new instance of `BigData` for each thread
if it does not exist already. The argument `exists` is used to check if `data` has been freshly
allocated. In this case, `data` is initialized. Otherwise, it was already initialized in a previous
`compute()` call.

The template class `PMI_TLS` is declared as follows:

```
template <typename T> class PMI_TLS {
public:
    T& local (bool& exists);
    T& local ();
    size_t size () const;
    T& operator [] (size_t index);
};
```

Both variants of the method `local()` return a reference to a thread-local element. The optional
argument `exists` indicates whether the element has been newly allocated (`false`), or if it was
already present (`true`).

The function `size()` returns the number of allocated elements. The array access operator `[]`
can be used to iterate over the elements of the container.

> **NOTE**   The array access operator `[]` should only be used in a sequential section
> of the code. For example, it may be used in the destructor of the PMI.

Debugging

Print statements represent the simplest approach for debugging a PMI. They can be inserted
anywhere in the code to print the values of a variable, for example:

```
void Auger_Recombination::
compute (const Input& input, Output& output)

{ output.r = C * (input.n + input.p) *
                (input.n*input.p - input.nie*input.nie);
    if (output.r < 0.0) {
        output.r = 0.0;
    }
    std::cout << "n   = " << input.n << std::endl;
    std::cout << "p   = " << input.p << std::endl;
```

```
        std::cout << "nie = " << input.nie << std::endl;
        std::cout << "r   = " << output.r << std::endl;
    }
```

It is also possible to use a debugger to catch errors in a PMI subroutine. The following instructions apply to `gdb`, the GNU debugger. The same approach also can be adjusted to work with other debuggers:

■ Compile the PMI source code in debug mode by using the `-g` option:

```
    cmi -g pmi_Auger.C
```

■ Determine the name of the Sentaurus Device binary. The command:

```
    sdevice -@ldd
```

should produce output similar to the following:

```
    path to executable: /usr/sentaurus/tcad/N-2017.09/linux64/bin
    executable: sdevice-1.4

    /usr/sentaurus/tcad/N-2017.09/linux64/bin/sdevice-1.4:
      ELF 64-bit LSB executable, AMD x86-64, version 1 (SYSV),
      for GNU/Linux 2.6.9, dynamically linked (uses shared libs), stripped
```

In this example, `/usr/sentaurus/tcad/N-2017.09/linux64/bin/sdevice-1.4` is the name of the Sentaurus Device binary.

■ Start the debugger `gdb` on the Sentaurus Device binary:

```
    gdb /usr/sentaurus/tcad/N-2017.09/linux64/bin/sdevice-1.4
```

■ Verify the setting of the environment variables:

```
    show environment
```

In particular, the variables `STROOT` and `STRELEASE` must be defined properly. If necessary, use the following `gdb` command to define these variables:

```
    set environment STROOT /usr/sentaurus
    set environment STRELEASE N-2017.09
```

■ It is not possible to define a break point in the PMI code until the corresponding shared object file has been loaded. Therefore, run your simulation:

```
    run pp1_des.cmd
```

and watch for messages regarding the loading of shared object files. All the shared object files for PMIs are loaded at the very beginning, usually within seconds of starting Sentaurus Device. Afterwards, use the shortcut keys Ctrl+C to interrupt the simulation.

■ You can now define a break point in the PMI source code, for example:

```
    break pmi_Auger.C:100
```

This command inserts a break point on line 100 in the file `pmi_Auger.C`.

■ After defining all required break points, you can resume the simulation with the command:

```
continue
```

The debugger will now stop whenever the control flow reaches a break point, and all the standard `gdb` commands are available for debugging.

Generation–Recombination Model

The recombination rate R_{net} appears in the electron and hole continuity equations (see).

Dependencies

The recombination rate R_{net} may depend on these variables:

`t`	Lattice temperature $[\mathrm{K}]$
`n`	Electron density $[\mathrm{cm}^{-3}]$
`p`	Hole density $[\mathrm{cm}^{-3}]$
`nie`	Effective intrinsic density $[\mathrm{cm}^{-3}]$
`f`	Absolute value of electric field $[\mathrm{Vcm}^{-1}]$

The PMI model must compute the following results:

`r`	Generation–recombination rate $[\mathrm{cm}^{-3}\mathrm{s}^{-1}]$

In the case of the standard interface, the following derivatives must be computed as well:

`drdt`	Derivative of `r` with respect to `t` $[\mathrm{cm}^{-3}\mathrm{s}^{-1}\mathrm{K}^{-1}]$
`drdn`	Derivative of `r` with respect to `n` $[\mathrm{s}^{-1}]$
`drdp`	Derivative of `r` with respect to `p` $[\mathrm{s}^{-1}]$
`drdnie`	Derivative of `r` with respect to `nie` $[\mathrm{s}^{-1}]$
`drdf`	Derivative of `r` with respect to `f` $[\mathrm{cm}^{-2}\mathrm{s}^{-1}\mathrm{V}^{-1}]$

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_Recombination : public PMI_Vertex_Interface {

public:
  PMI_Recombination (const PMI_Environment& env);
  virtual ~PMI_Recombination ();
  virtual useCorrectedDensities() {return false;}

  virtual void Compute_r
    (const double t, const double n, const double p,
     const double nie, const double f, double& r) = 0;

  virtual void Compute_drdt
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdt) = 0;

  virtual void Compute_drdn
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdn) = 0;

  virtual void Compute_drdp
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdp) = 0;

  virtual void Compute_drdnie
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdnie) = 0;
  virtual void Compute_drdf
    (const double t, const double n, const double p,
     const double nie, const double f, double& drdf) = 0;
};
```

The prototype for the virtual constructor is:

```
typedef PMI_Recombination* new_PMI_Recombination_func
  (const PMI_Environment& env);
extern "C" new_PMI_Recombination_func new_PMI_Recombination;
```

By default, Sentaurus Device assumes that a PMI generation–recombination model depends on the electric field. However, you can implement the optional function `PMI_Recombination_ElectricField()` to indicate whether the model depends on the electric field.

By default, the generation–recombination PMI passes uncorrected carrier and intrinsic densities regardless of quantum corrections or Fermi statistics activation in the Sentaurus Device command file.

To force Sentaurus Device to pass the corrected carrier and intrinsic densities to the generation–recombination PMI, the virtual function `useCorrectedDensity()` in the PMI must return `true`. For visualization purposes, two new data entries are available:

- `QCEffectiveIntrinsicDensity` is an improved version of `EffectiveIntrinsicDensity` and contains corrections due to Fermi statistics and quantization effects.

- `QCEffectiveBandgap` is the `EffectiveBandgap` with extra narrowing due to the quantum potentials and all the effects implemented through the quantum-potential framework.

If the model does not depend on the electric field (return value of 0), the method `Compute_drdf()` is not called, and the matrix assembly in Sentaurus Device works more efficiently:

```
typedef int PMI_Recombination_ElectricField_func ();
extern "C"
PMI_Recombination_ElectricField_func PMI_Recombination_ElectricField;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_Recombination_Base : public PMI_Vertex_Base {

public:
  class Input : public PMI_Vertex_Input_Base {
  public:
    pmi_float t;    // lattice temperature
    pmi_float n;    // electron density
    pmi_float p;    // hole density
    pmi_float nie;  // effective intrinsic density
    pmi_float f;    // absolute value of electric field
  };

  class Output {
  public:
    pmi_float r;    // recombination rate
  };

  PMI_Recombination_Base (const PMI_Environment& env);
  virtual ~PMI_Recombination_Base ();
```

```
    virtual useCorrectedDensities() {return false;}

    virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_Recombination_Base* new_PMI_Recombination_Base_func
    (const PMI_Environment& env);
extern "C" new_PMI_Recombination_Base_func new_PMI_Recombination_Base;
```

The optional function `PMI_Recombination_ElectricField()` is recognized as well, as in the case of the standard interface.

Example: Auger Recombination

See and .

Nonlocal Generation–Recombination Model

The nonlocal generation–recombination model computes individual electron and hole recombination rates in . The name of the PMI model must appear as a recombination model within the `Physics` section of the command file:

```
Physics {
    Recombination (pmi_model_name)
}
```

The computed electron and hole recombination rates also can be plotted in the `Plot` section:

```
Plot {
    PMIeNonLocalRecombination
    PMIhNonLocalRecombination
}
```

Dependencies

discusses the supported dependencies of nonlocal models. The actual dependencies must be defined with the method `DefineDependencies()`, and the Jacobian matrices must be defined with the method `DefineJacobians()`.

The method `Compute_parallel()` must compute the following results for the vertices defined in the `input` argument:

`elec`	Vector of electron recombination rates $[\text{cm}^{-3}\text{s}^{-1}]$
`hole`	Vector of hole recombination rates $[\text{cm}^{-3}\text{s}^{-1}]$
`J_elec`	Map of electron Jacobian matrices
`J_hole`	Map of hole Jacobian matrices

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_NonLocal_Recombination : public PMI_Device_Interface {

public:
   class Input {
   public:
      const des_region* region;       // all vertices belong to this region
      const std::vector<int>& vertices;  // list of vertices
   };

   class Output {
   public:
      std::vector<double>& elec;   // nonlocal recombination rates (electrons)
      std::vector<double>& hole;   // nonlocal recombination rates (holes)
      des_id_to_jacobian_map& J_elec;  // derivatives (electrons)
      des_id_to_jacobian_map& J_hole;  // derivatives (holes)
   };

   PMI_NonLocal_Recombination (const PMI_Device_Environment& env);
   virtual ~PMI_NonLocal_Recombination ();

   virtual void DefineDependencies
      (std::vector<des_data::des_id>& dependencies) = 0;

   virtual void DefineJacobians (des_id_to_jacobian_map& J_elec,
                                 des_id_to_jacobian_map& J_hole) = 0;

   virtual void Compute_parallel (const Input& input, Output& output) = 0;

   virtual bool NeedNewEdges () { return false; }
};
```

The prototype for the virtual constructor is:

```
typedef PMI_NonLocal_Recombination* new_PMI_NonLocal_Recombination_func
   (const PMI_Device_Environment& env);
extern "C" new_PMI_NonLocal_Recombination_func new_PMI_NonLocal_Recombination;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_NonLocal_Recombination_Base : public PMI_Device_Base {

public:
   class Input : public PMI_Device_Input_Base {
   public:
      const des_region* region;          // all vertices belong to this region
      const std::vector<int>& vertices;  // list of vertices
   };

   class Output {
   public:
      std::vector<pmi_float>& elec;
                                   // nonlocal recombination rates (electrons)
      std::vector<pmi_float>& hole;  // nonlocal recombination rates (holes)
      sdevice_id_to_jacobian_map& J_elec;  // derivatives (electrons)
      sdevice_id_to_jacobian_map& J_hole;  // derivatives (holes)
   };

   PMI_NonLocal_Recombination_Base (const PMI_Device_Environment& env);
   virtual ~PMI_NonLocal_Recombination_Base ();

   virtual void DefineDependencies
      (std::vector<sdevice_data::sdevice_id>& dependencies) = 0;

   virtual void DefineJacobians (sdevice_id_to_jacobian_map& J_elec,
                                 sdevice_id_to_jacobian_map& J_hole) = 0;

   virtual void Compute_parallel (const Input& input, Output& output) = 0;

   virtual bool NeedNewEdges () { return false; }
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_NonLocal_Recombination_Base*
   new_PMI_NonLocal_Recombination_Base_func
      (const PMI_Device_Environment& env);
```

```
extern "C" new_PMI_NonLocal_Recombination_Base_func
   new_PMI_NonLocal_Recombination_Base;
```

Example: Point-to-Point Tunneling Model

This example is presented in Example: Point-to-Point Tunneling Model on page 1056.

Avalanche Generation Model

The generation rate due to impact ionization can be expressed as:

$$G^{\parallel} = \alpha_n n v_n + \alpha_p p v_p \tag{1251}$$

where α_n and α_p are the ionization coefficients for electrons and holes, respectively (compare with Eq. 419, p. 406). The PMI in Sentaurus Device allows you to redefine the calculation of α_n and α_p.

Dependencies

The ionization coefficients α_n and α_p may depend on the following variables:

`F`	Driving force [Vcm^{-1}]
`t`	Lattice temperature [K]
`bg`	Band gap [eV]
`ct`	Carrier temperature [K]
`currentWoMob[3]`	Current without mobility [cm^{-4}AVs]

The parameter `ct` represents the electron temperature during the calculation of α_n and the hole temperature during the calculation of α_p.

The parameter `currentWoMob` can be used to compute anisotropic avalanche generation. Only the first d components of the vector `currentWoMob` are defined, where d is equal to the dimension of the problem. It is recommended that only the direction of the vector `currentWoMob` is taken into account, but not its magnitude.

The PMI model must compute the following results:

`alpha`	Ionization coefficient $[\text{cm}^{-1}]$

In the case of the standard interface, the following derivatives must be computed as well:

`dalphadF`	Derivative of `alpha` with respect to `F` $[\text{V}^{-1}]$
`dalphadt`	Derivative of `alpha` with respect to `t` $[\text{cm}^{-1}\text{K}^{-1}]$
`dalphadbg`	Derivative of `alpha` with respect to `bg` $[\text{cm}^{-1}\text{eV}^{-1}]$
`dalphadct`	Derivative of `alpha` with respect to `ct` $[\text{cm}^{-1}\text{K}^{-1}]$
`dalphadcurrentWoMob[3]`	Derivative of `alpha` with respect to `currentWoMob` $[\text{cm}^3\text{A}^{-1}\text{V}^{-1}\text{s}^{-1}]$

Only the first d components of the vector `dalphadcurrentWoMob` need to be computed.

Standard C++ Interface

Different driving forces for avalanche generation can be selected in the command file. The enumeration type `PMI_AvalancheDrivingForce`, defined in `PMIModels.h`, is used to reflect your selection:

```
enum PMI_AvalancheDrivingForce {
   PMI_AvalancheElectricField,
   PMI_AvalancheParallelElectricField,
   PMI_AvalancheGradQuasiFermi,
   PMI_AvalancheCarrierTemperatureCanali
};
```

The following base class is declared in the file `PMIModels.h`:

```
class PMI_Avalanche : public PMI_Vertex_Interface {

private:
  const PMI_AvalancheDrivingForce drivingForce;

public:
  PMI_Avalanche (const PMI_Environment& env,
                 const PMI_AvalancheDrivingForce force);
  virtual ~PMI_Avalanche ();

  PMI_AvalancheDrivingForce AvalancheDrivingForce () const
    { return drivingForce; }
```

```
virtual void Compute_alpha
  (const double F, const double t, const double bg,
   const double ct, const double currentWoMob[3], double& alpha) = 0;

virtual void Compute_dalphadF
  (const double F, const double t, const double bg,
   const double ct, const double currentWoMob[3], double& dalphadF) = 0;

virtual void Compute_dalphadt
  (const double F, const double t, const double bg,
   const double ct, const double currentWoMob[3], double& dalphadt) = 0;

virtual void Compute_dalphadbg
  (const double F, const double t, const double bg,
   const double ct, const double currentWoMob[3], double& dalphadbg) = 0;

virtual void Compute_dalphadct
  (const double F, const double t, const double bg,
   const double ct, const double currentWoMob[3], double& dalphadct) = 0;

virtual void Compute_dalphadcurrentWoMob
  (const double F, const double t, const double bg,
   const double ct, const double currentWoMob[3],
   double dalphadcurrentWoMob[3]) = 0;
};
```

Two virtual constructors are required for the calculation of the ionization coefficients α_n and α_p:

```
typedef PMI_Avalanche* new_PMI_Avalanche_func
  (const PMI_Environment& env, const PMI_AvalancheDrivingForce force);
extern "C" new_PMI_Avalanche_func new_PMI_e_Avalanche;
extern "C" new_PMI_Avalanche_func new_PMI_h_Avalanche;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_Avalanche_Base : public PMI_Vertex_Base {

public:
  class Input : public PMI_Vertex_Input_Base {
  public:
    pmi_float F;               // driving force
    pmi_float t;               // lattice temperature
    pmi_float bg;              // band gap
```

```
  pmi_float ct;                // carrier temperature
  pmi_float currentWoMob[3];   // current density (without mobility)
};

class Output {
public:
  pmi_float alpha;             // ionization coefficient
};

PMI_Avalanche_Base (const PMI_Environment& env,
                    const PMI_AvalancheDrivingForce force);
virtual ~PMI_Avalanche_Base ();

PMI_AvalancheDrivingForce AvalancheDrivingForce () const;

virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_Avalanche_Base* new_PMI_Avalanche_Base_func
  (const PMI_Environment& env, const PMI_AvalancheDrivingForce force);
extern "C" new_PMI_Avalanche_Base_func new_PMI_e_Avalanche_Base;
extern "C" new_PMI_Avalanche_Base_func new_PMI_h_Avalanche_Base;
```

Example: Okuto Model

Okuto and Crowell propose the following expression for the ionization coefficient α:

$$\alpha(F) = a[1 + c(T - T_0)]F\exp\left[-\left(\frac{b[1 + d(T - T_0)]}{F}\right)^2\right] \tag{1252}$$

This built-in model is discussed in Okuto–Crowell Model on page 417 and its implementation as a PMI model is:

```
#include "PMIModels.h"

class Okuto_Avalanche : public PMI_Avalanche {

protected:
  const double T0;
  double a, b, c, d;

public:
  Okuto_Avalanche (const PMI_Environment& env,
                   const PMI_AvalancheDrivingForce force);
```

```
  ~Okuto_Avalanche ();

  void Compute_alpha
    (const double F, const double t, const double bg,
     const double ct, const double currentWoMob[3], double& alpha);

  void Compute_dalphadF
    (const double F, const double t, const double bg,
     const double ct, const double currentWoMob[3], double& dalphadF);

  void Compute_dalphadt
    (const double F, const double t, const double bg,
     const double ct, const double currentWoMob[3], double& dalphadt);

  void Compute_dalphadbg
    (const double F, const double t, const double bg,
     const double ct, const double currentWoMob[3], double& dalphadbg);

  void Compute_dalphadct
    (const double F, const double t, const double bg,
     const double ct, const double currentWoMob[3], double& dalphadct);

  void Compute_dalphadcurrentWoMob
    (const double F, const double t, const double bg,
     const double ct, const double currentWoMob[3], double
dalphadcurrentWoMob[3]);
};

Okuto_Avalanche::
Okuto_Avalanche (const PMI_Environment& env,
                const PMI_AvalancheDrivingForce force) :
  PMI_Avalanche (env, force),
  T0 (300.0)
{
}

Okuto_Avalanche::
~Okuto_Avalanche ()
{
}

void Okuto_Avalanche::
Compute_alpha (const double F, const double t, const double bg,
               const double ct, const double currentWoMob[3], double& alpha)
{ const double aa = a * (1.0 + c * (t - T0));
  const double bb = b * (1.0 + d * (t - T0)) / F;
  alpha = aa * F * exp (-bb*bb);
}
```

```
void Okuto_Avalanche::
Compute_dalphadF (const double F, const double t, const double bg,
                    const double ct, const double currentWoMob[3], double&
dalphadF)
{ const double aa = a * (1.0 + c * (t - T0));
  const double bb = b * (1.0 + d * (t - T0)) / F;
  const double alpha = aa * F * exp (-bb*bb);
  dalphadF = (alpha / F) * (1.0 + 2.0*bb*bb);
}

void Okuto_Avalanche::
Compute_dalphadt (const double F, const double t, const double bg,
                    const double ct, const double currentWoMob[3], double&
dalphadt)
{ const double aa = a * (1.0 + c * (t - T0));
  const double bb = b * (1.0 + d * (t - T0)) / F;
  const double tmp = F * exp (-bb*bb);
  dalphadt = tmp * (a * c - 2.0 * aa * bb * b * d / F);
}

void Okuto_Avalanche::
Compute_dalphadbg (const double F, const double t, const double bg,
                    const double ct, const double currentWoMob[3], double&
dalphadbg)
{ dalphadbg = 0.0;
}

void Okuto_Avalanche::
Compute_dalphadct (const double F, const double t, const double bg,
                    const double ct, const double currentWoMob[3], double&
dalphadct)
{ dalphadct = 0.0;
}

void Okuto_Avalanche::
Compute_dalphadcurrentWoMob (const double F, const double t, const double bg,
                              const double ct, const double currentWoMob[3],
                              double dalphadcurrentWoMob[3])
{ const int dim = ReadDimension ();
  for (int k = 0; k < dim; k++) {
    dalphadcurrentWoMob [k] = 0.0;
  }
}

class Okuto_e_Avalanche : public Okuto_Avalanche {

public:
```

```
      Okuto_e_Avalanche (const PMI_Environment& env,
                          const PMI_AvalancheDrivingForce force);

      ~Okuto_e_Avalanche () {}
    };

    Okuto_e_Avalanche::
    Okuto_e_Avalanche (const PMI_Environment& env,
                       const PMI_AvalancheDrivingForce force) :
      Okuto_Avalanche (env, force)
    { // default values
      a = InitParameter ("a_e", 0.426);
      b = InitParameter ("b_e", 4.81e5);
      c = InitParameter ("c_e", 3.05e-4);
      d = InitParameter ("d_e", 6.86e-4);
    }

    class Okuto_h_Avalanche : public Okuto_Avalanche {

    public:
      Okuto_h_Avalanche (const PMI_Environment& env,
                          const PMI_AvalancheDrivingForce force);

      ~Okuto_h_Avalanche () {}
    };

    Okuto_h_Avalanche::
    Okuto_h_Avalanche (const PMI_Environment& env,
                       const PMI_AvalancheDrivingForce force) :
      Okuto_Avalanche (env, force)
    { // default values
      a = InitParameter ("a_h", 0.243);
      b = InitParameter ("b_h", 6.53e+5);
      c = InitParameter ("c_h", 5.35e-4);
      d = InitParameter ("d_h", 5.67e-4);
    }

    extern "C"
    PMI_Avalanche* new_PMI_e_Avalanche
      (const PMI_Environment& env, const PMI_AvalancheDrivingForce force)
    { return new Okuto_e_Avalanche (env, force);
    }

    extern "C"
    PMI_Avalanche* new_PMI_h_Avalanche
      (const PMI_Environment& env, const PMI_AvalancheDrivingForce force)
    { return new Okuto_h_Avalanche (env, force);
    }
```

Mobility Models

Sentaurus Device supports three types of PMI mobility models:

- Doping-dependent mobility
- Mobility degradation at interfaces
- High-field saturation

PMI and built-in models can be used simultaneously. See Chapter 15 on page 317 for more information about how the contributions of the different models are combined. PMI mobility models support anisotropic calculations and can be evaluated along different crystallographic axes. The enumeration type:

```
enum PMI_AnisotropyType {
    PMI_Isotropic,
    PMI_Anisotropic
};
```

determines the axis. The default is isotropic mobility. If anisotropic mobilities are activated in the command file, the PMI mobility classes are also instantiated in the anisotropic direction.

Doping-Dependent Mobility

A doping-dependent PMI model must account for both the constant mobility and doping-dependent mobility models discussed in Mobility due to Phonon Scattering on page 318 and Doping-Dependent Mobility Degradation on page 318.

Dependencies

The constant mobility and doping-dependent mobility μ_{dop} may depend on the following variables:

t	Lattice temperature [K]
n	Electron density [cm^{-3}]
p	Hole density [cm^{-3}]

The PMI model must compute the following results:

m   Mobility μ_{dop} $[cm^2 V^{-1} s^{-1}]$

In the case of the standard interface, the following derivatives must be computed as well:

dmdn   Derivative of μ_{dop} with respect to n $[cm^5 V^{-1} s^{-1}]$

dmdp   Derivative of μ_{dop} with respect to p $[cm^5 V^{-1} s^{-1}]$

dmdt   Derivative of μ_{dop} with respect to t $[cm^2 V^{-1} s^{-1} K^{-1}]$

In most cases, it is not necessary to compute the derivatives with respect to the dopant concentrations.

However, to model random dopant fluctuations (see Random Dopant Fluctuations on page 683), the PMI model must override the functions that compute the following values:

dmdNa   Derivative of μ_{dop} with respect to the acceptor concentration $[cm^5 V^{-1} s^{-1}]$

dmdNd   Derivative of μ_{dop} with respect to the donor concentration $[cm^5 V^{-1} s^{-1}]$

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```cpp
class PMI_DopingDepMobility : public PMI_Vertex_Interface {

private:
  const PMI_AnisotropyType anisoType;

public:
  PMI_DopingDepMobility (const PMI_Environment& env,
                         const PMI_AnisotropyType anisotype);
  virtual ~PMI_DopingDepMobility ();

  PMI_AnisotropyType AnisotropyType () const { return anisoType; }

  virtual void Compute_m
    (const double n, const double p,
     const double t, double& m) = 0;

  virtual void Compute_dmdn
    (const double n, const double p,
     const double t, double& dmdn) = 0;
```

```
virtual void Compute_dmdp
  (const double n, const double p,
   const double t, double& dmdp) = 0;

virtual void Compute_dmdt
  (const double n, const double p,
   const double t, double& dmdt) = 0;

virtual void Compute_dmdNa
  (const double n, const double p,
   const double t, double& dmdNa);

virtual void Compute_dmdNd
  (const double n, const double p,
   const double t, double& dmdNd);
};
```

Two virtual constructors are required for electron and hole mobilities:

```
typedef PMI_DopingDepMobility* new_PMI_DopingDepMobility_func
   (const PMI_Environment& env, const PMI_AnisotropyType anisotype);
extern "C" new_PMI_DopingDepMobility_func new_PMI_DopingDep_e_Mobility;
extern "C" new_PMI_DopingDepMobility_func new_PMI_DopingDep_h_Mobility;
```

Simplified C++ Interface

The following base class is declared in the file PMI.h:

```
class PMI_DopingDepMobility_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
     pmi_float n;         // electron density
     pmi_float p;         // hole density
     pmi_float t;         // lattice temperature
     pmi_float acceptor;  // total acceptor concentration
     pmi_float donor;     // total donor concentration
   };

   class Output {
   public:
     pmi_float m;         // doping-dependent mobility
   };

   PMI_DopingDepMobility_Base (const PMI_Environment& env,
```

```
                                      const PMI_AnisotropyType anisotype);
    virtual ~PMI_DopingDepMobility_Base ();

    PMI_AnisotropyType AnisotropyType () const;

    virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_DopingDepMobility_Base* new_PMI_DopingDepMobility_Base_func
   (const PMI_Environment& env, const PMI_AnisotropyType anisotype);
extern "C" new_PMI_DopingDepMobility_Base_func
   new_PMI_DopingDep_e_Mobility_Base;
extern "C" new_PMI_DopingDepMobility_Base_func
   new_PMI_DopingDep_h_Mobility_Base;
```

Example: Masetti Model

The built-in Masetti model (see Masetti Model on page 320) can also be implemented as a PMI
model:

```
#include "PMIModels.h"

class Masetti_DopingDepMobility : public PMI_DopingDepMobility {
protected:
  const double T0;
  double mumax, Exponent, mumin1, mumin2, mu1, Pc, Cr, Cs, alpha, beta;

public:
  Masetti_DopingDepMobility (const PMI_Environment& env,
                             const PMI_AnisotropyType anisotype);
  ~Masetti_DopingDepMobility () {}

  void Compute_m
    (const double n, const double p,
     const double t, double& m);

  void Compute_dmdn
    (const double n, const double p,
     const double t, double& dmdn);

  void Compute_dmdp
    (const double n, const double p,
     const double t, double& dmdp);

  void Compute_dmdt
```

```
       (const double n, const double p,
        const double t, double& dmdt);
};


Masetti_DopingDepMobility::
Masetti_DopingDepMobility (const PMI_Environment& env,
                           const PMI_AnisotropyType anisotype) :
  PMI_DopingDepMobility (env, anisotype),
  T0 (300.0)
{
}

void Masetti_DopingDepMobility::
Compute_m (const double n, const double p,
           const double t, double& m)
{ const double mu_const = mumax * pow (t/T0, -Exponent);
  const double Ni = Max (ReadDoping (PMI_Donor) +
                         ReadDoping (PMI_Acceptor), 1.0);
  m = mumin1 * exp (-Pc / Ni) +
      (mu_const - mumin2) / (1.0 + pow (Ni / Cr, alpha)) -
      mu1 / (1.0 + pow (Cs / Ni, beta));
}

void Masetti_DopingDepMobility::
Compute_dmdn (const double n, const double p,
              const double t, double& dmdn)
{ dmdn = 0.0;
}

void Masetti_DopingDepMobility::
Compute_dmdp (const double n, const double p,
              const double t, double& dmdp)
{ dmdp = 0.0;
}

void Masetti_DopingDepMobility::
Compute_dmdt (const double n, const double p,
              const double t, double& dmdt)
{ const double Ni = Max (ReadDoping (PMI_Donor) +
                         ReadDoping (PMI_Acceptor), 1.0);
  dmdt = mumax * (-Exponent/T0) * pow (t/T0, -Exponent - 1.0) /
         (1.0 + pow (Ni / Cr, alpha));
}

class Masetti_e_DopingDepMobility : public Masetti_DopingDepMobility {
public:
  Masetti_e_DopingDepMobility (const PMI_Environment& env,
```

```
                                    const PMI_AnisotropyType anisotype);
  ~Masetti_e_DopingDepMobility () {}
};

Masetti_e_DopingDepMobility::
Masetti_e_DopingDepMobility (const PMI_Environment& env,
                            const PMI_AnisotropyType anisotype) :
  Masetti_DopingDepMobility (env, anisotype)

{ // default values
  mumax = InitParameter ("mumax_e", 1417.0);
  Exponent = InitParameter ("Exponent_e", 2.5);
  mumin1 = InitParameter ("mumin1_e", 52.2);
  mumin2 = InitParameter ("mumin2_e", 52.2);
  mu1 = InitParameter ("mu1_e", 43.4);
  Pc = InitParameter ("Pc_e", 0.0);
  Cr = InitParameter ("Cr_e", 9.68e16);
  Cs = InitParameter ("Cs_e", 3.43e20);
  alpha = InitParameter ("alpha_e", 0.680);
  beta = InitParameter ("beta_e", 2.0);
}

class Masetti_h_DopingDepMobility : public Masetti_DopingDepMobility {
public:
  Masetti_h_DopingDepMobility (const PMI_Environment& env,
                              const PMI_AnisotropyType anisotype);
  ~Masetti_h_DopingDepMobility () {}
};

Masetti_h_DopingDepMobility::
Masetti_h_DopingDepMobility (const PMI_Environment& env,
                            const PMI_AnisotropyType anisotype) :
  Masetti_DopingDepMobility (env, anisotype)

{ // default values
  mumax = InitParameter ("mumax_h", 470.5);
  Exponent = InitParameter ("Exponent_h", 2.2);
  mumin1 = InitParameter ("mumin1_h", 44.9);
  mumin2 = InitParameter ("mumin2_h", 0.0);
  mu1 = InitParameter ("mu1_h", 29.0);
  Pc = InitParameter ("Pc_h", 9.23e16);
  Cr = InitParameter ("Cr_h", 2.23e17);
  Cs = InitParameter ("Cs_h", 6.10e20);
  alpha = InitParameter ("alpha_h", 0.719);
  beta = InitParameter ("beta_h", 2.0);
}

extern "C"
```

```
PMI_DopingDepMobility* new_PMI_DopingDep_e_Mobility
  (const PMI_Environment& env, const PMI_AnisotropyType anisotype)
{ return new Masetti_e_DopingDepMobility (env, anisotype);
}

extern "C"
PMI_DopingDepMobility* new_PMI_DopingDep_h_Mobility
  (const PMI_Environment& env, const PMI_AnisotropyType anisotype)
{ return new Masetti_h_DopingDepMobility (env, anisotype);
}
```

Multistate Configuration–Dependent Bulk Mobility

This PMI allows you to implement multistate configuration (MSC)–dependent bulk mobility models.

Command File

To activate a PMI of this type, as an option to `eMobility`, `hMobility`, or `Mobility` in the `Physics` section, specify:

```
DopingDependence(
  PMIModel (
    Name = <string>
    MSConfig = <string>
    Index = <int>
    String = <string>
  )
)
```

The options of `PMIModel` are described in .

Dependencies

The mobility may depend on the variables:

n   Electron density $[\text{cm}^{-3}]$

p   Hole density $[\text{cm}^{-3}]$

T   Lattice temperature $[\text{K}]$

eT   Electron temperature $[K]$

hT   Hole temperature $[K]$

s   Multistate configuration occupation probabilities $[1]$

The model must compute the following quantities:

val   Mobility μ_{dop} $[\mathrm{cm^2V^{-1}s^{-1}}]$

In the case of the standard interface, the following derivatives must be computed as well:

dval_dn   Derivative with respect to electron density $[\mathrm{cm^5V^{-1}s^{-1}}]$

dval_dp   Derivative with respect to hole density $[\mathrm{cm^5V^{-1}s^{-1}}]$

dval_dT   Derivative with respect to lattice temperature $[\mathrm{cm^2V^{-1}s^{-1}K^{-1}}]$

dval_deT   Derivative with respect to electron temperature $[\mathrm{cm^2V^{-1}s^{-1}K^{-1}}]$

dval_dhT   Derivative with respect to hole temperature $[\mathrm{cm^2V^{-1}s^{-1}K^{-1}}]$

dval_ds   Derivative with respect to multistate configuration occupation probabilities $[\mathrm{cm^2V^{-1}s^{-1}}]$

Standard C++ Interface

The PMI offers a base class that presents the following interface:

```
class PMI_MSC_Mobility : public PMI_MSC_Vertex_Interface
{
public:
  PMI_MSC_Mobility (const PMI_Environment& env,
    const std::string& msconfig_name,
    const int model_index,
    const std::string& model_string,
    const PMI_AnisotropyType aniso);
  // otherwise, see Standard C++ Interface on page 1175
};
```

Apart from the name of the base class and the constructor, the explanations in Standard C++ Interface on page 1175 apply here as well.

The following virtual constructor must be implemented:

```
typedef PMI_MSC_Mobility* new_PMI_MSC_Mobility_func
  (const PMI_Environment& env, const std::string& msconfig_name,
   int model_index, const std::string& model_string,
   const PMI_AnisotropyType anisotype);
extern "C" new_PMI_MSC_Mobility_func new_PMI_MSC_Mobility;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_MSC_Mobility_Base : public PMI_MSC_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      const pmi_float& n () const;   // electron density
      const pmi_float& p () const;   // hole density
      const pmi_float& T () const;   // lattice temperature
      const pmi_float& eT () const;  // electron temperature
      const pmi_float& hT () const;  // hole temperature
      const pmi_float& s (size_t ind) const;  // phase fraction
   };

   class Output {
   public:
      pmi_float& val ();    // mobility
   };

   PMI_MSC_Mobility_Base (const PMI_Environment& env,
                          const std::string& msconfig_name,
                          const int model_index,
                          const std::string& model_string,
                          const PMI_AnisotropyType anisotype);
   virtual ~PMI_MSC_Mobility_Base ();

   PMI_AnisotropyType AnisotropyType () const;

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_MSC_Mobility_Base* new_PMI_MSC_Mobility_Base_func
   (const PMI_Environment& env, const std::string& msconfig_name,
    const int model_index, const std::string& model_string,
```

```
        const PMI_AnisotropyType anisotype);
    extern "C" new_PMI_MSC_Mobility_Base_func new_PMI_MSC_Mobility_Base;
```

Mobility Degradation at Interfaces

Sentaurus Device uses Mathiessen's rule:

$$\frac{1}{\mu} = \frac{1}{\mu_{dop}} + \frac{1}{\mu_{enormal}} \tag{1253}$$

to combine the constant and doping-dependent mobility μ_{dop}, and the surface contribution $\mu_{enormal}$ (see Mobility Degradation at Interfaces on page 332). To express no mobility degradation, for example, in the bulk of a device, it is necessary to set $\mu_{enormal} = \infty$. To avoid numeric difficulties, the PMI requires the calculation of the inverse mobility $1/\mu_{enormal}$ instead of $\mu_{enormal}$.

As an additional precaution, Sentaurus Device does not evaluate the PMI model if the normal electric field $F_{\perp}$ is less than `EnormMinimum`, where `EnormMinimum` is a parameter that can be specified in the `PMI_model_name` section of the parameter file. By default, `EnormMinimum = 1 V/cm` is used.

Dependencies

The mobility degradation at interfaces may depend on the following variables:

`dist`	Distance to nearest interface [cm]
`pot`	Electrostatic potential [V]
`enorm`	Normal electric field $[\mathrm{Vcm}^{-1}]$
`t`	Lattice temperature [K]
`n`	Electron density $[\mathrm{cm}^{-3}]$
`p`	Hole density $[\mathrm{cm}^{-3}]$
`ct`	Carrier temperature [K]

> **NOTE** If Sentaurus Device cannot determine the distance to the nearest interface, the value of $dist = 10^{10}$ is used.

NOTE   The carrier temperature `ct` represents the electron temperature during the evaluation of the model for electrons, and the hole temperature during the evaluation of the model for holes. The parameter `ct` is only defined for hydrodynamic simulations. Otherwise, the value of `ct = 0` is used.

The PMI model must compute the following results:

`muinv`   Inverse of mobility $1/\mu_{enormal}$ $[\,cm^{-2}Vs\,]$

In the case of the standard interface, the following derivatives must be computed as well:

`dmuinvdpot`   Derivative of $1/\mu_{enormal}$ with respect to `pot` $[\,cm^{-2}s\,]$

`dmuinvdenorm` Derivative of $1/\mu_{enormal}$ with respect to `enorm` $[\,cm^{-1}s\,]$

`dmuinvdn`   Derivative of $1/\mu_{enormal}$ with respect to `n` $[\,cmVs\,]$

`dmuinvdp`   Derivative of $1/\mu_{enormal}$ with respect to `p` $[\,cmVs\,]$

`dmuinvdt`   Derivative of $1/\mu_{enormal}$ with respect to `t` $[\,cm^{-2}VsK^{-1}\,]$

`dmuinvdct`   Derivative of $1/\mu_{enormal}$ with respect to `ct` $[\,cm^{-2}VsK^{-1}\,]$

In most cases, it is not necessary to compute the derivatives with respect to the dopant concentrations. However, to model random dopant fluctuations (see Random Dopant Fluctuations on page 683), the PMI model must override the functions that compute the following values:

`dmuinvdNa`   Derivative of $1/\mu_{enormal}$ with respect to the acceptor concentration $[\,cmVs\,]$

`dmuinvdNd`   Derivative of $1/\mu_{enormal}$ with respect to the donor concentration $[\,cmVs\,]$

Standard C++ Interface

The enumeration type `PMI_EnormalType` describes the type of the normal electric field $F_\perp$:

```
enum PMI_EnormalType {
   PMI_EnormalToCurrent,
   PMI_EnormalToInterface
};
```

The following base class is declared in the file `PMIModels.h`:

```
class PMI_EnormalMobility : public PMI_Vertex_Interface {

public:
  PMI_EnormalMobility (const PMI_Environment& env,
                       const PMI_EnormalType type,
                       const PMI_AnisotropyType anisotype);

  virtual ~PMI_EnormalMobility ();

  PMI_EnormalType EnormalType () const;
  PMI_AnisotropyType AnisotropyType () const;

  virtual void Compute_muinv
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& muinv) = 0;

  virtual void Compute_dmuinvdpot
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& dmuinvdpot) = 0;

  virtual void Compute_dmuinvdenorm
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& dmuinvdenorm) = 0;

  virtual void Compute_dmuinvdn
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& dmuinvdn) = 0;

  virtual void Compute_dmuinvdp
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& dmuinvdp) = 0;

  virtual void Compute_dmuinvdt
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& dmuinvdt) = 0;

  virtual void Compute_dmuinvdct
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& dmuinvdct) = 0;
```

```
   virtual void Compute_dmuinvdNa
     (const double dist, const double pot,
      const double enorm, const double n, const double p,
      const double t, const double ct, double& dmuinvdNa);

   virtual void Compute_dmuinvdNd
     (const double dist, const double pot,
      const double enorm, const double n, const double p,
      const double t, const double ct, double& dmuinvdNd);
};
```

Two virtual constructors are required for electron and hole mobilities:

```
typedef PMI_EnormalMobility* new_PMI_EnormalMobility_func
  (const PMI_Environment& env, const PMI_EnormalType type,
   const PMI_AnisotropyType anisotype);
extern "C" new_PMI_EnormalMobility_func new_PMI_Enormal_e_Mobility;
extern "C" new_PMI_EnormalMobility_func new_PMI_Enormal_h_Mobility;
```

Simplified C++ Interface

The following base class is declared in the file PMI.h:

```
class PMI_EnormalMobility_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      pmi_float dist;      // distance to nearest interface
      pmi_float pot;       // electrostatic potential
      pmi_float enorm;     // normal electric field
      pmi_float n;         // electron density
      pmi_float p;         // hole density
      pmi_float t;         // lattice temperature
      pmi_float ct;        // carrier temperature
      pmi_float acceptor;  // total acceptor concentration
      pmi_float donor;     // total donor concentration
   };

   class Output {
   public:
      pmi_float muinv;     // inverse of mobility degradation
   };

   PMI_EnormalMobility_Base (const PMI_Environment& env,
                             const PMI_EnormalType type,
                             const PMI_AnisotropyType anisotype);
```

```
    virtual ~PMI_EnormalMobility_Base ();

    PMI_EnormalType EnormalType () const;
    PMI_AnisotropyType AnisotropyType () const;

    virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_EnormalMobility_Base* new_PMI_EnormalMobility_Base_func
   (const PMI_Environment& env, const PMI_EnormalType type,
    const PMI_AnisotropyType anisotype);
extern "C" new_PMI_EnormalMobility_Base_func new_PMI_Enormal_e_Mobility_Base;
extern "C" new_PMI_EnormalMobility_Base_func new_PMI_Enormal_h_Mobility_Base;
```

Example: Lombardi Model

This example illustrates the implementation of a slightly simplified Lombardi model (see Mobility Degradation at Interfaces on page 332) using the PMI. The contribution due to acoustic phonon-scattering has the form:

$$\mu_{ac} = \frac{B}{F_\perp} + \frac{CN_i^\lambda}{F_\perp^{1/3}(T/T_0)} \tag{1254}$$

where $T_0 = 300\ \mathrm{K}$.

The contribution due to surface roughness scattering is given by:

$$\mu_{sr} = \left(\frac{F_\perp^2}{\delta} + \frac{F_\perp^3}{\eta}\right)^{-1} \tag{1255}$$

The mobilities μ_{ac} and μ_{sr} are combined according to Mathiessen's rule with an additional damping factor:

$$\frac{1}{\mu_{enormal}} = e^{-\frac{l}{l_{crit}}} \cdot \left(\frac{1}{\mu_{ac}} + \frac{1}{\mu_{sr}}\right) \tag{1256}$$

where l is the distance to the nearest semiconductor–insulator interface point:

```
#include "PMIModels.h"

class Lombardi_EnormalMobility : public PMI_EnormalMobility {
```

```
protected:
  const double T0;
  double B, C, lambda, delta, eta, l_crit;

public:
  Lombardi_EnormalMobility (const PMI_Environment& env,
                            const PMI_EnormalType type,
                            const PMI_AnisotropyType anisotype);


  ~Lombardi_EnormalMobility ();

  void Compute_muinv
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& muinv);

  void Compute_dmuinvdpot
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& dmuinvdpot);

  void Compute_dmuinvdenorm
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& dmuinvdenorm);

  void Compute_dmuinvdn
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& dmuinvdn);

  void Compute_dmuinvdp
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& dmuinvdp);

  void Compute_dmuinvdt
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& dmuinvdt);

  void Compute_dmuinvdct
    (const double dist, const double pot,
     const double enorm, const double n, const double p,
     const double t, const double ct, double& dmuinvdct);
};
```

```
Lombardi_EnormalMobility::
Lombardi_EnormalMobility (const PMI_Environment& env,
                          const PMI_EnormalType type,
                          const PMI_AnisotropyType anisotype) :
  PMI_EnormalMobility (env, type, anisotype),
  T0 (300.0)
{
}


Lombardi_EnormalMobility::
~Lombardi_EnormalMobility ()
{
}


void Lombardi_EnormalMobility::
Compute_muinv (const double dist, const double pot,
               const double enorm, const double n, const double p,
               const double t, const double ct, double& muinv)
{ const double Ni = ReadDoping (PMI_Donor) + ReadDoping (PMI_Acceptor);
  const double denom_ac_inv =
    B + pow (enorm, 2.0/3.0) * C * pow (Ni, lambda) * T0 / t;
  const double mu_ac_inv = enorm / denom_ac_inv;
  const double mu_sr_inv = enorm * enorm / delta + pow (enorm, 3.0) / eta;
  const double damping = exp (-dist/l_crit);
  muinv = damping * (mu_ac_inv + mu_sr_inv);
}


void Lombardi_EnormalMobility::
Compute_dmuinvdpot (const double dist, const double pot,
                    const double enorm, const double n, const double p,
                    const double t, const double ct, double& dmuinvdpot)
{ dmuinvdpot = 0.0;
}


void Lombardi_EnormalMobility::
Compute_dmuinvdenorm (const double dist, const double pot,
                      const double enorm, const double n, const double p,
                      const double t, const double ct, double& dmuinvdenorm)
{ const double Ni = ReadDoping (PMI_Donor) + ReadDoping (PMI_Acceptor);
  const double denom_ac_inv =
    B + pow (enorm, 2.0/3.0) * C * pow (Ni, lambda) * T0 / t;
  const double dmu_ac_inv_denorm =
    (2.0 * B + denom_ac_inv) / (3.0 * denom_ac_inv * denom_ac_inv);
  const double mu_sr_inv_denorm =
    2.0 * enorm / delta + 3.0 * enorm * enorm / eta;
  const double damping = exp (-dist/l_crit);
  dmuinvdenorm = damping * (dmu_ac_inv_denorm + mu_sr_inv_denorm);
}
```

```
void Lombardi_EnormalMobility::
Compute_dmuinvdn (const double dist, const double pot,
                  const double enorm, const double n, const double p,
                  const double t, const double ct, double& dmuinvdn)
{ dmuinvdn = 0.0;
}

void Lombardi_EnormalMobility::
Compute_dmuinvdp (const double dist, const double pot,
                  const double enorm, const double n, const double p,
                  const double t, const double ct, double& dmuinvdp)
{ dmuinvdp = 0.0;
}

void Lombardi_EnormalMobility::
Compute_dmuinvdt (const double dist, const double pot,
                  const double enorm, const double n, const double p,
                  const double t, const double ct, double& dmuinvdt)
{ const double Ni = ReadDoping (PMI_Donor) + ReadDoping (PMI_Acceptor);
  const double factor = pow (enorm, 2.0/3.0) * C * pow (Ni, lambda) * T0;
  const double denom_ac_inv = B + factor / t;
  const double dmu_ac_inv_dt =
    enorm * factor / (denom_ac_inv * denom_ac_inv * t * t);
  const double damping = exp (-dist/l_crit);
  dmuinvdt = damping * dmu_ac_inv_dt;
}

void Lombardi_EnormalMobility::
Compute_dmuinvdct (const double dist, const double pot,
                   const double enorm, const double n, const double p,
                   const double t, const double ct, double& dmuinvdct)
{ dmuinvdct = 0.0;
}

class Lombardi_e_EnormalMobility : public Lombardi_EnormalMobility {
public:
  Lombardi_e_EnormalMobility (const PMI_Environment& env,
                              const PMI_EnormalType type,
                              const PMI_AnisotropyType anisotype);

  ~Lombardi_e_EnormalMobility () {}
};

Lombardi_e_EnormalMobility::
Lombardi_e_EnormalMobility (const PMI_Environment& env,
                            const PMI_EnormalType type,
                            const PMI_AnisotropyType anisotype) :
```

```
      Lombardi_EnormalMobility (env, type, anisotype)
{ // default values
  B = InitParameter ("B_e", 4.750e7);
  C = InitParameter ("C_e", 580.0);
  lambda = InitParameter ("lambda_e", 0.125);
  delta = InitParameter ("delta_e", 5.82e14);
  eta = InitParameter ("eta_e", 5.82e30);
  l_crit = InitParameter ("l_crit_e", 1.0e-6);
}

class Lombardi_h_EnormalMobility : public Lombardi_EnormalMobility {
public:
  Lombardi_h_EnormalMobility (const PMI_Environment& env,
                              const PMI_EnormalType type,
                              const PMI_AnisotropyType anisotype);

  ~Lombardi_h_EnormalMobility () {}
};

Lombardi_h_EnormalMobility::
Lombardi_h_EnormalMobility (const PMI_Environment& env,
                            const PMI_EnormalType type,
                            const PMI_AnisotropyType anisotype) :
  Lombardi_EnormalMobility (env, type, anisotype)
{ // default values
  B = InitParameter ("B_h", 9.925e6);
  C = InitParameter ("C_h", 2947.0);
  lambda = InitParameter ("lambda_h", 0.0317);
  delta = InitParameter ("delta_h", 2.0546e14);
  eta = InitParameter ("eta_h", 2.0546e30);
  l_crit = InitParameter ("l_crit_h", 1.0e-6);
}

extern "C"
PMI_EnormalMobility* new_PMI_Enormal_e_Mobility
  (const PMI_Environment& env, const PMI_EnormalType type,
   const PMI_AnisotropyType anisotype)
{ return new Lombardi_e_EnormalMobility (env, type, anisotype);
}

extern "C"
PMI_EnormalMobility* new_PMI_Enormal_h_Mobility
  (const PMI_Environment& env, const PMI_EnormalType type,
   const PMI_AnisotropyType anisotype)
{ return new Lombardi_h_EnormalMobility (env, type, anisotype);
}
```

High-Field Saturation Model

The high-field saturation model computes the final mobility μ as a function of the low-field mobility μ_{low} and the driving force F_{hfs} (see High-Field Saturation on page 361).

Dependencies

The mobility μ computed by a high-field mobility model may depend on the following variables:

`pot`	Electrostatic potential [V]
`t`	Lattice temperature [K]
`n`	Electron density [cm^{-3}]
`p`	Hole density [cm^{-3}]
`ct`	Carrier temperature [K]
`mulow`	Low-field mobility μ_{low} [$\text{cm}^2\text{V}^{-1}\text{s}^{-1}$]
`F`	Driving force [Vcm^{-1}]

> **NOTE** The carrier temperature `ct` represents the electron temperature during the evaluation of the model for electrons, and the hole temperature during the evaluation of the model for holes. The parameter `ct` is only defined for hydrodynamic simulations. Otherwise, the value of `ct = 0` is used.

The PMI model must compute the following results:

`mu`	Mobility μ [$\text{cm}^2\text{V}^{-1}\text{s}^{-1}$]

In the case of the standard interface, the following derivatives must be computed as well:

`dmudpot`	Derivative of μ with respect to `pot` [$\text{cm}^2\text{V}^{-2}\text{s}^{-1}$]
`dmudn`	Derivative of μ with respect to `n` [$\text{cm}^5\text{V}^{-1}\text{s}^{-1}$]
`dmudp`	Derivative of μ with respect to `p` [$\text{cm}^5\text{V}^{-1}\text{s}^{-1}$]
`dmudt`	Derivative of μ with respect to `t` [$\text{cm}^2\text{V}^{-1}\text{s}^{-1}\text{K}^{-1}$]

dmudct   Derivative of μ with respect to `ct` $[\mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1}\mathrm{K}^{-1}]$

dmudmulow   Derivative of μ with respect to `mulow` (1)

dmudF   Derivative of μ with respect to `F` $[\mathrm{cm}^3\mathrm{V}^{-2}\mathrm{s}^{-1}]$

In most cases, it is not necessary to compute the derivatives with respect to the dopant concentrations. However, to model random dopant fluctuations (see Random Dopant Fluctuations on page 683), the PMI model must override the functions that compute the following values:

dmudNa   Derivative of μ with respect to the acceptor concentration $[\mathrm{cm}^5\mathrm{V}^{-1}\mathrm{s}^{-1}]$

dmudNd   Derivative of μ with respect to the donor concentration $[\mathrm{cm}^5\mathrm{V}^{-1}\mathrm{s}^{-1}]$

Standard C++ Interface

The enumeration type `PMI_HighFieldDrivingForce` describes the driving force as specified in the command file:

```
enum PMI_HighFieldDrivingForce {
  PMI_HighFieldParallelElectricField,
  PMI_HighFieldParallelToInterfaceElectricField,
  PMI_HighFieldGradQuasiFermi
};
```

The following base class is declared in the file `PMIModels.h`:

```
class PMI_HighFieldMobility : public PMI_Vertex_Interface {

private:
  const PMI_HighFieldDrivingForce drivingForce;
  const PMI_AnisotropyType anisoType;

public:
  PMI_HighFieldMobility (const PMI_Environment& env,
                         const PMI_HighFieldDrivingForce force,
                         const PMI_AnisotropyType anisotype);

  virtual ~PMI_HighFieldMobility ();

  PMI_HighFieldDrivingForce HighFieldDrivingForce () const;
  PMI_AnisotropyType AnisotropyType () const;

  virtual void Compute_mu
    (const double pot, const double n,
```

```
        const double p, const double t, const double ct,
        const double mulow, const double F, double& mu) = 0;

    virtual void Compute_dmudpot
      (const double pot, const double n,
       const double p, const double t, const double ct,
       const double mulow, const double F, double& dmudpot) = 0;

    virtual void Compute_dmudn
      (const double pot, const double n,
       const double p, const double t, const double ct,
       const double mulow, const double F, double& dmudn) = 0;

    virtual void Compute_dmudp
      (const double pot, const double n,
       const double p, const double t, const double ct,
       const double mulow, const double F, double& dmudp) = 0;

    virtual void Compute_dmudt
      (const double pot, const double n,
       const double p, const double t, const double ct,
       const double mulow, const double F, double& dmudt) = 0;

    virtual void Compute_dmudct
      (const double pot, const double n,
       const double p, const double t, const double ct,
       const double mulow, const double F, double& dmudct) = 0;

    virtual void Compute_dmudmulow
      (const double pot, const double n,
       const double p, const double t, const double ct,
       const double mulow, const double F, double& dmudmulow) = 0;

    virtual void Compute_dmudF
      (const double pot, const double n,
       const double p, const double t, const double ct,
       const double mulow, const double F, double& dmudF) = 0;

    virtual void Compute_dmudNa
      (const double pot, const double n,
       const double p, const double t, const double ct,
       const double mulow, const double F, double& dmudNa);

    virtual void Compute_dmudNd
      (const double pot, const double n,
       const double p, const double t, const double ct,
       const double mulow, const double F, double& dmudNd);
};
```

Two virtual constructors are required for electron and hole mobilities:

```
typedef PMI_HighFieldMobility* new_PMI_HighFieldMobility_func
   (const PMI_Environment& env, const PMI_HighFieldDrivingForce force,
    const PMI_AnisotropyType anisotype);
extern "C" new_PMI_HighFieldMobility_func new_PMI_HighField_e_Mobility;
extern "C" new_PMI_HighFieldMobility_func new_PMI_HighField_h_Mobility;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_HighFieldMobility_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      pmi_float pot;       // electrostatic potential
      pmi_float n;         // electron density
      pmi_float p;         // hole density
      pmi_float t;         // lattice temperature
      pmi_float ct;        // carrier temperature
      pmi_float mulow;     // low field mobility
      pmi_float F;         // driving force
      pmi_float acceptor;  // total acceptor concentration
      pmi_float donor;     // total donor concentration
   };

   class Output {
   public:
      pmi_float mu;        // mobility
   };

   PMI_HighFieldMobility_Base (const PMI_Environment& env,
                               const PMI_HighFieldDrivingForce force,
                               const PMI_AnisotropyType anisotype);
   virtual ~PMI_HighFieldMobility_Base ();

   PMI_HighFieldDrivingForce HighFieldDrivingForce () const;
   PMI_AnisotropyType AnisotropyType () const;

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_HighFieldMobility_Base* new_PMI_HighFieldMobility_Base_func
   (const PMI_Environment& env, const PMI_HighFieldDrivingForce force,
    const PMI_AnisotropyType anisotype);
extern "C" new_PMI_HighFieldMobility_Base_func
   new_PMI_HighField_e_Mobility_Base;
extern "C" new_PMI_HighFieldMobility_Base_func
   new_PMI_HighField_h_Mobility_Base;
```

Example: Canali Model

This example presents the PMI implementation of the Canali model:

$$\mu = \frac{\mu_{low}}{\left[1 + \left(\frac{\mu_{low}F_{hfs}}{v_{sat}}\right)^{\beta}\right]^{1/\beta}}$$ (1257)

where:

$$\beta = \beta_0 \left(\frac{T}{T_0}\right)^{\beta_{exp}}$$ (1258)

and:

$$v_{sat} = v_{sat0}\left(\frac{T}{T_0}\right)^{v_{sat,exp}}$$ (1259)

The built-in Canali model is discussed in Extended Canali Model on page 363.

```
#include "PMIModels.h"

class Canali_HighFieldMobility : public PMI_HighFieldMobility {

private:
  double beta, vsat, Fabs, val, valb, valb1, valb11b;
  void Compute_internal (const double t, const double mulow,
                         const double F);

protected:
  const double T0;
  double beta0, betaexp, vsat0, vsatexp;

public:
  Canali_HighFieldMobility (const PMI_Environment& env,
                            const PMI_HighFieldDrivingForce force,
```

```
                                const PMI_AnisotropyType anisotype);

   ~Canali_HighFieldMobility ();

   void Compute_mu
     (const double pot, const double n,
      const double p, const double t, const double ct,
      const double mulow, const double F,
      double& mu);

   void Compute_dmudpot
     (const double pot, const double n,
      const double p, const double t, const double ct,
      const double mulow, const double F, double& dmudpot);

   void Compute_dmudn
     (const double pot, const double n,
      const double p, const double t, const double ct,
      const double mulow, const double F, double& dmudn);

   void Compute_dmudp
     (const double pot, const double n,
      const double p, const double t, const double ct,
      const double mulow, const double F, double& dmudp);

   void Compute_dmudt
     (const double pot, const double n,
      const double p, const double t, const double ct,
      const double mulow, const double F, double& dmudt);

   void Compute_dmudct
     (const double pot, const double n,
      const double p, const double t, const double ct,
      const double mulow, const double F, double& dmudct);

   void Compute_dmudmulow
     (const double pot, const double n,
      const double p, const double t, const double ct,
      const double mulow, const double F, double& dmudmulow);

   void Compute_dmudF
     (const double pot, const double n,
      const double p, const double t, const double ct,
      const double mulow, const double F, double& dmudF);
};

void Canali_HighFieldMobility::
Compute_internal (const double t, const double mulow, const double F)
```

```
{ beta = beta0 * pow (t/T0, betaexp);
  vsat = vsat0 * pow (t/T0, -vsatexp);
  Fabs = fabs (F);
  val = mulow * Fabs / vsat;
  valb = pow (val, beta);
  valb1 = 1.0 + valb;
  valb11b = pow (valb1, 1.0/beta);
}

Canali_HighFieldMobility::
Canali_HighFieldMobility (const PMI_Environment& env,
                          const PMI_HighFieldDrivingForce force,
                          const PMI_AnisotropyType anisotype) :
  PMI_HighFieldMobility (env, force, anisotype),
  T0 (300.0)
{
}

Canali_HighFieldMobility::
~Canali_HighFieldMobility ()
{
}


void Canali_HighFieldMobility::
Compute_mu (const double pot, const double n,
            const double p, const double t, const double ct,
            const double mulow, const double F, double& mu)
{ Compute_internal (t, mulow, F);
  mu = mulow / valb11b;
}

void Canali_HighFieldMobility::
Compute_dmudpot (const double pot, const double n,
                 const double p, const double t, const double ct,
                 const double mulow, const double F, double& dmudpot)
{ dmudpot = 0.0;
}

void Canali_HighFieldMobility::
Compute_dmudn (const double pot, const double n,
               const double p, const double t, const double ct,
               const double mulow, const double F, double& dmudn)
{ dmudn = 0.0;
}

void Canali_HighFieldMobility::
Compute_dmudp (const double pot, const double n,
```

```
                    const double p, const double t, const double ct,
                    const double mulow, const double F, double& dmudp)
        { dmudp = 0.0;
        }


        void Canali_HighFieldMobility::
        Compute_dmudt (const double pot, const double n,
                       const double p, const double t, const double ct,
                       const double mulow, const double F, double& dmudt)
        { Compute_internal (t, mulow, F);
          const double mu = mulow / valb11b;
          const double dmudbeta = mu * (log (valb1) / (beta*beta) -
                                        valb * log (val) / (beta * valb1));
          const double dmudvsat = (mu * valb) / (valb1 * vsat);
          const double dbetadt = beta * betaexp / t;
          const double dvsatdt = -vsat * vsatexp / t;
          dmudt = dmudbeta * dbetadt + dmudvsat * dvsatdt;
        }


        void Canali_HighFieldMobility::
        Compute_dmudct (const double pot, const double n,
                        const double p, const double t, const double ct,
                        const double mulow, const double F, double& dmudct)
        { dmudct = 0.0;
        }


        void Canali_HighFieldMobility::
        Compute_dmudmulow (const double pot, const double n,
                           const double p, const double t, const double ct,
                           const double mulow, const double F, double& dmudmulow)
        { Compute_internal (t, mulow, F);
          dmudmulow = 1.0 / (valb1 * valb11b);
        }


        void Canali_HighFieldMobility::
        Compute_dmudF (const double pot, const double n,
                       const double p, const double t, const double ct,
                       const double mulow, const double F, double& dmudF)
        { Compute_internal (t, mulow, F);
          const double mu = mulow / valb11b;
          const double signF = (F >= 0.0) ? 1.0 : -1.0;
          dmudF = -mu * pow (mulow/vsat, beta) * pow (Fabs, beta-1.0) *
                  signF / valb1;
        }


        class Canali_e_HighFieldMobility : public Canali_HighFieldMobility {
        public:
          Canali_e_HighFieldMobility (const PMI_Environment& env,
```

```
                                    const PMI_HighFieldDrivingForce force,
                                    const PMI_AnisotropyType anisotype);

    ~Canali_e_HighFieldMobility () {}
};

Canali_e_HighFieldMobility::
Canali_e_HighFieldMobility (const PMI_Environment& env,
                               const PMI_HighFieldDrivingForce force,
                               const PMI_AnisotropyType anisotype) :
    Canali_HighFieldMobility (env, force, anisotype)
{ // default values
    beta0 = InitParameter ("beta0_e", 1.109);
    betaexp = InitParameter ("betaexp_e", 0.66);
    vsat0 = InitParameter ("vsat0_e", 1.07e7);
    vsatexp = InitParameter ("vsatexp_e", 0.87);
}

class Canali_h_HighFieldMobility : public Canali_HighFieldMobility {
public:
    Canali_h_HighFieldMobility (const PMI_Environment& env,
                                  const PMI_HighFieldDrivingForce force,
                                  const PMI_AnisotropyType anisotype);

    ~Canali_h_HighFieldMobility () {}
};

Canali_h_HighFieldMobility::
Canali_h_HighFieldMobility (const PMI_Environment& env,
                               const PMI_HighFieldDrivingForce force,
                               const PMI_AnisotropyType anisotype) :
    Canali_HighFieldMobility (env, force, anisotype)
{ // default values
    beta0 = InitParameter ("beta0_h", 1.213);
    betaexp = InitParameter ("betaexp_h", 0.17);
    vsat0 = InitParameter ("vsat0_h", 8.37e6);
    vsatexp = InitParameter ("vsatexp_h", 0.52);
}

extern "C"
PMI_HighFieldMobility* new_PMI_HighField_e_Mobility
    (const PMI_Environment& env, const PMI_HighFieldDrivingForce force,
     const PMI_AnisotropyType anisotype)
{ return new Canali_e_HighFieldMobility (env, force, anisotype);
}

extern "C"
PMI_HighFieldMobility* new_PMI_HighField_h_Mobility
```

```
         (const PMI_Environment& env, const PMI_HighFieldDrivingForce force,
          const PMI_AnisotropyType anisotype)
      { return new Canali_h_HighFieldMobility (env, force, anisotype);
      }
```

High-Field Saturation With Two Driving Forces

This PMI allows you to compute the final mobility μ as a function of the low-field mobility μ_{low} and two driving fields (see High-Field Saturation on page 361). One field is the gradient of the quasi-Fermi energy; the other is derived from the electric field (see Driving Force Models on page 369).

Command File

The model is specified using `PMIModel` as an option to `HighFieldSaturation`, `eHighFieldSaturation`, or `hHighFieldSaturation`. The name of the model must be provided with the `Name` parameter of `PMIModel`. Optionally, an index and a string can be specified, which will be passed to and interpreted by the model:

```
eMobility(
   HighFieldSaturation(
      PMIModel (
         Name = <string>
         Index = <int>
         String = <string>)
      EparallelToInterface | Eparallel | ElectricField)
)
```

Dependencies

The high-field mobility may depend on the following variables:

`mulow`	Low-field mobility μ_{low} [$cm^2V^{-1}s^{-1}$]
`n`	Electron density [cm^{-3}]
`p`	Hole density [cm^{-3}]
`T`	Lattice temperature [K]
`cT`	Carrier temperature [K]

`Epar`	Modulus of electric field driving force $[\mathrm{Vcm^{-1}}]$
`gradQF`	Modulus of gradient of the quasi-Fermi energy $[\mathrm{eVcm^{-1}}]$
`EprodQF`	Scalar product of electric field driving force and gradient of quasi-Fermi energy $[\mathrm{eVVcm^{-2}}]$
`Na0`	Acceptor concentration $[\mathrm{cm^{-3}}]$
`Nd0`	Donor concentration $[\mathrm{cm^{-3}}]$

The electric field used to obtain `Epar` is determined by `EparallelToInterface`, `Eparallel`, or `ElectricField` as for other high-field mobility models (see Driving Force Models on page 369). With `EparallelToInterface`, the electric field used to compute `EprodQF` is the projection of the electric field parallel to the interface; otherwise, the full electric field is used to obtain `EprodQF`.

The PMI model must compute the following results:

`val`	High-field mobility μ $[\mathrm{cm^2V^{-1}s^{-1}}]$

In the case of the standard interface, the following derivatives must be computed as well:

`dval_dmulow`	Derivative of μ with respect to `mulow` $[\,1\,]$
`dval_dn`	Derivative of μ with respect to `n` $[\mathrm{cm^5V^{-1}s^{-1}}]$
`dval_dp`	Derivative of μ with respect to `p` $[\mathrm{cm^5V^{-1}s^{-1}}]$
`dval_dT`	Derivative of μ with respect to `T` $[\mathrm{cm^2V^{-1}s^{-1}K^{-1}}]$
`dval_dcT`	Derivative of μ with respect to `cT` $[\mathrm{cm^2V^{-1}s^{-1}K^{-1}}]$
`dval_dEpar`	Derivative of μ with respect to `Epar` $[\mathrm{cm^3V^{-2}s^{-1}}]$
`dval_dgradQF`	Derivative of μ with respect to `gradQF` $[\mathrm{cm^3eV^{-1}V^{-1}s^{-1}}]$
`dval_dEprodQF`	Derivative of μ with respect to `EprodQF` $[\mathrm{cm^4eV^{-1}V^{-2}s^{-1}}]$
`dval_dNa0`	Derivative of μ with respect to `Na0` $[\mathrm{cm^5V^{-1}s^{-1}}]$
`dval_dNd0`	Derivative of μ with respect to `Nd0` $[\mathrm{cm^5V^{-1}s^{-1}}]$

Standard C++ Interface

The PMI base class is declared in `PMIModels.h` as:

```cpp
class PMI_HighFieldMobility2 : public PMI_Vertex_Interface {

public:
   // the input data coming from the simulator
   class idata {
   public:
      double mulow() const;      // low-field mobility
      double n() const;          // electron density
      double p() const;          // hole density
      double T() const;          // lattice temperature
      double cT() const;         // carrier temperature
      double Epar() const;       // parallel electric field
      double gradQF() const;     // gradient of quasi-Fermi energy
      double EprodQF() const;    // product gradient QF and electric field
      double Na0() const;        // acceptor concentration
      double Nd0() const;        // donor concentration
   };

   // the results computed by the PMI
   class odata {
   public:
      double& val();             // mobility
      double& dval_dmulow();     // derivative wrt. low-field mobility
      double& dval_dn();         // wrt. electron density
      double& dval_dp();         // wrt. hole density
      double& dval_dT();         // wrt. lattice temperature
      double& dval_dcT();        // wrt. carrier temperature
      double& dval_dEpar();      // wrt. parallel electric field
      double& dval_dgradQF();    // wrt. gradient of quasi-Fermi energy
      double& dval_dEprodQF();   // wrt. product gradient QF and field
      double& dval_dNa0();       // wrt. acceptor concentration
      double& dval_dNd0();       // wrt. donor concentration
   };

   // constructor and destructor
   PMI_HighFieldMobility2(const PMI_Environment& env,
                          const int model_index,
                          const std::string& model_string,
                          const PMI_AnisotropyType anisotype);
   virtual ~PMI_HighFieldMobility2();

   PMI_AnisotropyType AnisotropyType () const;
```

```
// compute value and derivatives
virtual void compute(const idata* id, odata* od) = 0;
};
```

The `Compute` function receives its input from `id`. It returns the results using `od` by assignment using the member functions of `od`. The framework initializes the values of the derivatives to zero, so you only have to compute derivatives for variables the PMI actually uses.

The following virtual constructor must be implemented:

```
typedef PMI_HighFieldMobility2* new_PMI_HighFieldMobility2_func
   (const PMI_Environment& env,
    int model_index,
    const std::string& model_string,
    const PMI_AnisotropyType anisotype);
extern "C" new_PMI_HighFieldMobility2_func new_PMI_HighFieldMobility2;
```

Simplified C++ Interface

The following base class is declared in `PMI.h`:

```
class PMI_HighFieldMobility2_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      Input (const PMI_HighFieldMobility2_Base* highfieldmobility2_base,
             const int vertex);
      pmi_float mulow;      // low-field mobility
      pmi_float n;          // electron density
      pmi_float p;          // hole density
      pmi_float T;          // lattice temperature
      pmi_float cT;         // carrier temperature
      pmi_float Epar;       // parallel electric field
      pmi_float gradQF;     // gradient of quasi-Fermi energy
      pmi_float EprodQF;    // product gradient QF and electric field
      pmi_float Na0;        // acceptor concentration
      pmi_float Nd0;        // donor concentration
   };

   class Output {
   public:
      pmi_float val;        // mobility
   };

   PMI_HighFieldMobility2_Base (const PMI_Environment& env,
                                const int model_index,
```

```
                                         const std::string& model_string,
                                         const PMI_AnisotropyType anisotype);
      virtual ~PMI_HighFieldMobility2_Base ();

      int model_index () const;
      const std::string& model_string () const;
      PMI_AnisotropyType AnisotropyType () const;

      virtual void compute (const Input& input, Output& output) = 0;
   };
```

The following virtual constructor is provided:

```
typedef PMI_HighFieldMobility2_Base* new_PMI_HighFieldMobility2_Base_func
   (const PMI_Environment& env, const int model_index,
    const std::string& model_string, const PMI_AnisotropyType anisotype);
extern "C"
new_PMI_HighFieldMobility2_Base_func new_PMI_HighField_Mobility2_Base;
```

Band Gap

Sentaurus Device provides a PMI to compute the energy band gap E_g in a semiconductor. It can be specified in the `Physics` section of the command file, for example:

```
Physics {
   EffectiveIntrinsicDensity (
      BandGap (pmi_model_name)
   )
}
```

The default bandgap model in Sentaurus Device is selected explicitly by the keyword `Default`:

```
Physics {
   EffectiveIntrinsicDensity (
      BandGap (Default)
   )
}
```

Dependencies

The band gap E_g may depend on:

t   Lattice temperature [K]

The PMI model must compute the following results:

bg   Band gap E_g [eV]

In the case of the standard interface, the following derivatives must be computed as well:

dbgdt   Derivative of bg with respect to t [eVK^{-1}]

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_BandGap : public PMI_Vertex_Interface {

public:
  PMI_BandGap (const PMI_Environment& env);
  virtual ~PMI_BandGap ();

  virtual void Compute_bg
    (const double t, double& bg) = 0;

  virtual void Compute_dbgdt
    (const double t, double& dbgdt) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_BandGap* new_PMI_BandGap_func (const PMI_Environment& env);
extern "C" new_PMI_BandGap_func new_PMI_BandGap;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_BandGap_Base : public PMI_Vertex_Base {

public:
  class Input : public PMI_Vertex_Input_Base {
  public:
    pmi_float t;    // lattice temperature
  };

  class Output {
  public:
```

```
    pmi_float bg;    // band gap
  };

  PMI_BandGap_Base (const PMI_Environment& env);
  virtual ~PMI_BandGap_Base ();

  virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_BandGap_Base* new_PMI_BandGap_Base_func
    (const PMI_Environment& env);
extern "C" new_PMI_BandGap_Base_func new_PMI_BandGap_Base;
```

Example: Default Bandgap Model

Sentaurus Device uses the following default bandgap model:

$$E_g(t) = E_g(0) - \frac{\alpha t^2}{t + \beta} \tag{1260}$$

$E_g(0)$ denotes the band gap at $0\,\mathrm{K}$.

```
#include "PMIModels.h"

class Default_BandGap : public PMI_BandGap {

private:
  double Eg0, alpha, beta;

public:
  Default_BandGap (const PMI_Environment& env);

  ~Default_BandGap ();

  void Compute_bg (const double t, double& bg);

  void Compute_dbgdt (const double t, double& dbgdt);
};

Default_BandGap::
Default_BandGap (const PMI_Environment& env) :
  PMI_BandGap (env)
{ Eg0 = InitParameter ("Eg0", 1.16964);
  alpha = InitParameter ("alpha", 4.73e-4);
  beta = InitParameter ("beta", 636);
```

```
}

Default_BandGap::
~Default_BandGap ()
{
}

void Default_BandGap::
Compute_bg (const double t, double& bg)
{ bg = Eg0 - alpha * t * t / (t + beta);
}

void Default_BandGap::
Compute_dbgdt (const double t, double& dbgdt)
{ dbgdt = - alpha * t * (t + 2.0 * beta) / ((t + beta) * (t + beta));
}
extern "C"
PMI_BandGap* new_PMI_BandGap
  (const PMI_Environment& env)
{ return new Default_BandGap (env);
}
```

Bandgap Narrowing

Sentaurus Device provides a PMI to compute bandgap narrowing (see Band Gap and Electron Affinity on page 249). A user model is activated with the keyword EffectiveIntrinsicDensity in the Physics section of the command file:

```
Physics {
   EffectiveIntrinsicDensity (pmi_model_name)
}
```

Dependencies

A PMI bandgap narrowing model has no explicit dependencies. However, it can depend on doping concentrations through the runtime support.

The PMI model must compute:

bgn   Bandgap narrowing ΔE_g^0 [eV]

In most cases, it is not necessary to compute the derivatives with respect to the dopant concentrations. However, to model dopant fluctuations (see Chapter 23 on page 675), in the

standard interface the PMI model must override the functions that compute the following values:

dbgndNa   Derivative of ΔE_g^0 with respect to the acceptor concentration $[\,cm^3 eV\,]$

dbgndNd   Derivative of ΔE_g^0 with respect to the donor concentration $[\,cm^3 eV\,]$

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_BandGapNarrowing : public PMI_Vertex_Interface {
public:
  PMI_BandGapNarrowing (const PMI_Environment& env);
    virtual ~PMI_BandGapNarrowing ();
    virtual void Compute_bgn (double& bgn) = 0;
    virtual void Compute_dbgndNa (double& dbgndNa);
    virtual void Compute_dbgndNd (double& dbgndNd);
};
```

The following virtual constructor must be implemented:

```
typedef PMI_BandGapNarrowing* new_PMI_BandGapNarrowing_func
  (const PMI_Environment& env);
extern "C" new_PMI_BandGapNarrowing_func new_PMI_BandGapNarrowing;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_BandGapNarrowing_Base : public PMI_Vertex_Base {

public:
  class Input : public PMI_Vertex_Input_Base {
  public:
    pmi_float acceptor;  // total acceptor concentration
    pmi_float donor;     // total donor concentration
  };

  class Output {
  public:
    pmi_float bgn;       // bandgap narrowing
  };

  PMI_BandGapNarrowing_Base (const PMI_Environment& env);
```

```
   virtual ~PMI_BandGapNarrowing_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_BandGapNarrowing_Base* new_PMI_BandGapNarrowing_Base_func
   (const PMI_Environment& env);
extern "C" new_PMI_BandGapNarrowing_Base_func new_PMI_BandGapNarrowing_Base;
```

Example: Default Model

The default bandgap narrowing model in Sentaurus Device (Bennett–Wilson) is given by:

$$\Delta E_g^0 = \begin{cases} E_{ref}\left[\ln\frac{N_{tot}}{N_{ref}}\right]^2, & N_{tot} > N_{ref}, \\ 0, & N_{tot} \le N_{ref}. \end{cases} \tag{1261}$$

See .

This model can be implemented as a PMI model as follows:

```
#include "PMIModels.h"

class Bennett_BandGapNarrowing : public PMI_BandGapNarrowing {

private:
   double Ebgn, Nref;

public:
   Bennett_BandGapNarrowing (const PMI_Environment& env);

   ~Bennett_BandGapNarrowing ();

   void Compute_bgn (double& bgn);
};

Bennett_BandGapNarrowing::
Bennett_BandGapNarrowing (const PMI_Environment& env) :
   PMI_BandGapNarrowing (env)
{ Ebgn = InitParameter ("Ebgn", 6.84e-3);
  Nref = InitParameter ("Nref", 3.162e18);
}

Bennett_BandGapNarrowing::
```

```
~Bennett_BandGapNarrowing ()
{
}

void Bennett_BandGapNarrowing::
Compute_bgn (double& bgn)
{ const double Na = ReadDoping (PMI_Acceptor);
  const double Nd = ReadDoping (PMI_Donor);
  const double Ni = Na + Nd;
  if (Ni > Nref) {
      const double tmp = log (Ni / Nref);
      bgn = Ebgn * tmp * tmp;
  } else {
      bgn = 0.0;
  }
}

extern "C"
PMI_BandGapNarrowing* new_PMI_BandGapNarrowing
   (const PMI_Environment& env)
{ return new Bennett_BandGapNarrowing (env);
}
```

Apparent Band-Edge Shift

The apparent band-edge shift Λ_{PMI} is a quantity similar to bandgap narrowing. In contrast to bandgap narrowing, the apparent band-edge shift can depend on the solution variables (electron and hole densities, lattice temperature, and electric field). Conversely, the apparent band-edge shift does not take effect in all situations where a real band-edge shift takes effect (this is why the band-edge shift is called 'apparent').

Implementationwise, the apparent band-edge shift is an extension of the density gradient model (see Density Gradient Quantization Model on page 294). For the PMI model, this implies:

- Sentaurus Device applies the apparent band-edge shift Λ_{PMI} everywhere where it applies quantization corrections.

- By default, the apparent band-edge shift that Sentaurus Device computes is not equal to Λ_{PMI}, but contains contributions from quantization. To remove them, set $\gamma = 0$ (see Density Gradient Quantization Model on page 294).

- Apart from a specification in the `Physics` section, it is necessary to specify additional equations in the `Solve` section (see Using the Density Gradient Model on page 296).

To select a model to compute Λ_{PMI}, specify its name using the `LocalModel` keyword (see Table 294 on page 1470). The same models for Λ_{PMI} can be used for the shift of the conduction

and valence bands. A positive value of Λ_{PMI} means that the band shifts outwards, away from midgap (therefore, the band gap widens).

Dependencies

The apparent band-edge shift Λ_{PMI} may depend on:

n	Electron density $[\text{cm}^{-3}]$
p	Hole density $[\text{cm}^{-3}]$
t	Lattice temperature $[\text{K}]$
F	Absolute value of the electric field $[\text{Vcm}^{-1}]$

The PMI model must compute the following values:

shift	Apparent band-edge shift Λ_{PMI} $[\text{eV}]$

In the case of the standard interface, the following derivatives must be computed as well:

dshiftdn	Derivative of Λ_{PMI} with respect to n $[\text{eVcm}^3]$
dshiftdp	Derivative of Λ_{PMI} with respect to p $[\text{eVcm}^3]$
dshiftdt	Derivative of Λ_{PMI} with respect to t $[\text{eVK}^{-1}]$
dshiftdf	Derivative of Λ_{PMI} with respect to f $[\text{eVcmV}^{-1}]$

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_ApparentBandEdgeShift : public PMI_Vertex_Interface {

public:
  PMI_ApparentBandEdgeShift (const PMI_Environment& env);
  virtual ~PMI_ApparentBandEdgeShift ();

  virtual void Compute_shift
    (const double n, const double p,
     const double t, const double f,
     double& shift) = 0;
```

```
virtual void Compute_dshiftdn
  (const double n, const double p,
   const double t, const double f,
   double& dshiftdn) = 0;

virtual void Compute_dshiftdp
  (const double n, const double p,
   const double t, const double f,
   double& dshiftdp) = 0;

virtual void Compute_dshiftdt
  (const double n, const double p,
   const double t, const double f,
   double& dshiftdt) = 0;

virtual void Compute_dshiftdf
  (const double n, const double p,
   const double t, const double f,
   double& dshiftdf) = 0;
};
```

The following virtual constructor must be implemented:

```
typedef PMI_ApparentBandEdgeShift* new_PMI_ApparentBandEdgeShift_func
  (const PMI_Environment& env);
extern "C" new_PMI_ApparentBandEdgeShift_func new_PMI_ApparentBandEdgeShift;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_ApparentBandEdgeShift_Base : public PMI_Vertex_Base {

public:
  class Input : public PMI_Vertex_Input_Base {
  public:
    pmi_float n;  // electron density
    pmi_float p;  // hole density
    pmi_float t;  // lattice temperature
    pmi_float f;  // absolute value of electric field
  };

  class Output {
  public:
    pmi_float shift;  // apparent band-edge shift
  };
```

```
    PMI_ApparentBandEdgeShift_Base (const PMI_Environment& env);
    virtual ~PMI_ApparentBandEdgeShift_Base ();

    virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_ApparentBandEdgeShift_Base*
    new_PMI_ApparentBandEdgeShift_Base_func (const PMI_Environment& env);
extern "C" new_PMI_ApparentBandEdgeShift_Base_func
    new_PMI_ApparentBandEdgeShift_Base;
```

Multistate Configuration–Dependent Apparent Band-Edge Shift

The multistate configuration (MSC)–dependent, apparent band-edge shift model is a variant of the apparent band-edge shift model (see Apparent Band-Edge Shift on page 1144). Besides dependencies on the solution variables, electron and hole densities, lattice temperature, and carrier temperatures, it allows dependencies on all state occupation rates of an arbitrary reference MSC defined by `MSConfig`. The remarks made for the apparent band-edge shift in connection with the density gradient model are valid here as well.

The model can be selected as arguments of the keywords `eBandEdgeShift`, `hBandEdgeShift`, and `BandEdgeShift` (see Apparent Band-Edge Shift on page 483) in the `MSConfig` specification. The optional model index parameter allows you to implement, in the same model, several variants that can be accessed from the command file.

Dependencies

The MSC apparent band-edge shift Λ_{PMI} may depend on:

n	Electron density $[\mathrm{cm}^{-3}]$
p	Hole density $[\mathrm{cm}^{-3}]$
t	Lattice temperature $[\mathrm{K}]$
ct	Carrier temperature$[\mathrm{K}]$
s	Vector of state occupation rates of the reference MSC $[1]$

The PMI model must compute the following values if the dependency is used:

shift   Apparent band-edge shift Λ_{PMI} [eV]

In the case of the standard interface, the following derivatives must be computed as well:

dshiftdn   Derivative of Λ_{PMI} with respect to n [eVcm^3]

dshiftdp   Derivative of Λ_{PMI} with respect to p [eVcm^3]

dshiftdt   Derivative of Λ_{PMI} with respect to t [eVK^{-1}]

dshiftdf   Derivative of Λ_{PMI} with respect to ct [eVK^{-1}]

dshiftds   Derivative of Λ_{PMI} with respect to s [eV]

Additional Functionality

The PMI model provides additional functionality.

Using Dependencies

You can use the function set_dependency_used to switch on or off the dependencies of this model explicitly (the default is on). For used dependencies, the function computing the corresponding derivative must be provided; for unused dependencies, the functions are not called.

Updating Actual Status

Before calling the computation functions (compute_val and compute_dval_dX), the simulator passes the actual values of the dependencies to the model using set_actual_status. The model parameters are updated by init_parameter before the actual status is updated.

Standard C++ Interface

The following base class (here, only an extract) is declared in the file `PMIModels.h`:

```
class PMI_MSC_ApparentBandEdgeShift : public PMI_MSC_Vertex_Interface {

public:
  enum e_var { var_n, var_p, var_T, var_eT, var_hT, var_s, var_undefined };

  class input_data {
  public:
    input_data ();
    ~input_data ();
    double& val ( e_var var, size_t ind );
    double val ( e_var var, size_t ind ) const;
  };

public:
  PMI_MSC_ApparentBandEdgeShift (const PMI_Environment& env,
    const std::string& msconfig_name, int model_index = 0);
  virtual ~PMI_MSC_ApparentBandEdgeShift ();

// get names of MSConfig and its states
  const std::string& msconfig_name () const;
  size_t nb_states () const;
  const std::string& state ( size_t index ) const;

  virtual void set_actual_status (
    const PMI_MSC_ApparentBandEdgeShift::input_data& id );

// compute value and derivatives
  virtual void compute_val ( double& val );
  virtual void compute_dval_dn ( double& val );
  virtual void compute_dval_dp ( double& val );
  virtual void compute_dval_dT ( double& val );
  virtual void compute_dval_deT ( double& val );
  virtual void compute_dval_dhT ( double& val );
  virtual void compute_dval_ds ( std::vector<double>& val );

// support ramping of parameters
  virtual void init_parameter ();

// handle dependencies
  void set_dependency_used (
    PMI_MSC_ApparentBandEdgeShift::e_var var, bool flag );
  bool dependency_used ( PMI_MSC_ApparentBandEdgeShift::e_var var ) const;
};
```

The following virtual constructor must be implemented:

```
typedef PMI_MSC_ApparentBandEdgeShift* new_PMI_MSC_ApparentBandEdgeShift_func
   (const PMI_Environment& env,
    const std::string& msconfig_name,
    int model_index);
extern "C" new_PMI_ApparentBandEdgeShift_func
   new_PMI_MSC_ApparentBandEdgeShift;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_MSC_ApparentBandEdgeShift_Base : public PMI_MSC_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
     pmi_float n;   // electron density
     pmi_float p;   // hole density
     pmi_float T;   // lattice temperature
     pmi_float eT;  // electron temperature
     pmi_float hT;  // hole temperature
     std::vector<pmi_float> s;  // phase fraction
   };

   class Output {
   public:
     pmi_float val;  // apparent band-edge shift
   };

   PMI_MSC_ApparentBandEdgeShift_Base (const PMI_Environment& env,
                                       const std::string& msconfig_name,
                                       const int model_index);
   virtual ~PMI_MSC_ApparentBandEdgeShift_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_MSC_ApparentBandEdgeShift_Base*
   new_PMI_MSC_ApparentBandEdgeShift_Base_func
      (const PMI_Environment& env, const std::string& msconfig_name,
       const int model_index);
extern "C" new_PMI_MSC_ApparentBandEdgeShift_Base_func
   new_PMI_MSC_ApparentBandEdgeShift_Base;
```

Electron Affinity

The electron affinity χ, that is, the energy separation between the conduction band and vacuum level, can be specified by using a PMI. The syntax in the command file is:

```
Physics {
   Affinity (pmi_model_name)
}
```

The default affinity model in Sentaurus Device can be selected explicitly by the keyword Default:

```
Physics {
   Affinity (Default)
}
```

Dependencies

The electron affinity χ may depend on:

t   Lattice temperature [K]

The PMI model must compute:

affinity   Electron affinity χ [eV]

In the case of the standard interface, the following derivative must be computed as well:

affinitydt   Derivative of affinity with respect to t $[\mathrm{eVK}^{-1}]$

Standard C++ Interface

The following base class is declared in the file PMIModels.h:

```
class PMI_Affinity : public PMI_Vertex_Interface {

public:
   PMI_Affinity (const PMI_Environment& env);
   virtual ~PMI_Affinity ();

   virtual void Compute_affinity
```

```
      (const double t, double& affinity) = 0;

   virtual void Compute_daffinitydt
      (const double t, double& daffinitydt) = 0;
};
```

The prototype for the virtual constructor is:

```
typedef PMI_Affinity* new_PMI_Affinity_func
   (const PMI_Environment& env);
extern "C" new_PMI_Affinity_func new_PMI_Affinity;
```

Simplified C++ Interface

The following base class is declared in the file PMI.h:

```
class PMI_Affinity_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      pmi_float t;  // lattice temperature
   };

   class Output {
   public:
      pmi_float affinity;  // electron affinity
   };

   PMI_Affinity_Base (const PMI_Environment& env);
   virtual ~PMI_Affinity_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_Affinity_Base* new_PMI_Affinity_Base_func
   (const PMI_Environment& env);
extern "C" new_PMI_Affinity_Base_func new_PMI_Affinity_Base;
```

Example: Default Affinity Model

By default, Sentaurus Device uses this formula to compute χ:

$$\chi(t) = \chi(0) + 0.5\frac{\alpha t^2}{t + \beta} \tag{1262}$$

$\chi(0)$ denotes the affinity at $0\,\mathrm{K}$.

```
#include "PMIModels.h"

class Default_Affinity : public PMI_Affinity {

private:
  double Affinity0, alpha, beta;

public:
  Default_Affinity (const PMI_Environment& env);

  ~Default_Affinity ();

  void Compute_affinity (const double t, double& affinity);

  void Compute_daffinitydt (const double t, double& daffinitydt);

};

Default_Affinity::
Default_Affinity (const PMI_Environment& env) :
  PMI_Affinity (env)
{ Affinity0 = InitParameter ("Affinity0", 4.05);
  alpha = InitParameter ("alpha", 4.73e-4);
  beta = InitParameter ("beta", 636);
}

Default_Affinity::
~Default_Affinity ()
{
}

void Default_Affinity::
Compute_affinity (const double t, double& affinity)
{ affinity = Affinity0 + 0.5 * alpha * t * t / (t + beta);
}

void Default_Affinity::
Compute_daffinitydt (const double t, double& daffinitydt)
```

```
{ daffinitydt = 0.5 * alpha * t * (t + 2.0 * beta) /
                ((t + beta) * (t + beta));
}
extern "C"
PMI_Affinity* new_PMI_Affinity
  (const PMI_Environment& env)
{ return new Default_Affinity (env);
}
```

Effective Mass

Sentaurus Device provides a PMI to compute the effective mass of electrons and holes. The effective mass is always expressed as a multiple of the electron mass in vacuum. The name of the PMI model must appear in the `Physics` section of the command file:

```
Physics {
   EffectiveMass (pmi_model_name)
}
```

Dependencies

The relative effective mass may depend on the following variables:

t   Lattice temperature [K]

bg   Band gap [eV]

The PMI model must compute the following results:

m   Relative effective mass (1)

In the case of the standard interface, the following derivatives must be computed as well:

dmdt   Derivative of m with respect to t $[\text{K}^{-1}]$

dmdbg   Derivative of m with respect to bg $[\text{eV}^{-1}]$

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_EffectiveMass : public PMI_Vertex_Interface {

public:
  PMI_EffectiveMass (const PMI_Environment& env);
  virtual ~PMI_EffectiveMass ();

  virtual void Compute_m
    (const double t, const double bg, double& m) = 0;

  virtual void Compute_dmdt
    (const double t, const double bg, double& dmdt) = 0;

virtual void Compute_dmdbg
(const double t, const double bg, double& dmdbg) = 0;
};
```

Two virtual constructors are necessary to compute the effective mass of electrons and holes:

```
typedef PMI_EffectiveMass* new_PMI_EffectiveMass_func
   (const PMI_Environment& env);
extern "C" new_PMI_EffectiveMass_func new_PMI_e_EffectiveMass;
extern "C" new_PMI_EffectiveMass_func new_PMI_h_EffectiveMass;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_EffectiveMass_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
     pmi_float t;   // lattice temperature
     pmi_float bg;  // band gap
   };

   class Output {
   public:
     pmi_float m;  // effective mass
   };
```

```
    PMI_EffectiveMass_Base (const PMI_Environment& env);
    virtual ~PMI_EffectiveMass_Base ();

    virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_EffectiveMass_Base* new_PMI_EffectiveMass_Base_func
    (const PMI_Environment& env);
extern "C" new_PMI_EffectiveMass_Base_func new_PMI_e_EffectiveMass_Base;
extern "C" new_PMI_EffectiveMass_Base_func new_PMI_h_EffectiveMass_Base;
```

Example: Linear Effective Mass Model

A simple, linear effective mass model is given by:

$$m = m_{300} + \frac{dm}{dt}(t - 300) \tag{1263}$$

m_{300} denotes the mass at $300\,\text{K}$. It can be implemented as follows:

```
#include "PMIModels.h"

class Linear_EffectiveMass : public PMI_EffectiveMass {

protected:
  double mass_300, dmass_dt;

public:
  Linear_EffectiveMass (const PMI_Environment& env);

  ~Linear_EffectiveMass ();

  void Compute_m (const double t, const double bg, double& m);

  void Compute_dmdt (const double t, const double bg, double& dmdt);

  void Compute_dmdbg (const double t, const double bg, double& dmdbg);
};

Linear_EffectiveMass::
Linear_EffectiveMass (const PMI_Environment& env) :
  PMI_EffectiveMass (env)
{
}
```

```
Linear_EffectiveMass::
~Linear_EffectiveMass ()
{
}

void Linear_EffectiveMass::
Compute_m (const double t, const double bg, double& m)
{ m = mass_300 + dmass_dt * (t - 300.0);
}

void Linear_EffectiveMass::
Compute_dmdt (const double t, const double bg, double& dmdt)
{ dmdt = dmass_dt;
}

void Linear_EffectiveMass::
Compute_dmdbg (const double t, const double bg, double& dmdbg)
{ dmdbg = 0.0;
}

class Linear_e_EffectiveMass : public Linear_EffectiveMass {

public:
  Linear_e_EffectiveMass (const PMI_Environment& env);

  ~Linear_e_EffectiveMass () {}

};

Linear_e_EffectiveMass::
Linear_e_EffectiveMass (const PMI_Environment& env) :
  Linear_EffectiveMass (env)
{ mass_300 = InitParameter ("mass_e_300", 1.09);
  dmass_dt = InitParameter ("dmass_e_dt", 1.6e-4);
}

class Linear_h_EffectiveMass : public Linear_EffectiveMass {

public:
  Linear_h_EffectiveMass (const PMI_Environment& env);

  ~Linear_h_EffectiveMass () {}

};

Linear_h_EffectiveMass::
Linear_h_EffectiveMass (const PMI_Environment& env) :
  Linear_EffectiveMass (env)
```

```
{ mass_300 = InitParameter ("mass_h_300", 1.15);
  dmass_dt = InitParameter ("dmass_h_dt", 9.2e-4);
}

extern "C"
PMI_EffectiveMass* new_PMI_e_EffectiveMass
  (const PMI_Environment& env)
{ return new Linear_e_EffectiveMass (env);
}


extern "C"
PMI_EffectiveMass* new_PMI_h_EffectiveMass
  (const PMI_Environment& env)
{ return new Linear_h_EffectiveMass (env);
}
```

Energy Relaxation Times

The model for the energy relaxation times τ in Eq. 83 and Eq. 84, p. 197 can be specified in the `Physics` section of the command file. The four available possibilities are:

```
Physics {
   EnergyRelaxationTimes (
      formula
      constant
      irrational
      pmi_model_name
   )
}
```

These entries have the following meaning:

formula	Use the value of `formula` in the parameter file (default)
constant	Use constant energy relaxation times (`formula = 1`)
irrational	Use the ratio of two irrational polynomials (`formula = 2`)
pmi_model_name	Call a PMI model to compute the energy relaxation times

Dependencies

The energy relaxation time τ may depend on the variable:

ct   Carrier temperature [K]

> **NOTE** The parameter ct represents the electron temperature during the calculation of τ_n and the hole temperature during the calculation of τ_p.

The PMI model must compute the following results:

tau   Energy relaxation time τ [s]

In the case of the standard interface, the following derivative must be computed as well:

dtaudct   Derivative of τ with respect to ct $[sK^{-1}]$

Standard C++ Interface

The following base class is declared in the file PMIModels.h:

```
class PMI_EnergyRelaxationTime : public PMI_Vertex_Interface {

public:
   PMI_EnergyRelaxationTime (const PMI_Environment& env);

   virtual ~PMI_EnergyRelaxationTime ();

   virtual void Compute_tau
      (const double ct, double& tau) = 0;

   virtual void Compute_dtaudct
      (const double ct, double& dtaudct) = 0;
};
```

The following two virtual constructors must be implemented for electron and hole energy relaxation times:

```
typedef PMI_EnergyRelaxationTime* new_PMI_EnergyRelaxationTime_func
   (const PMI_Environment& env);
extern "C" new_PMI_EnergyRelaxationTime_func new_PMI_e_EnergyRelaxationTime;
extern "C" new_PMI_EnergyRelaxationTime_func new_PMI_h_EnergyRelaxationTime;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_EnergyRelaxationTime_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      pmi_float ct;  // carrier temperature
   };

   class Output {
   public:
      pmi_float tau;  // energy relaxation time
   };

   PMI_EnergyRelaxationTime_Base (const PMI_Environment& env);
   virtual ~PMI_EnergyRelaxationTime_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_EnergyRelaxationTime_Base* new_PMI_EnergyRelaxationTime_Base_func
   (const PMI_Environment& env);
extern "C" new_PMI_EnergyRelaxationTime_Base_func
   new_PMI_e_EnergyRelaxationTime_Base;
extern "C" new_PMI_EnergyRelaxationTime_Base_func
   new_PMI_h_EnergyRelaxationTime_Base;
```

Example: Constant Energy Relaxation Times

The following C++ code implements constant energy relaxation times:

```
#include "PMIModels.h"

class Const_EnergyRelaxationTime : public PMI_EnergyRelaxationTime {

protected:
  double tau_const;

public:
  Const_EnergyRelaxationTime (const PMI_Environment& env);
```

```
  ~Const_EnergyRelaxationTime ();

  void Compute_tau
    (const double ct, double& tau);

  void Compute_dtaudct
    (const double ct, double& dtaudct);

};

Const_EnergyRelaxationTime::
Const_EnergyRelaxationTime (const PMI_Environment& env) :
  PMI_EnergyRelaxationTime (env)
{
}

Const_EnergyRelaxationTime::
~Const_EnergyRelaxationTime ()
{
}

void Const_EnergyRelaxationTime::
Compute_tau (const double ct, double& tau)
{ tau = tau_const;
}

void Const_EnergyRelaxationTime::
Compute_dtaudct (const double ct, double& dtaudct)
{ dtaudct = 0.0;
}

class Const_e_EnergyRelaxationTime : public Const_EnergyRelaxationTime {

public:
  Const_e_EnergyRelaxationTime (const PMI_Environment& env);

  ~Const_e_EnergyRelaxationTime () {}

};

Const_e_EnergyRelaxationTime::
Const_e_EnergyRelaxationTime (const PMI_Environment& env) :
  Const_EnergyRelaxationTime (env)
{ tau_const = InitParameter ("tau_const_e", 0.3e-12);
}

class Const_h_EnergyRelaxationTime : public Const_EnergyRelaxationTime {
```

```
public:
   Const_h_EnergyRelaxationTime (const PMI_Environment& env);

   ~Const_h_EnergyRelaxationTime () {}

};

Const_h_EnergyRelaxationTime::
Const_h_EnergyRelaxationTime (const PMI_Environment& env) :
   Const_EnergyRelaxationTime (env)

{ tau_const = InitParameter ("tau_const_h", 0.25e-12);
}

extern "C"
PMI_EnergyRelaxationTime* new_PMI_e_EnergyRelaxationTime
   (const PMI_Environment& env)
{ return new Const_e_EnergyRelaxationTime (env);
}

extern "C"
PMI_EnergyRelaxationTime* new_PMI_h_EnergyRelaxationTime
   (const PMI_Environment& env)
{ return new Const_h_EnergyRelaxationTime (env);
}
```

Lifetimes

This PMI provides access to the electron and hole lifetimes, τ_n and τ_p, in the SRH recombination (see Eq. 275, p. 331) and the coupled defect level (CDL) recombination (see Eq. 395, p. 398). In the command file, the names of the lifetime models are given as arguments to the SRH or CDL keywords:

```
Physics {
   Recombination (SRH (pmi_model_name))
}
```

or:

```
Physics {
   Recombination (CDL (pmi_model_name))
}
```

   NOTE   A PMI model overrides all other keywords in an SRH or a CDL statement.

Dependencies

A PMI lifetime model may depend on the variable:

t   Lattice temperature [K]

It must compute the following results:

tau   Lifetime τ [s]

In the case of the standard interface, the following derivative must be computed as well:

dtaudt   Derivative of τ with respect to lattice temperature $[sK^{-1}]$

Standard C++ Interface

The enumeration type `PMI_LifetimeModel` describes where the PMI lifetime is used:

```
enum PMI_LifetimeModel {
   PMI_SRH,
   PMI_CDL1,
   PMI_CDL2
};
```

The following base class is declared in the file `PMIModels.h`:

```
class PMI_Lifetime : public PMI_Vertex_Interface {

private:
   const PMI_LifetimeModel lifetimeModel;

public:
   PMI_Lifetime (const PMI_Environment& env,
                 const PMI_LifetimeModel model);

   virtual ~PMI_Lifetime ();

   PMI_LifetimeModel LifetimeModel () const { return lifetimeModel; }

   virtual void Compute_tau
      (const double t, double& tau) = 0;
```

```
      virtual void Compute_dtaudt
         (const double t, double& dtaudt) = 0;
   };
```

Two virtual constructors must be implemented for electron and hole lifetimes:

```
typedef PMI_Lifetime* new_PMI_Lifetime_func
   (const PMI_Environment& env, const PMI_LifetimeModel model);
extern "C" new_PMI_Lifetime_func new_PMI_e_Lifetime;
extern "C" new_PMI_Lifetime_func new_PMI_h_Lifetime;
```

Simplified C++ Interface

The following base class is declared in the file PMI.h:

```
class PMI_Lifetime_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
     pmi_float t;  // lattice temperature
   };

   class Output {
   public:
     pmi_float tau;  // lifetime
   };

   PMI_Lifetime_Base (const PMI_Environment& env,
                      const PMI_LifetimeModel model);
   virtual ~PMI_Lifetime_Base ();

   PMI_LifetimeModel LifetimeModel () const;

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_Lifetime_Base* new_PMI_Lifetime_Base_func
   (const PMI_Environment& env, const PMI_LifetimeModel model);
extern "C" new_PMI_Lifetime_Base_func new_PMI_e_Lifetime_Base;
extern "C" new_PMI_Lifetime_Base_func new_PMI_h_Lifetime_Base;
```

Example: Doping- and Temperature-Dependent Lifetimes

The following example combines doping-dependent lifetimes (Scharfetter) and temperature dependence (power law):

$$\tau = \left(\tau_{min} + \frac{\tau_{max} - \tau_{min}}{1 + \left(\dfrac{N_{A,0} + N_{D,0}}{N_{ref}} \right)^{\gamma}} \right) \left(\frac{T}{300\,K} \right)^{\alpha} \tag{1264}$$

```
#include "PMIModels.h"

class Scharfetter_Lifetime : public PMI_Lifetime {

protected:
  const double T0;
  double taumin, taumax, Nref, gamma, Talpha;

public:
  Scharfetter_Lifetime (const PMI_Environment& env,
                        const PMI_LifetimeModel model);

  ~Scharfetter_Lifetime ();
  void Compute_tau
    (const double t, double& tau);

  void Compute_dtaudt
    (const double t, double& dtaudt);

};

Scharfetter_Lifetime::
Scharfetter_Lifetime (const PMI_Environment& env,
                      const PMI_LifetimeModel model) :
  PMI_Lifetime (env, model),
  T0 (300.0)
{
}

Scharfetter_Lifetime::
~Scharfetter_Lifetime ()
{
}

void Scharfetter_Lifetime::
Compute_tau (const double t, double& tau)
{ const double Ni = ReadDoping (PMI_Acceptor) + ReadDoping (PMI_Donor);
```

```
    tau = taumin + (taumax - taumin) / (1.0 + pow (Ni/Nref, gamma));
    tau *= pow (t/T0, Talpha);
}

void Scharfetter_Lifetime::
Compute_dtaudt (const double t, double& dtaudt)
{ const double Ni = ReadDoping (PMI_Acceptor) + ReadDoping (PMI_Donor);
    dtaudt = taumin + (taumax - taumin) / (1.0 + pow (Ni/Nref, gamma));
    dtaudt *= (Talpha/T0) * pow (t/T0, Talpha-1.0);
}

class Scharfetter_e_Lifetime : public Scharfetter_Lifetime {

public:
    Scharfetter_e_Lifetime (const PMI_Environment& env,
                            const PMI_LifetimeModel model);

    ~Scharfetter_e_Lifetime () {}

};
Scharfetter_e_Lifetime::
Scharfetter_e_Lifetime (const PMI_Environment& env,
                        const PMI_LifetimeModel model) :
    Scharfetter_Lifetime (env, model)
{ taumin = InitParameter ("taumin_e", 0.0);
    taumax = InitParameter ("taumax_e", 1.0e-5);
    Nref = InitParameter ("Nref_e", 1.0e16);
    gamma = InitParameter ("gamma_e", 1.0);
    Talpha = InitParameter ("Talpha_e", -1.5);
}

class Scharfetter_h_Lifetime : public Scharfetter_Lifetime {

public:
    Scharfetter_h_Lifetime (const PMI_Environment& env,
                            const PMI_LifetimeModel model);

    ~Scharfetter_h_Lifetime () {}

};

Scharfetter_h_Lifetime::
Scharfetter_h_Lifetime (const PMI_Environment& env,
                        const PMI_LifetimeModel model) :
    Scharfetter_Lifetime (env, model)

{ taumin = InitParameter ("taumin_h", 0.0);
    taumax = InitParameter ("taumax_h", 3.0e-6);
```

```
    Nref = InitParameter ("Nref_h", 1.0e16);
    gamma = InitParameter ("gamma_h", 1.0);
    Talpha = InitParameter ("Talpha_h", -1.5);
}

extern "C"
PMI_Lifetime* new_PMI_e_Lifetime
    (const PMI_Environment& env, const PMI_LifetimeModel model)
{ return new Scharfetter_e_Lifetime (env, model);
}

extern "C"
PMI_Lifetime* new_PMI_h_Lifetime
    (const PMI_Environment& env, const PMI_LifetimeModel model)
{ return new Scharfetter_h_Lifetime (env, model);
}
```

Thermal Conductivity

The PMI provides access to the lattice thermal conductivity κ in Eq. 68, p. 192. To activate it, in the `Physics` section of the command file, specify:

```
Physics {
    ThermalConductivity (
        <string>
    )
}
```

where the string is the name of the PMI model.

The PMI supports anisotropic thermal conductivity, and the model can be evaluated along different crystallographic axes. The enumeration type `PMI_AnisotropyType` as defined in Mobility Models on page 1107 determines the axis. The default is isotropic thermal conductivity. If anisotropic thermal conductivity is activated in the command file, the PMI class `PMI_ThermalConductivity` is also instantiated in the anisotropic direction.

Dependencies

The thermal conductivity κ may depend on the variable:

t   Lattice temperature [K]

The PMI model must compute the following results:

kappa   Thermal conductivity κ $[\mathrm{Wcm^{-1}K^{-1}}]$

In the case of the standard interface, the following derivative must be computed as well:

dkappadt derivative of κ with respect to t $[\mathrm{Wcm^{-1}K^{-2}}]$

Standard C++ Interface

The following base class is declared in the file PMIModels.h:

```
class PMI_ThermalConductivity : public PMI_Vertex_Interface {

public:
   PMI_ThermalConductivity (const PMI_Environment& env,
                            const PMI_AnisotropyType anisotype);

   virtual ~PMI_ThermalConductivity ();

   PMI_AnisotropyType AnisotropyType () const { return anisoType; }

   virtual void Compute_kappa
      (const double t, double& kappa) = 0;

   virtual void Compute_dkappadt
      (const double t, double& dkappadt) = 0;
};
```

The following virtual constructor must be implemented:

```
typedef PMI_ThermalConductivity* new_PMI_ThermalConductivity_func
   (const PMI_Environment& env, const PMI_AnisotropyType anisotype);
extern "C" new_PMI_ThermalConductivity_func
   new_PMI_ThermalConductivity;
```

Simplified C++ Interface

The following base class is declared in the file PMI.h:

```
class PMI_ThermalConductivity_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
```

```
public:
   pmi_float t;   // lattice temperature
};

class Output {
public:
   pmi_float kappa;   // thermal conductivity
};

PMI_ThermalConductivity_Base (const PMI_Environment& env,
                              const PMI_AnisotropyType anisotype);

virtual ~PMI_ThermalConductivity_Base ();

PMI_AnisotropyType AnisotropyType () const;

virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_ThermalConductivity_Base* new_PMI_ThermalConductivity_Base_func
   (const PMI_Environment& env, const PMI_AnisotropyType anisotype);
extern "C" new_PMI_ThermalConductivity_Base_func
   new_PMI_ThermalConductivity_Base;
```

Example: Temperature-Dependent Thermal Conductivity

The following C++ code implements the temperature-dependent thermal conductivity:

$$\kappa(T) = \frac{1}{a + bT + cT^2} \tag{1265}$$

as given in .

```
#include "PMIModels.h"

class TempDep_ThermalConductivity : public PMI_ThermalConductivity {
private:
  double a, b, c;

public:
  TempDep_ThermalConductivity (const PMI_Environment& env, const
PMI_AnisotropyType anisotype);
  ~TempDep_ThermalConductivity ();

  void Compute_kappa
```

```
      (const double t, double& kappa);

   void Compute_dkappadt
      (const double t, double& dkappadt);
};


TempDep_ThermalConductivity::
TempDep_ThermalConductivity (const PMI_Environment& env, const
PMI_AnisotropyType anisotype) :
   PMI_ThermalConductivity (env, anisotype)
{ // default values
   a = InitParameter ("a", 0.03);
   b = InitParameter ("b", 1.56e-03);
   c = InitParameter ("c", 1.65e-06);
}

TempDep_ThermalConductivity::
~TempDep_ThermalConductivity ()
{
}

void TempDep_ThermalConductivity::
Compute_kappa (const double t, double& kappa)
{ kappa = 1.0 / (a + b*t + c*t*t);
}

void TempDep_ThermalConductivity::
Compute_dkappadt (const double t, double& dkappadt)
{ const double kappa = 1.0 / (a + b*t + c*t*t);
   dkappadt = -kappa * kappa * (b + 2.0*c*t);
}

extern "C"
PMI_ThermalConductivity* new_PMI_ThermalConductivity
   (const PMI_Environment& env, const PMI_AnisotropyType anisotype)
{ return new TempDep_ThermalConductivity (env, anisotype);
}
```

Example: Thin-Layer Thermal Conductivity

In this example, thermal conductivity depends on the doping and thickness of layers. In this case, the external `LayerThickness` command (see LayerThickness Command on page 310) must be specified in the command file:

```
Physics (Material="Silicon") {
   LayerThickness(<parameters>)    # external command for thickness extraction
   ThermalConductivity (ThinLayerKappa)
}
```

The following C++ code implements the thin-layer doping-dependent thermal conductivity (see `$STROOT/tcad/$STRELEASE/lib/sdevice/src/pmi_ThinLayerKappa/ThinLayerKappa.C`):

$$\kappa = \kappa_0 \cdot \kappa_d(d) \cdot \kappa_h(h) \tag{1266}$$

where:

κ_0 Constant value $[\mathrm{Wcm^{-1}K^{-1}}]$

d `Doping`/`ScaleDoping` (unitless doping)

h `LayerThickness`/`ScaleThickness` (unitless layer thickness)

$$\kappa_d(d) = (a_2(d-d_0)^2 + a_1(d-d_0) + a_0) \cdot \exp(\alpha(d-d_0))$$

$$\kappa_h(h) = (b_2(h-h_0)^2 + b_1(h-h_0) + b_0) \cdot \exp(\beta(h-h_0))$$

```
#include <math.h>
#include "PMI.h"

class ThinLayer_ThermalConductivity : public PMI_ThermalConductivity_Base
{
private:
  double kappa0;                    //  [W/(K*cm)]
  double ScaleDoping;               //  [cm-3]
  double ScaleThickness;       //  [um]
  double d0, a0, a1, a2, alpha;    //  [1]
  double h0, b0, b1, b2, beta;     //  [1]

public:
  ThinLayer_ThermalConductivity (const PMI_Environment& env,
                                 const PMI_AnisotropyType anisotype);
  ~ThinLayer_ThermalConductivity ();

  void compute (const Input& input, Output& output);
```

```
  };

  ThinLayer_ThermalConductivity::
  ThinLayer_ThermalConductivity (const PMI_Environment& env,
                                 const PMI_AnisotropyType anisotype) :
    PMI_ThermalConductivity_Base (env, anisotype)
  { // default values
    kappa0 = InitParameter("kappa0", 1.);              // [W/(K*cm)]

    ScaleDoping = InitParameter("ScaleDoping", 1.e+18);    // [cm-3]
    d0   = InitParameter("d0", 1.);      // [1]
    a0   = InitParameter("a0", 1.);      // [1]
    a1   = InitParameter("a1", 0.);      // [1]
    a2   = InitParameter("a2", 0.);      // [1]
    alpha = InitParameter("alpha", 0.);  // [1]

    ScaleThickness = InitParameter("ScaleThickness", 1.e-3);  // [um] = 1 nm
    h0   = InitParameter("h0", 1.);      // [1]
    b0   = InitParameter("b0", 1.);      // [1]
    b1   = InitParameter("b1", 0.);      // [1]
    b2   = InitParameter("b2", 0.);      // [1]
    beta = InitParameter("beta", 0.);    // [1]
  }

  ThinLayer_ThermalConductivity::
  ~ThinLayer_ThermalConductivity ()
  {}

  void ThinLayer_ThermalConductivity::
  compute (const Input& input, Output& output)
  {
    const double h  = input.ReadLayerThickness()/ScaleThickness;
    pmi_float Nd = input.ReadDoping(PMI_Donor);
    pmi_float Na = input.ReadDoping(PMI_Acceptor);
    pmi_float d  = (Nd - Na)/ScaleDoping;

    pmi_float kd = (a2*(d-d0)*(d-d0) + a1*(d-d0) + a0)*exp(alpha*(d-d0));
    pmi_float kh = (b2*(h-h0)*(h-h0) + b1*(h-h0) + b0)*exp(beta*(h-h0));

    pmi_float kappa = kappa0*kd*kh;

    output.kappa = kappa;  //  [W/(K*cm)]
  }
```

```
extern "C"
PMI_ThermalConductivity_Base* new_PMI_ThermalConductivity_Base
   (const PMI_Environment& env, const PMI_AnisotropyType anisotype)
{ return new ThinLayer_ThermalConductivity (env, anisotype);
}
```

The following example is a parameter file for the formula $\kappa = (2d^2 + d + 1) \cdot \exp(0.1 \cdot h)$:

```
Material = "Silicon" {

   ThinLayerKappa {
      kappa0 = 1  # [W/(K*cm)]

      ScaleDoping = 1.e+18    # [cm-3]
      d0    = 0     # [1]
      a0    = 1     # [1]
      a1    = 1     # [1]
      a2    = 2     # [1]
      alpha = 0     # [1]

      ScaleThickness = 1.e-3  # [um] = 1 nm
      h0    = 0     # [1]
      b0    = 1     # [1]
      b1    = 0     # [1]
      b2    = 0     # [1]
      beta  = 0.1   # [1]
   }
}
```

Multistate Configuration–Dependent Thermal Conductivity

This PMI provides access to the lattice thermal conductivity κ in Eq. 68, p. 192 and allows it to depend on a multistate configuration (see Chapter 18 on page 473).

Command File

To activate a PMI of this type, in the `Physics` section, specify:

```
ThermalConductivity(
   PMIModel (
      Name = <string>
      MSConfig = <string>
      Index = <int>
```

```
        String = <string>
    )
)
```

Here, `Name` is the name of the PMI model; its specification is mandatory. `MSConfig` selects the name of the multistate configuration. `MSConfig` defaults to an empty string, which means the model does not depend on any multistate configuration. `Index` and `String` are optional; they determine the arguments `model_index` and `model_string` that are passed to the virtual constructor (see below); the interpretation of those arguments is up to the PMI model. `Index` defaults to zero, and `String` defaults to the empty string.

Dependencies

The thermal conductivity may depend on the variables:

n	Electron density $[\,\text{cm}^{-3}\,]$
p	Hole density $[\,\text{cm}^{-3}\,]$
T	Lattice temperature $[\,\text{K}\,]$
eT	Electron temperature $[\,\text{K}\,]$
hT	Hole temperature $[\,\text{K}\,]$
s	Multistate configuration occupation probabilities $[\,1\,]$

The model must compute the following quantities:

val	Thermal conductivity $[\,\text{Wcm}^{-1}\text{K}^{-1}\,]$

In the case of the standard interface, the following derivatives must be computed as well:

dval_dn	Derivative with respect to electron density $[\,\text{Wcm}^2\text{K}^{-1}\,]$
dval_dp	Derivative with respect to hole density $[\,\text{Wcm}^2\text{K}^{-1}\,]$
dval_dT	Derivative with respect to lattice temperature $[\,\text{Wcm}^{-1}\text{K}^{-2}\,]$
dval_deT	Derivative with respect to electron temperature $[\,\text{Wcm}^{-1}\text{K}^{-2}\,]$
dval_dhT	Derivative with respect to hole temperature $[\,\text{Wcm}^{-1}\text{K}^{-2}\,]$
dval_ds	Derivative with respect to multistate configuration occupation probabilities $[\,\text{Wcm}^{-1}\text{K}^{-1}\,]$

Standard C++ Interface

The PMI offers a base class that presents the following interface:

```
class PMI_MSC_ThermalConductivity : public PMI_MSC_Vertex_Interface
{
public:
  class idata {
  public:
    double n () const;
    double p () const;
    double T () const;
    double eT () const;
    double hT () const;
    double s (size_t ind) const;
  };

  class odata {
  public:
    double& val ();
    double& dval_dn ();
    double& dval_dp ();
    double& dval_dT ();
    double& dval_deT ();
    double& dval_dhT ();
    double& dval_ds ( size_t ind );
  };

  PMI_MSC_ThermalConductivity(const PMI_Environment& env,
    const std::string& msconfig_name,
    const int model_index,
    const std::string& model_string,
    const PMI_AnisotropyType anisotype);
  virtual ~PMI_MSC_ThermalConductivity ();

  PMI_AnisotropyType AnisotropyType () const;

  virtual void compute
    (const idata* id,
     odata* od ) = 0;
};
```

The `Compute` function receives its input from `id`. It returns the results using `od` by assignment using the member functions of `od`. The PMI framework initializes the values of the derivatives to zero, so you do not have to do anything for derivatives with respect to the variables on which your model does not depend.

The following virtual constructor must be implemented:

```
typedef PMI_MSC_ThermalConductivity* new_PMI_MSC_ThermalConductivity_func
   (const PMI_Environment& env, const std::string& msconfig_name,
   int model_index, const std::string& model_string,
   const PMI_AnisotropyType anisotype);
extern "C" new_PMI_MSC_ThermalConductivity_func
   new_PMI_MSC_ThermalConductivity;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_MSC_ThermalConductivity_Base : public PMI_MSC_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      const pmi_float& n () const;   // electron density
      const pmi_float& p () const;   // hole density
      const pmi_float& T () const;   // lattice temperature
      const pmi_float& eT () const;  // electron temperature
      const pmi_float& hT () const;  // hole temperature
      const pmi_float& s (size_t ind) const;  // phase fraction
   };

   class Output {
   public:
      pmi_float& val ();   // thermal conductivity
   };

   PMI_MSC_ThermalConductivity_Base (const PMI_Environment& env,
                                      const std::string& msconfig_name,
                                      const int model_index,
                                      const std::string& model_string,
                                      const PMI_AnisotropyType anisotype);
   virtual ~PMI_MSC_ThermalConductivity_Base ();

   PMI_AnisotropyType AnisotropyType () const;

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_MSC_ThermalConductivity_Base*
   new_PMI_MSC_ThermalConductivity_Base_func
      (const PMI_Environment& env, const std::string& msconfig_name,
       const int model_index, const std::string& model_string,
       const PMI_AnisotropyType anisotype);
extern "C" new_PMI_MSC_ThermalConductivity_Base_func
   new_PMI_MSC_ThermalConductivity_Base;
```

Heat Capacity

The model for lattice heat capacity in Eq. 68, p. 192 can be specified in the `Physics` section of the command file. The following two possibilities are available:

```
Physics {
   HeatCapacity (
      constant
      pmi_model_name
   )
}
```

These entries have the following meaning:

`constant`	Use constant heat capacity (default)
`pmi_model_name`	Call a PMI model to compute the heat capacity

Dependencies

The heat capacity c_L may depend on the variable:

`t`	Lattice temperature [K]

The PMI model must compute the following results:

`c`	Heat capacity c_L [$JK^{-1}cm^{-3}$]

In the case of the standard interface, the following derivative must be computed as well:

`dcdt`	Derivative of c_L with respect to `t` [$JK^{-2}cm^{-3}$]

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_HeatCapacity : public PMI_Vertex_Interface {

public:
   PMI_HeatCapacity (const PMI_Environment& env);

   virtual ~PMI_HeatCapacity ();

   virtual void Compute_c
      (const double t, double& c) = 0;

   virtual void Compute_dcdt
      (const double t, double& dcdt) = 0
};
```

The following virtual constructor must be implemented:

```
typedef PMI_HeatCapacity* new_PMI_HeatCapacity_func
   (const PMI_Environment& env);
extern "C" new_PMI_HeatCapacity_func new_PMI_HeatCapacity;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_HeatCapacity_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      pmi_float t;   // lattice temperature
   };

   class Output {
   public:
      pmi_float c;   // heat capacity
   };

   PMI_HeatCapacity_Base (const PMI_Environment& env);
   virtual ~PMI_HeatCapacity_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_HeatCapacity_Base* new_PMI_HeatCapacity_Base_func
   (const PMI_Environment& env);
extern "C" new_PMI_HeatCapacity_Base_func new_PMI_HeatCapacity_Base;
```

Example: Constant Heat Capacity

The following C++ code implements constant heat capacity:

```
#include "PMIModels.h"

class Constant_HeatCapacity : public PMI_HeatCapacity {
private:
  double cv;

public:
  Constant_HeatCapacity (const PMI_Environment& env);
  ~Constant_HeatCapacity ();

  void Compute_c
    (const double t, double& c);

  void Compute_dcdt
    (const double t, double& dcdt);
};

Constant_HeatCapacity::
Constant_HeatCapacity (const PMI_Environment& env) :
  PMI_HeatCapacity (env)
{ // default values
  cv = InitParameter ("cv", 1.63);
}

Constant_HeatCapacity::
~Constant_HeatCapacity ()
{
}

void Constant_HeatCapacity::
Compute_c (const double t, double& c)
{ c = cv;
}

void Constant_HeatCapacity::
Compute_dcdt (const double t, double& dcdt)
{ dcdt = 0.0;
```

```
   }

   extern "C"
   PMI_HeatCapacity* new_PMI_HeatCapacity
     (const PMI_Environment& env)
   { return new Constant_HeatCapacity (env);
   }
```

Multistate Configuration–Dependent Heat Capacity

This PMI computes the lattice heat capacity and allows it to depend on a multistate configuration (see Chapter 18 on page 473).

Command File

To activate a PMI of this type, in the `Physics` section, specify:

```
HeatCapacity(
   PMIModel (
      Name = <string>
      MSConfig = <string>
      Index = <int>
      String = <string>
   )
)
```

The options of `PMIModel` are described in Command File on page 1173.

Dependencies

The heat capacity may depend on the variables:

n	Electron density [cm^{-3}]
p	Hole density [cm^{-3}]
T	Lattice temperature [K]
eT	Electron temperature [K]
hT	Hole temperature [K]
s	Multistate configuration occupation probabilities [1]

The model must compute the following quantities:

`val`   Heat capacity $[\mathrm{Jcm^{-3}K^{-1}}]$

In the case of the standard interface, the following derivatives must be computed as well:

`dval_dn`   Derivative with respect to electron density $[\mathrm{JK^{-1}}]$

`dval_dp`   Derivative with respect to hole density $[\mathrm{JK^{-1}}]$

`dval_dT`   Derivative with respect to lattice temperature $[\mathrm{Jcm^{-3}K^{-2}}]$

`dval_deT`   Derivative with respect to electron temperature $[\mathrm{Jcm^{-3}K^{-2}}]$

`dval_dhT`   Derivative with respect to hole temperature $[\mathrm{Jcm^{-3}K^{-2}}]$

`dval_ds`   Derivative with respect to multistate configuration occupation probabilities $[\mathrm{Jcm^{-3}K^{-1}}]$

Standard C++ Interface

The PMI offers a base class that presents the following interface:

```
class PMI_MSC_HeatCapacity : public PMI_MSC_Vertex_Interface
{
public:
  PMI_MSC_HeatCapacity (const PMI_Environment& env,
    const std::string& msconfig_name,
    const int model_index,
    const std::string& model_string);
  // otherwise, see Standard C++ Interface on page 1175
};
```

Apart from the base class name and the constructor, the explanations in Standard C++ Interface on page 1175 apply here as well.

The following virtual constructor must be implemented:

```
typedef PMI_MSC_HeatCapacity* new_PMI_MSC_HeatCapacity_func
   (const PMI_Environment& env, const std::string& msconfig_name,
   int model_index, const std::string& model_string);
extern "C" new_PMI_MSC_HeatCapacity_func new_PMI_MSC_HeatCapacity;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_MSC_HeatCapacity_Base : public PMI_MSC_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      const pmi_float& n () const;   // electron density
      const pmi_float& p () const;   // hole density
      const pmi_float& T () const;   // lattice temperature
      const pmi_float& eT () const;  // electron temperature
      const pmi_float& hT () const;  // hole temperature
      const pmi_float& s (size_t ind) const;  // phase fraction
   };

   class Output {
   public:
      Output (NS_PMI_MSC::odata* odata);

      pmi_float& val ();   // heat capacity
   };

   PMI_MSC_HeatCapacity_Base (const PMI_Environment& env,
                              const std::string& msconfig_name,
                              const int model_index,
                              const std::string& model_string);
   virtual ~PMI_MSC_HeatCapacity_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_MSC_Mobility_Base* new_PMI_MSC_Mobility_Base_func
   (const PMI_Environment& env, const std::string& msconfig_name,
    const int model_index, const std::string& model_string,
    const PMI_AnisotropyType anisotype);
extern "C" new_PMI_MSC_HeatCapacity_Base_func new_PMI_MSC_HeatCapacity_Base;
```

Optical Quantum Yield

The quantum yield factors η_G, $\eta_{T_{E_g}}$, and η_{T_0} defined by Eq. 643, p. 546 can be accessed through a PMI. In the command file, the PMI is specified in the QuantumYield section as follows:

```
Physics {
   Optics (
      OpticalGeneration (
         QuantumYield (
            ...
            pmiModel = "<pmi_model_name>"
         )
      )
   )
}
```

Dependencies

The quantum yield factors η_G, $\eta_{T_{E_g}}$, and η_{T_0} may depend on the variables:

n	Electron density $[\text{cm}^{-3}]$
p	Hole density $[\text{cm}^{-3}]$
T	Lattice temperature $[\text{K}]$
bg	Bandgap energy E_g $[\text{eV}]$
bg_eff	Effective bandgap energy (includes bandgap narrowing) $E_{g,eff}$ $[\text{eV}]$
wavelength	Wavelength of incident light λ $[\mu\text{m}]$
cplxRefIndex	Refractive index
cplxExtCoeff	Extinction coefficient
n_0	Base refractive index
k_0	Base extinction coefficient
d_n_lambda	Wavelength-dependent part of refractive index
d_k_lambda	Wavelength-dependent part of extinction coefficient
d_n_temp	Temperature-dependent part of refractive index

`d_n_carr`	Carrier-dependent part of refractive index
`d_k_carr`	Carrier-dependent part of extinction coefficient
`d_n_gain`	Gain-dependent part of refractive index

The PMI model must compute the following results:

`eta_G`	Quantum yield
`eta_T_Eg`	Thermalization yield (band gap)
`eta_T0`	Thermalization yield (vacuum)

Standard C++ Interface

The following base class (public interface) is declared in the file `PMIModels.h`:

```
class PMI_OpticalQuantumYield : public PMI_Vertex_Interface
{
public:
   // the input data coming from the simulator

   class idata {
   public:
      idata(const void*);
      double n() const;
      double p() const;
      double T() const;
      double bg() const;
      double bg_eff() const;
      double wavelength() const;
      double cplxRefIndex() const;
      double cplxExtCoeff() const;
      double n_0() const;
      double k_0() const;
      double d_n_lambda() const;
      double d_k_lambda() const;
      double d_n_temp() const;
      double d_n_carr() const;
      double d_k_carr() const;
      double d_n_gain() const;
   };

   // the results computed by the PMI
   class odata {
      public:
```

```
      odata(void*);
      double& eta_G();
      double& eta_T_Eg();
      double& eta_T0();
   };

   // constructor and destructor
   PMI_OpticalQuantumYield(const PMI_Environment& env);
   virtual ~PMI_OpticalQuantumYield();

   // compute value and derivatives
   virtual void compute(const idata* id, odata* od ) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_OpticalQuantumYield* new_PMI_OpticalQuantumYield_func
   (const PMI_Environment& env);
extern "C" new_PMI_OpticalQuantumYield_func new_PMI_OpticalQuantumYield;
```

Simplified C++ Interface

The following base class (public interface) is declared in the file `PMI.h`:

```
class PMI_OpticalQuantumYield_Base : public PMI_Vertex_Base {
public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      Input (const PMI_OpticalQuantumYield_Base* opticalquantumyield_base,
      const int vertex);
      pmi_float n;
      pmi_float p;
      pmi_float T;
      pmi_float bg;
      pmi_float bg_eff;
      pmi_float wavelength;
      pmi_float cplxRefIndex;
      pmi_float cplxExtCoeff;
      pmi_float n_0;
      pmi_float k_0;
      pmi_float d_n_lambda;
      pmi_float d_k_lambda;
      pmi_float d_n_temp;
      pmi_float d_n_carr;
      pmi_float d_k_carr;
      pmi_float d_n_gain;
   };
```

```
      class Output {
      public:
         pmi_float eta_G;
         pmi_float eta_T_Eg;
         pmi_float eta_T0;
      };

      PMI_OpticalQuantumYield_Base (const PMI_Environment& env);
      virtual ~PMI_OpticalQuantumYield_Base ();
      virtual void compute (const Input& input, Output& output) = 0;
   };
```

The prototype for the virtual constructor is given as:

```
typedef PMI_OpticalQuantumYield_Base* new_PMI_OpticalQuantumYield_Base_func
   (const PMI_Environment& env);
extern "C" new_PMI_OpticalQuantumYield_Base_func
new_PMI_OpticalQuantumYield_Base;
```

Stress

Sentaurus Device supports a PMI for mechanical stress (see Chapter 31 on page 821). The name of the PMI model must appear in the `Piezo` section of the command file:

```
Physics {
   Piezo (
      Stress = pmi_model_name
   )
}
```

Dependencies

A PMI stress model has no explicit dependencies. However, it can depend on doping concentrations and mole fractions through the runtime support.

The PMI model must compute the following results:

`stress_xx`	XX component of stress tensor [Pa]
`stress_yy`	YY component of stress tensor [Pa]
`stress_zz`	ZZ component of stress tensor [Pa]

stress_yz   YZ component of stress tensor [Pa]

stress_xz   XZ component of stress tensor [Pa]

stress_xy   XY component of stress tensor [Pa]

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_Stress : public PMI_Vertex_Interface {

public:
   PMI_Stress (const PMI_Environment& env);
   virtual ~PMI_Stress ();

   virtual void Compute_StressXX
      (double& stress_xx) = 0;

   virtual void Compute_StressYY
      (double& stress_yy) = 0;

   virtual void Compute_StressZZ
      (double& stress_zz) = 0;

   virtual void Compute_StressYZ
      (double& stress_yz) = 0;

   virtual void Compute_StressXZ
      (double& stress_xz) = 0;

   virtual void Compute_StressXY
      (double& stress_xy) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_Stress* new_PMI_Stress_func
   (const PMI_Environment& env);
extern "C" new_PMI_Stress_func new_PMI_Stress;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```cpp
class PMI_Stress_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
   };

   class Output {
   public:
      pmi_float stress_xx;  // xx component of stress
      pmi_float stress_yy;  // yy component of stress
      pmi_float stress_zz;  // zz component of stress
      pmi_float stress_yz;  // yz component of stress
      pmi_float stress_xz;  // xz component of stress
      pmi_float stress_xy;  // xy component of stress
   };

   PMI_Stress_Base (const PMI_Environment& env);
   virtual ~PMI_Stress_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```cpp
typedef PMI_Stress_Base* new_PMI_Stress_Base_func
   (const PMI_Environment& env);
extern "C" new_PMI_Stress_Base_func new_PMI_Stress_Base;
```

Example: Constant Stress Model

The following code returns constant values for the stress tensor:

```cpp
#include "PMIModels.h"

class Constant_Stress : public PMI_Stress {

private:
   double xx, yy, zz, yz, xz, xy;

public:
   Constant_Stress (const PMI_Environment& env);
```

```
  ~Constant_Stress ();

  void Compute_StressXX (double& stress_xx);
  void Compute_StressYY (double& stress_yy);
  void Compute_StressZZ (double& stress_zz);
  void Compute_StressYZ (double& stress_yz);
  void Compute_StressXZ (double& stress_xz);
  void Compute_StressXY (double& stress_xy);

};

Constant_Stress::
Constant_Stress (const PMI_Environment& env) :
  PMI_Stress (env)
{ xx = InitParameter ("xx", 100);
  yy = InitParameter ("yy", -4e9);
  zz = InitParameter ("zz", 300);
  yz = InitParameter ("yz", 400);
  xz = InitParameter ("xz", 500);
  xy = InitParameter ("xy", 600);
}

Constant_Stress::
~Constant_Stress ()
{
}

void Constant_Stress::
Compute_StressXX (double& stress_xx)
{ stress_xx = xx;
}

void Constant_Stress::
Compute_StressYY (double& stress_yy)
{ stress_yy = yy;
}

void Constant_Stress::
Compute_StressZZ (double& stress_zz)
{ stress_zz = zz;
}

void Constant_Stress::
Compute_StressYZ (double& stress_yz)
{ stress_yz = yz;
}
```

```
void Constant_Stress::
Compute_StressXZ (double& stress_xz)
{ stress_xz = xz;
}

void Constant_Stress::
Compute_StressXY (double& stress_xy)
{ stress_xy = xy;
}

extern "C"
PMI_Stress* new_PMI_Stress (const PMI_Environment& env)
{ return new Constant_Stress (env);
}
```

Space Factor

The space distribution of the metal workfunction (see Metal Workfunction on page 242), traps (see Energetic and Spatial Distribution of Traps on page 450), the bond concentration (see Using the Trap Degradation Model on page 495), the extended nonradiative multiphonon (eNMP) model precursor concentration (see Using the eNMP Model on page 516), and piezoresistance enhancement factors (see SFactor Dataset or PMI Model on page 876) can be computed by a space factor PMI. The name of the PMI is specified in the appropriate `Physics` section as follows:

```
Physics (Material | Region = "<name>") {
   MetalWorkfunction (SFactor=pmi_model_name ...)
}
```

or:

```
Physics {
   Traps (SFactor=pmi_model_name ...)
}
```

or:

```
Physics {
   Traps (BondConcSFactor=pmi_model_name ...)
}
```

or:

```
Physics (MaterialInterface | RegionInterface = "<name1>/<name2>"){
   eNMP (SFactor=pmi_model_name ...)
}
```

or:

```
Physics {
   Piezo (
      Model (
         Mobility (
            Factor (
               SFactor=pmi_model_name
               [ChannelDirection=<n>]
               [AutoOrientation | ParameterSetName="<psname>"]
            )
         )
      )
   )
}
```

In the last specification, the `Factor` options `ChannelDirection=<n>`, `AutoOrientation`, and `ParameterSetName="<psname>"`, if specified, are passed as parameters to the space factor PMI model (`AutoOrientation` is passed as `AutoOrientation=1`).

NOTE The name of the PMI model must not coincide with the name of an internal field of Sentaurus Device. Otherwise, Sentaurus Device takes the value of the internal field as the space factor.

Dependencies

A PMI space factor model has no explicit dependencies. The model must compute:

`spacefactor`   Space factor (1) or $[\text{cm}^{-3}]$

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_SpaceFactor : public PMI_Vertex_Interface {

public:
   PMI_SpaceFactor (const PMI_Environment& env);
   virtual ~PMI_SpaceFactor ();

   virtual void Compute_spacefactor
      (double& spacefactor) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_SpaceFactor* new_PMI_SpaceFactor_func
   (const PMI_Environment& env);
extern "C" new_PMI_SpaceFactor_func new_PMI_SpaceFactor;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_SpaceFactor_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
   };

   class Output {
   public:
      pmi_float spacefactor;  // space factor
   };

   PMI_SpaceFactor_Base (const PMI_Environment& env);
   virtual ~PMI_SpaceFactor_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_SpaceFactor_Base* new_PMI_SpaceFactor_Base_func
   (const PMI_Environment& env);
extern "C" new_PMI_SpaceFactor_Base_func new_PMI_SpaceFactor_Base;
```

Example: PMI User Field as Space Factor

The following code reads the space factor from a PMI user field:

```
#include "PMIModels.h"

class pmi_spacefactor : public PMI_SpaceFactor {

public:
  pmi_spacefactor (const PMI_Environment& env);
  ~pmi_spacefactor ();
```

```
      void Compute_spacefactor (double& spacefactor);
   };

   pmi_spacefactor::
   pmi_spacefactor (const PMI_Environment& env) :
     PMI_SpaceFactor (env)
   {
   }

   pmi_spacefactor::
   ~pmi_spacefactor ()
   {
   }

   void pmi_spacefactor::
   Compute_spacefactor (double& spacefactor)
   { spacefactor = ReadUserField (PMI_UserField1);
   }

   extern "C"
   PMI_SpaceFactor* new_PMI_SpaceFactor
     (const PMI_Environment& env)
   { return new pmi_spacefactor (env);
   }
```

Mobility Stress Factor

Stress-dependent isotropic mobility enhancement factors can be computed by a mobility stress factor PMI. These factors are applied to total low-field mobility or mobility components as described in Isotropic Factor Models on page 870.

The name of a mobility stress factor PMI model is specified as a `Factor` option in the command file (see Using Isotropic Factor Models on page 871):

```
Physics {
   Piezo (
      Model (
         Mobility (
            Factor (
               pmi_model_name
               [ChannelDirection=<n>]
               [AutoOrientation | ParameterSetName="<psname>"]
            )
         )
      )
```

```
      )
   }
```

If specified, the `Factor` options `ChannelDirection=<n>`, `AutoOrientation`, and `ParameterSetName="<psname>"` are passed as parameters to the mobility stress factor PMI model (`AutoOrientation` is passed as `AutoOrientation=1`).

Dependencies

A mobility stress factor PMI model may depend on the following variable:

`enorm`   Normal electric field [Vcm^{-1}]

The PMI model must compute the following result:

`mobilitystressfactor`   Stress-dependent mobility enhancement factor [1]

In the case of the standard interface, the following derivative must be computed as well:

`dmobilitystressfactordenorm` Derivative of the mobility stress factor with respect to E_{normal} [cmV^{-1}]

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```cpp
class PMI_MobilityStressFactor : public PMI_Vertex_Interface {

public:
  PMI_MobilityStressFactor (const PMI_Environment& env);

  virtual ~PMI_MobilityStressFactor ();

  virtual void Compute_mobilitystressfactor
    (const double enorm, double& mobilitystressfactor,
     double& dmobilitystressfactordenorm) = 0;
};
```

Two virtual constructors are required for electron and hole mobility factors:

```
typedef PMI_MobilityStressFactor* new_PMI_MobilityStressFactor_func
  (const PMI_Environment& env);
extern "C" new_PMI_MobilityStressFactor_func new_PMI_e_MobilityStressFactor;
extern "C" new_PMI_MobilityStressFactor_func new_PMI_h_MobilityStressFactor;
```

Simplified C++ Interface

The following base class is declared in the file PMI.h:

```
class PMI_MobilityStressFactor_Base : public PMI_Vertex_Base {

public:
  class Input : public PMI_Vertex_Input_Base {
  public:
    pmi_float enorm;  // normal to interface electric field
  };

  class Output {
  public:
    pmi_float mobilitystressfactor;  // mobility enhancement stress factor
  };
  PMI_MobilityStressFactor_Base (const PMI_Environment& env);
  virtual ~PMI_MobilityStressFactor_Base ();
  virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_MobilityStressFactor_Base* new_PMI_MobilityStressFactor_Base_func
  (const PMI_Environment& env);
extern "C" new_PMI_MobilityStressFactor_Base_func
  new_PMI_e_MobilityStressFactor_Base;
extern "C" new_PMI_MobilityStressFactor_Base_func
  new_PMI_h_MobilityStressFactor_Base;
```

Example: Effective Stress Model

This example illustrates the implementation of the EffectiveStressModel (see Effective Stress Model on page 872) using the standard C++ interface:

```
#include "PMI.h"
#include <cmath>

class pmi_EffectiveStressModel : public PMI_MobilityStressFactor {
```

```
protected:
  int cd, dim;
  double alpha1,alpha2,alpha3,beta11,beta12,beta13,beta22,beta23,beta33;
  double mu0,a10,a11,a12,a20,a21,a22,s00,s01,s02,t0,t1,t2,F0;

public:
  pmi_EffectiveStressModel (const PMI_Environment& env);
  ~pmi_EffectiveStressModel ();
  void Compute_mobilitystressfactor (const double enorm,
                                     double& mobilitystressfactor,
                                     double& dmobilitystressfactordenorm);
};

pmi_EffectiveStressModel::
pmi_EffectiveStressModel (const PMI_Environment& env) :
  PMI_MobilityStressFactor (env)
{
}

pmi_EffectiveStressModel::
~pmi_EffectiveStressModel ()
{
}
void pmi_EffectiveStressModel::
Compute_mobilitystressfactor (const double enorm,
                              double& mobilitystressfactor,
                              double& dmobilitystressfactordenorm)
{
  // Get stress components and convert to MPa.
  double stress[6];
  stress[0] = 1.e-6*ReadStress(PMI_StressXX);
  stress[1] = 1.e-6*ReadStress(PMI_StressYY);
  stress[2] = 1.e-6*ReadStress(PMI_StressZZ);
  stress[3] = 1.e-6*ReadStress(PMI_StressYZ);
  stress[4] = 1.e-6*ReadStress(PMI_StressXZ);
  stress[5] = 1.e-6*ReadStress(PMI_StressXY);

  // Get the diagonal stresses used in the calculation.
  double S11 = 0.0, S22 = 0.0, S33 = 0.0;

  // 1D cases and 2D cases where cd != 2.
  if (dim == 1 || (dim == 2 && cd <2)) {
    const int nd = (cd == 0) ? 1 : 0;
    const int pd = 3-cd-nd;
    S11 = stress[cd];
    S22 = stress[nd];
    S33 = stress[pd];
```

```
        }

// Otherwise, do a stress transformation to get the stress components.
else {
  // Normal direction vector.
  double norm[3];
  ReadNearestInterfaceNormal(norm[0], norm[1], norm[2]);
  norm[cd] = 0.0;
  if (norm[0] == 0. && norm[1] == 0. && norm[2] == 0.0) {
    if (cd == 0) norm[1] = 1.0;
    else norm[0] = 1.0;
  }
  else {
    const double mag=sqrt(norm[0]*norm[0]+norm[1]*norm[1]+norm[2]*norm[2]);
    norm[0] /= mag; norm[1] /= mag; norm[2] /= mag;
  }

  // Channel direction vector.
  double chan[3] = {0.0};
  chan[cd] = 1.0;

  // In-plane direction vector.
  double plan[3];
  plan[0] = chan[1]*norm[2] - chan[2]*norm[1];
  plan[1] = chan[2]*norm[0] - chan[0]*norm[2];
  plan[2] = chan[0]*norm[1] - chan[1]*norm[0];

  // Rotation matrix.
  double a[3][3];
  a[0][0]=chan[0]; a[0][1]=chan[1]; a[0][2]=chan[2];
  a[1][0]=norm[0]; a[1][1]=norm[1]; a[1][2]=norm[2];
  a[2][0]=plan[0]; a[2][1]=plan[1]; a[2][2]=plan[2];

  // Get the diagonal components of the transformed stress tensor.
  double SD[3][3];
  SD[0][0] = stress[0]; SD[1][1] = stress[1]; SD[2][2] = stress[2];
  SD[0][1] = SD[1][0] = stress[5];
  SD[0][2] = SD[2][0] = stress[4];
  SD[1][2] = SD[2][1] = stress[3];

  // Channel direction.
  S11 = SD[cd][cd];

  // Normal direction.
  for (int i=0; i<3; ++i) {
    for (int j=0; j<3; ++j) {
      S22 += a[1][i]*a[1][j]*SD[i][j];
    }
```

```
    }

    // In-plane direction.
    for (int i=0; i<3; ++i) {
      for (int j=0; j<3; ++j) {
        S33 += a[2][i]*a[2][j]*SD[i][j];
      }
    }
  }

  // Effective stress.
  const double Seff = alpha1*S11 + alpha2*S22 + alpha3*S33
    + beta11*S11*S11 + beta12*S11*S22 + beta13*S11*S33
    + beta22*S22*S22 + beta23*S22*S33 + beta33*S33*S33;

  // Convert field to MV/cm.
  const double F = 1.e-6*enorm;

  // Get the stress factor.
  const double FF = (F < F0) ? F : F0;
  const double F2 = FF*FF;
  const double A1 = a10 + a11*FF + a12*F2;
  const double A2 = a20 + a21*FF + a22*F2;
  const double S0 = s00 + s01*FF + s02*F2;
  const double t  =  t0 +  t1*F +  t2*F*F;
  const double sarg = (Seff - S0)/t;
  const double expsarg = exp(sarg);
  const double expsargp1 = 1. + expsarg;
  mobilitystressfactor = ((A1-A2)/expsargp1 + A2)/mu0;

  // Derivative wrt enorm.
  const double dA1dF = (F < F0) ? a11 + 2.*a12*F : 0.0;
  const double dA2dF = (F < F0) ? a21 + 2.*a22*F : 0.0;
  const double dS0dF = (F < F0) ? s01 + 2.*s02*F : 0.0;
  const double dtdF  =  t1 + 2.*t2*F;
  const double dsfdF = (dA1dF + expsarg*dA2dF + (A1-A2)*expsarg*
        (dS0dF + sarg*dtdF)/(t*expsargp1))/(mu0*expsargp1);
  dmobilitystressfactordenorm = 1.e-6*dsfdF;
}

class pmi_e_EffectiveStressModel : public pmi_EffectiveStressModel {
public:
  pmi_e_EffectiveStressModel (const PMI_Environment& env);
  ~pmi_e_EffectiveStressModel () {}
};

pmi_e_EffectiveStressModel::
pmi_e_EffectiveStressModel (const PMI_Environment& env)
```

```
                   : pmi_EffectiveStressModel (env)
               {
                 // Get channel direction and dimension.
                 const double dchannelDirection = InitParameter("ChannelDirection", 1.0);
                 cd = (dchannelDirection == 2.0) ? 1 : ((dchannelDirection == 3.0) ? 2 : 0);
                 dim = ReadDimension();

                 alpha1 = InitParameter ("alpha1_e",  1.0);
                 alpha2 = InitParameter ("alpha2_e", -1.7);
                 alpha3 = InitParameter ("alpha3_e",  0.7);
                 beta11 = InitParameter ("beta11_e",  0.0);
                 beta12 = InitParameter ("beta12_e",  0.0);
                 beta13 = InitParameter ("beta13_e",  0.0);
                 beta22 = InitParameter ("beta22_e",  0.0);
                 beta23 = InitParameter ("beta23_e",  0.0);
                 beta33 = InitParameter ("beta33_e",  0.0);
                 mu0 = InitParameter ("mu0_e",    810.0);
                 a10 = InitParameter ("a10_e",    565.0);
                 a11 = InitParameter ("a11_e",    -81.0);
                 a12 = InitParameter ("a12_e",    -44.0);
                 a20 = InitParameter ("a20_e",   2028.0);
                 a21 = InitParameter ("a21_e",  -1992.0);
                 a22 = InitParameter ("a22_e",    920.0);
                 s00 = InitParameter ("s00_e",   1334.0);
                 s01 = InitParameter ("s01_e",  -2646.0);
                 s02 = InitParameter ("s02_e",    875.0);
                 t0 = InitParameter ("t0_e" ,    882.0);
                 t1 = InitParameter ("t1_e" ,   -987.0);
                 t2 = InitParameter ("t2_e" ,    604.0);
                 F0 = InitParameter ("F0_e" ,   1.e10);
               }

               class pmi_h_EffectiveStressModel : public pmi_EffectiveStressModel {
               public:
                 pmi_h_EffectiveStressModel (const PMI_Environment& env);
                 ~pmi_h_EffectiveStressModel () {}
               };

               pmi_h_EffectiveStressModel::
               pmi_h_EffectiveStressModel (const PMI_Environment& env)
                 : pmi_EffectiveStressModel (env)
               {
                 // Get channel direction and dimension.
                 const double dchannelDirection = InitParameter("ChannelDirection", 1.0);
                 cd = (dchannelDirection == 2.0) ? 1 : ((dchannelDirection == 3.0) ? 2 : 0);
                 dim = ReadDimension();

                 alpha1 = InitParameter ("alpha1_h",  1.0);
```

```
        alpha2 = InitParameter ("alpha2_h", -0.4);
        alpha3 = InitParameter ("alpha3_h", -0.6);
        beta11 = InitParameter ("beta11_h",  0.0);
        beta12 = InitParameter ("beta12_h",  0.0);
        beta13 = InitParameter ("beta13_h", -0.00004);
        beta22 = InitParameter ("beta22_h",  0.00006);
        beta23 = InitParameter ("beta23_h", -0.00018);
        beta33 = InitParameter ("beta33_h",  0.00011);
        mu0 = InitParameter ("mu0_h",   212.0);
        a10 = InitParameter ("a10_h",  2460.0);
        a11 = InitParameter ("a11_h",     0.0);
        a12 = InitParameter ("a12_h",     0.0);
        a20 = InitParameter ("a20_h",    42.0);
        a21 = InitParameter ("a21_h",     0.0);
        a22 = InitParameter ("a22_h",     0.0);
        s00 = InitParameter ("s00_h", -1338.0);
        s01 = InitParameter ("s01_h",     0.0);
        s02 = InitParameter ("s02_h",     0.0);
        t0 = InitParameter ("t0_h" ,   524.0);
        t1 = InitParameter ("t1_h" ,     0.0);
        t2 = InitParameter ("t2_h" ,     0.0);
        F0 = InitParameter ("F0_h" ,   1.e10);
    }

    extern "C"
    PMI_MobilityStressFactor* new_PMI_e_MobilityStressFactor
      (const PMI_Environment& env)
    { return new pmi_e_EffectiveStressModel (env);
    }

    extern "C"
    PMI_MobilityStressFactor* new_PMI_h_MobilityStressFactor
      (const PMI_Environment& env)
    { return new pmi_h_EffectiveStressModel (env);
    }
```

Trap Capture and Emission Rates

The present PMI model can be used to define either capture and emission rates for traps (see c_C^n, c_V^p, e_C^n, and e_V^p in Trap Occupation Dynamics on page 455) or the transitions between states of multistate configurations (see Specifying Multistate Configurations on page 475). The model is an arbitrary function of n, p, T, T_n, T_p, and F.

Traps

In the command file, specify the model with the `CBRate` and `VBRate` options to `Traps`.

For example:

```
Traps((CBRate=("modelX",17) VBRate="modelY") ... )
```

uses the user-specified model `modelX` to compute c_C^n and e_C^n (see Local Trap Capture and Emission on page 457), and `modelY` to compute c_V^p and e_V^p. The `17` is passed as the second argument to the virtual constructor for `modelX`; `modelY` is passed as a default value of `0` instead. The interpretation of these integers is left to the user-specified models. They allow you to select among different parameters or model variants, without having to reimplement the full model for each different choice of parameters or each minor model variation.

Multistate Configurations

The present model is used for transitions of multistate configurations by the keyword `CEModel` (see Specifying Multistate Configurations on page 475), for example:

```
MSConfig { ...
   Transition ( Name="t1" To = "c" From="a" CEModel ("modelX" 5) )
}
```

where `5` is the optional model index parameter that defaults to 0.

Dependencies

The capture and emission rates may depend on the variables:

`n`	Electron density $[\text{cm}^{-3}]$
`p`	Hole density $[\text{cm}^{-3}]$
`t`	Lattice temperature $[\text{K}]$
`tn`	Electron temperature $[\text{K}]$
`tp`	Hole temperature $[\text{K}]$
`f`	Electric field $[\text{Vcm}^{-1}]$

The PMI model must compute the following results (note that the carrier type that is captured and emitted is determined by the band to which the model is applied):

`capture`	Capture rate $[\text{s}^{-1}]$
`emission`	Emission rate $[\text{s}^{-1}]$

In the case of the standard interface, the following derivatives must be computed as well:

`dcapturedn`	Derivative of capture rate with respect to n $[\text{s}^{-1}\text{cm}^3]$
`demissiondn`	Derivative of emission rate with respect to n $[\text{s}^{-1}\text{cm}^3]$
`dcapturedp`	Derivative of capture rate with respect to p $[\text{s}^{-1}\text{cm}^3]$
`demissiondp`	Derivative of emission rate with respect to p $[\text{s}^{-1}\text{cm}^3]$
`dcapturedt`	Derivative of capture rate with respect to t $[\text{s}^{-1}\text{K}^{-1}]$
`demissiondt`	Derivative of emission rate with respect to t $[\text{s}^{-1}\text{K}^{-1}]$
`dcapturedtn`	Derivative of capture rate with respect to tn $[\text{s}^{-1}\text{K}^{-1}]$
`demissiondtn`	Derivative of emission rate with respect to tn $[\text{s}^{-1}\text{K}^{-1}]$
`dcapturedtp`	Derivative of capture rate with respect to tp $[\text{s}^{-1}\text{K}^{-1}]$
`demissiondtp`	Derivative of emission rate with respect to tp $[\text{s}^{-1}\text{K}^{-1}]$
`dcapturedf`	Derivative of capture rate with respect to f $[\text{s}^{-1}\text{V}^{-1}\text{cm}]$
`demissiondf`	Derivative of emission rate with respect to f $[\text{s}^{-1}\text{V}^{-1}\text{cm}]$

Standard C++ Interface

The following base class is declared in `PMIModels.h`:

```
class PMI_TrapCaptureEmission : public PMI_Vertex_Interface {
public:
  PMI_TrapCaptureEmission(const PMI_Environment& env);
  virtual ~PMI_TrapCaptureEmission();

  virtual void Compute_rates
    (const double n, const double p, const double t,
     const double tn, const double tp, const double f,
     double& capture, double& emission) = 0;

  virtual void Compute_dratesdn
```

```
     (const double n, const double p, const double t,
      const double tn, const double tp, const double f,
      double& dcapturedn, double& demissiondn) = 0;

   virtual void Compute_dratesdp
     (const double n, const double p, const double t,
      const double tn, const double tp, const double f,
      double& dcapturedp, double& demissiondp) = 0;

   virtual void Compute_dratesdt
     (const double n, const double p, const double t,
      const double tn, const double tp, const double f,
      double& dcapturedt, double& demissiondt) = 0;

   virtual void Compute_dratesdtn
     (const double n, const double p, const double t,
      const double tn, const double tp, const double f,
      double& dcapturedtn, double& demissiondtn) = 0;

   virtual void Compute_dratesdtp
     (const double n, const double p, const double t,
      const double tn, const double tp, const double f,
      double& dcapturedtp, double& demissiondtp) = 0;

   virtual void Compute_dratesdf
     (const double n, const double p, const double t,
      const double tn, const double tp, const double f,
      double& dcapturedf, double& demissiondf) = 0;
};
```

The following virtual constructor must be implemented:

```
typedef PMI_TrapCaptureEmission* new_PMI_TrapCaptureEmission_func
   (const PMI_Environment& env, int id);
extern "C" new_PMI_TrapCaptureEmission_func new_PMI_TrapCaptureEmission;
```

Simplified C++ Interface

The following base class is declared in the file PMI.h:

```
class PMI_TrapCaptureEmission_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      pmi_float n;   // electron density
      pmi_float p;   // hole density
```

```
      pmi_float t;   // lattice temperature
      pmi_float tn;  // electron temperature
      pmi_float tp;  // hole temperature
      pmi_float f;   // absolute value of electric field
      pmi_float nc;  // lattice effective state density for electrons
      pmi_float nv;  // lattice effective state density for holes
      pmi_float egeff;  // effective band gap
    };

    class Output {
    public:
      pmi_float capture;   // capture rate
      pmi_float emission;  // emission rate
    };

    PMI_TrapCaptureEmission_Base (const PMI_Environment& env);
    virtual ~PMI_TrapCaptureEmission_Base ();

    virtual void compute (const Input& input, Output& output) = 0;
  };
```

The prototype for the virtual constructor is given as:

```
typedef PMI_TrapCaptureEmission_Base* new_PMI_TrapCaptureEmission_Base_func
    (const PMI_Environment& env, int id);
extern "C" new_PMI_TrapCaptureEmission_Base_func
    new_PMI_TrapCaptureEmission_Base;
```

Example: CEModel_ArrheniusLaw

The model has the structure of the Arrhenius law. It depends on the temperature.

Table 174   Model parameters

Symbol	Parameter name	Default	Unit	Description
δE	DeltaE	0.	eV	Energy difference
g	g	1.	1	Degeneracy factor
r_0	r0	1.	s^{-1}	Maximal transition rate
E_{act}	Eact	0.	eV	Activation energy

Let δE and E_{act} be the energy difference and activation energy. The capture and emission rates are given by:

$$c = r_0 \exp(-E_{act}/kT) \tag{1267}$$

$$e = r_0 g \exp(-\langle E_{act} + \delta E\rangle/kT) \tag{1268}$$

The model is shipped with Sentaurus Device. A more flexible and general way to specify Arrhenius law transitions is provided by the transition model `pmi_ce_msc` (see Arrhenius Law (Formula=0) on page 479).

Trap Energy Shift

The present PMI determines a shift E_{shift} of trap energies that depends on the electric field and the lattice temperature at the location of the vertex or at a position given with `ReferencePoint` (see Energetic and Spatial Distribution of Traps on page 450).

Command File

The energy shift model is specified by `EnergyShift=<model name>` or `EnergyShift=(<model name>, <int>)` as an option to `Traps` in the `Physics` section. The optional integer defaults to zero and is passed as the argument `id` to the virtual constructor of the PMI (see below). The interpretation of `id` is dependent on the user-specified model.

Dependencies

The trap energy shift can depend on the variables:

`f`	Electric field vector $[\mathrm{Vcm^{-1}}]$, a vector with up to three components, for the field in the x-, y-, and z-direction
`t`	Lattice temperature $[\mathrm{K}]$

The PMI model must compute the following results:

`shift`	Energy shift $[\mathrm{eV}]$

In the case of the standard interface, the following derivatives must be computed as well:

dshiftdf   Derivative of energy shift with respect to each component of f $[\mathrm{eVcmV}^{-1}]$, a vector with up to three entries

dshiftdt   Derivative of energy shift with respect to t $[\mathrm{eVK}^{-1}]$

Standard C++ Interface

The following base class is declared in `PMIModels.h`:

```
class PMI_TrapEnergyShift : public PMI_Vertex_Interface {

public:
   PMI_TrapEnergyShift(const PMI_Environment& env);
   virtual ~PMI_TrapEnergyShift();

   virtual void Compute_shift(
      const double f[3], const double t, double& shift) = 0;
   virtual void Compute_dshiftdf(
      const double f[3], const double t, double df[3]) = 0;
   virtual void Compute_dshiftdt(
      const double f[3], const double t, double& dt) = 0;
};
```

The following virtual constructor must be implemented:

```
typedef PMI_TrapEnergyShift* new_PMI_TrapEnergyShift_func
   (const PMI_Environment& env, int id);
extern "C" new_PMI_TrapEnergyShift_func new_PMI_TrapEnergyShift;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_TrapEnergyShift_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      pmi_float f[3];  // electric field vector
      pmi_float t;     // lattice temperature
   };

   class Output {
```

```
      public:
        pmi_float shift;  // trap energy shift
      };

      PMI_TrapEnergyShift_Base (const PMI_Environment& env);
      virtual ~PMI_TrapEnergyShift_Base ();

      virtual void compute (const Input& input, Output& output) = 0;
   };
```

The prototype for the virtual constructor is given as:

```
typedef PMI_TrapEnergyShift_Base* new_PMI_TrapEnergyShift_Base_func
   (const PMI_Environment& env, int id);
extern "C" new_PMI_TrapEnergyShift_Base_func new_PMI_TrapEnergyShift_Base;
```

eNMP Transition Rates

Transition rates used in the extended nonradiative multiphonon (eNMP) model can be computed by an eNMP transition rates PMI model. The computed transition rates are used in the solution of the eNMP model rate equations (see eNMP Model Description on page 514).

To use a PMI for calculating the transition rates, specify the PMI model name as an option to eNMP in the Physics section of the command file:

```
Physics (MaterialInterface | RegionInterface = "<name1>/<name2>") {
   eNMP (
      pmi_model_name [StateCharge=<1 or -1>] ...
   )
}
```

The eNMP model requires the calculation of eight transition rates occurring between four states. For the built-in eNMP model, the metastable states are designated with primes (that is, 1' and 2'). To simplify the naming of the transition rates for the PMI, the following definitions are made:

- state 3 = state 1'
- state 4 = state 2'

In addition, when a PMI model is used to calculate the transition rates, the sign of the charge states can be specified with the StateCharge parameter in the command file. By default, the charge states are assumed to be positive (StateCharge > 0). To designate that the charge states are negative, specify StateCharge < 0.

With these definitions, the transition rates that must be calculated by the PMI model are shown in Figure 84.

Figure 84   State diagram for the eNMP transition rates PMI

Distinction Between Electron and Hole Transitions

For transitions involving a change in charge ($1 \leftrightarrow 4$ and $2 \leftrightarrow 3$), the PMI requires a distinction between transitions that involve holes (hole capture and hole emission) and electrons (electron capture and electron emission). This distinction is necessary so that Sentaurus Device correctly accounts for changes in carrier recombination when the eNMP model is used. The component of a transition rate involving holes is designated with an "h" suffix, and an "e" suffix designates the electron component:

$$k_{14} = k_{14h} + k_{14e} \tag{1269}$$

$$k_{41} = k_{41h} + k_{41e} \tag{1270}$$

$$k_{23} = k_{23h} + k_{23e} \tag{1271}$$

$$k_{32} = k_{32h} + k_{32e} \tag{1272}$$

The transition rate components have the meanings shown in Table 175 depending on StateCharge.

Table 175   Definition of eNMP transition rate depending on StateCharge

Rates	StateCharge > 0	StateCharge < 0
k_{14h}, k_{32h}	Hole capture	Hole emission
k_{14e}, k_{32e}	Electron emission	Electron capture
k_{41h}, k_{23h}	Hole emission	Hole capture
k_{41e}, k_{23e}	Electron capture	Electron emission

It is not required to compute both electron and hole transition components in the PMI. For example, the built-in eNMP model includes only hole transitions, and electron transitions are ignored.

Transition Rates for All Sample Defects

Since the eNMP model uses a random sampling technique to obtain the average behavior of multiple defects, the eNMP transition rates PMI model must calculate transition rates for all of the sample defects at each vertex. For this purpose, the following parameters are passed automatically to the eNMP transition rates PMI and can be accessed using the runtime support function `InitParameter()`:

```
NumberOfSamples  = InitParameter("NumberOfSamples", 1000);
NumberOfVertices = InitParameter("NumberOfVertices", 1);
```

The `NumberOfSamples` keyword represents the value specified in the `eNMP` section of the command file. The `NumberOfVertices` keyword represents the number of interface vertices at the interface where the eNMP model is being used.

Parameter Randomization

Since transition rates must be obtained for all of the sample defects, it is likely that some model parameters will need to be randomized (either using a uniform distribution or a Gaussian distribution). In this case, the randomized parameter values should be obtained and stored in the constructor of the eNMP transition rates PMI for *all* `NumberOfSamples` defects *and* for all `NumberOfVertices` interface vertices. Therefore, a total of `NumberOfSamples` × `NumberOfVertices` values should be obtained for each parameter to be randomized. The requirement to obtain randomized parameter values for all interface vertices in the PMI constructor is to ensure that each vertex uses *different* `NumberOfSamples` values for each randomized parameter.

The eNMP transition rates PMI includes two member functions to assist in randomizing parameter values:

- `double UnifRanNum(int &idum)` – returns a random number between 0 and 1, exclusive of the endpoints.
- `double GausRanNum(int &idum)` – returns a random number that follows a normal distribution with zero mean and unit variance.

These functions must be initialized with `idum < 0` and, thereafter, `idum` must not be changed during the sequence. For example, the following code fragment shows how two parameters can be randomized and stored for later use:

```
std::vector<double> Eti;
std::vector<double> xti;
...
NumberOfSamples = InitParameter("NumberOfSamples", 1000);
NumberOfVertices = InitParameter("NumberOfVertices", 1);
double Et0   = InitParameter("Et", -0.5);
double Etsig = InitParameter("Etsig", 0.1);
double xtmin = InitParameter("xtmin", 0.0);
double xtmax = InitParameter("xtmax", 0.0);
...
int idum = -1;
for (int i = 0; i < NumberOfSamples*NumberOfVertices; ++i) {
   double Et = Et0 + Etsig*GausRanNum(idum);
   double xt = xtmin + (xtmax - xtmin)*UnifRanNum(idum);
   ...
   Eti.push_back(Et);
   xti.push_back(xt);
   ...
}
```

Dependencies

The eNMP transition rates PMI may depend on the interface values of the following variables:

`n`	Electron density $[\mathrm{cm}^{-3}]$
`p`	Hole density $[\mathrm{cm}^{-3}]$
`Nc`	Conduction band density-of-states $[\mathrm{cm}^{-3}]$
`Nv`	Valence band density-of-states $[\mathrm{cm}^{-3}]$
`Eg`	Band gap [eV]
`T`	Lattice temperature [K]
`F`	Magnitude of insulator electric field $[\mathrm{V\ cm}^{-1}]$

The PMI model must compute the following results:

`k[0]`$_i$ = $(k_{14h})_i$	Hole component of transition rates from state 1 to state 4 $[\mathrm{s}^{-1}]$
`k[1]`$_i$ = $(k_{14e})_i$	Electron component of transition rates from state 1 to state 4 $[\mathrm{s}^{-1}]$

$\mathtt{k[2]}_i = (k_{41h})_i$ Hole component of transition rates from state 4 to state 1 $[\mathrm{s}^{-1}]$

$\mathtt{k[3]}_i = (k_{41e})_i$ Electron component of transition rates from state 4 to state 1 $[\mathrm{s}^{-1}]$

$\mathtt{k[4]}_i = (k_{23h})_i$ Hole component of transition rates from state 2 to state 3 $[\mathrm{s}^{-1}]$

$\mathtt{k[5]}_i = (k_{23e})_i$ Electron component of transition rates from state 2 to state 3 $[\mathrm{s}^{-1}]$

$\mathtt{k[6]}_i = (k_{32h})_i$ Hole component of transition rates from state 3 to state 2 $[\mathrm{s}^{-1}]$

$\mathtt{k[7]}_i = (k_{32e})_i$ Electron component of transition rates from state 3 to state 2 $[\mathrm{s}^{-1}]$

$\mathtt{k[8]}_i = (k_{13})_i$ Transition rates from state 1 to state 3 $[\mathrm{s}^{-1}]$

$\mathtt{k[9]}_i = (k_{31})_i$ Transition rates from state 3 to state 1 $[\mathrm{s}^{-1}]$

$\mathtt{k[10]}_i = (k_{24})_i$ Transition rates from state 2 to state 4 $[\mathrm{s}^{-1}]$

$\mathtt{k[11]}_i = (k_{42})_i$ Transition rates from state 4 to state 2 $[\mathrm{s}^{-1}]$

> **NOTE** The subscript i in the above transition rates is shorthand that indicates that the transition rate must be computed for all `NumberOfSamples` sample defects at the interface vertex, for example:

$$\mathtt{k[0]}_i \rightarrow \mathtt{k[0]}_0, \mathtt{k[0]}_1, \mathtt{k[0]}_2, ..., \mathtt{k[0]}_{\mathrm{NumberOfSamples - 1}} \tag{1273}$$

In the case of the standard PMI interface, the following derivatives must also be computed:

$\mathtt{dkdn[0]}_i, \mathtt{dkdn[1]}_i, ..., \mathtt{dkdn[11]}_i$ Derivatives of all transition rates with respect to $\mathtt{n}$ $[\mathrm{cm}^3\mathrm{s}^{-1}]$

$\mathtt{dkdp[0]}_i, \mathtt{dkdp[1]}_i, ..., \mathtt{dkdp[11]}_i$ Derivatives of all transition rates with respect to $\mathtt{p}$ $[\mathrm{cm}^3\mathrm{s}^{-1}]$

$\mathtt{dkdNc[0]}_i, \mathtt{dkdNc[1]}_i, ..., \mathtt{dkdNc[11]}_i$ Derivatives of all transition rates with respect to $\mathtt{Nc}$ $[\mathrm{cm}^3\mathrm{s}^{-1}]$

$\mathtt{dkdNv[0]}_i, \mathtt{dkdNv[1]}_i, ..., \mathtt{dkdNv[11]}_i$ Derivatives of all transition rates with respect to $\mathtt{Nv}$ $[\mathrm{cm}^3\mathrm{s}^{-1}]$

$\mathtt{dkdEg[0]}_i, \mathtt{dkdEg[1]}_i, ..., \mathtt{dkdEg[11]}_i$ Derivatives of all transition rates with respect to $\mathtt{Eg}$ $[\mathrm{eV}^{-1}\mathrm{s}^{-1}]$

$\mathtt{dkdT[0]}_i, \mathtt{dkdT[1]}_i, ..., \mathtt{dkdT[11]}_i$ Derivatives of all transition rates with respect to $\mathtt{T}$ $[\mathrm{K}^{-1}\mathrm{s}^{-1}]$

$\mathtt{dkdF[0]}_i, \mathtt{dkdF[1]}_i, ..., \mathtt{dkdF[11]}_i$ Derivatives of all transition rates with respect to $\mathtt{F}$ $[\mathrm{cm}\,\mathrm{V}^{-1}\mathrm{s}^{-1}]$

> **NOTE** Similar to the transition rates, the subscript i in the above derivatives is shorthand that indicates that the derivatives must be computed for all `NumberOfSamples` sample defects at the interface vertex, for example:

$$\mathtt{dkdn[0]}_i \rightarrow \mathtt{dkdn[0]}_0, \mathtt{dkdn[0]}_1, \mathtt{dkdn[0]}_2, ..., \mathtt{dkdn[0]}_{\mathrm{NumberOfSamples - 1}} \tag{1274}$$

The derivative array indices correspond to the array indices for the transition rates, for example:

$$\mathtt{dkdn[0]}_i = \frac{d(k_{14h})_i}{dn}, \mathtt{dkdn[1]}_i = \frac{d(k_{14e})_i}{dn}, \dots \tag{1275}$$

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```cpp
class PMI_eNMPTransitionRates : public PMI_Vertex_Interface {

public:
   class Input {
   public:
      double n;   // electron density
      double p;   // hole density
      double Nc; // conduction-band effective density-of-states
      double Nv; // valence-band effective density-of-states
      double Eg; // bandgap
      double T;   // lattice temperature
      double F;   // insulator electric field
      int vindex; // vertex index (0 ≤ vindex ≤ NumberOfVertices – 1)
   };

   class Output {
   public:
      std::vector<double> k[12];      // transition rates
      std::vector<double> dkdn[12];  // derivatives wrt electron density
      std::vector<double> dkdp[12];  // derivatives wrt hole density
      std::vector<double> dkdNc[12]; // derivatives wrt to conduction band DOS
      std::vector<double> dkdNv[12]; // derivatives wrt to valence band DOS
      std::vector<double> dkdEg[12]; // derivatives wrt bandgap
      std::vector<double> dkdT[12];  // derivatives wrt lattice temperature
      std::vector<double> dkdF[12];  // derivatives wrt insulator electric
      field
   };

   PMI_eNMPTransitionRates (const PMI_Environment& env);

   virtual ~PMI_eNMPTransitionRates ();

   // method to be implemented by user
   virtual void compute(const Input& input, Output& output) = 0;
```

```
   // random number generators
   double UnifRanNum (int &idum);
   double GausRanNum (int &idum);
};
```

The following virtual constructor must be implemented:

```
typedef PMI_eNMPTransitionRates*
   new_PMI_eNMPTransitionRates_func (const PMI_Environment& env);
extern "C" new_PMI_eNMPTransitionRates_func new_PMI_eNMPTransitionRates;
```

Simplified C++ Interface

The following base class is declared in the file PMI.h:

```
class PMI_eNMPTransitionRates_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      Input (const PMI_eNMPTransitionRates_Base* enmprates_base, const int
      vertex);
      pmi_float n;  // electron density
      pmi_float p;  // hole density
      pmi_float Nc; // conduction-band effective density-of-states
      pmi_float Nv; // valence-band effective density-of-states
      pmi_float Eg; // bandgap
      pmi_float T;  // lattice temperature
      pmi_float F;  // insulator electric field
      int vindex;   // vertex index (0 ≤ vindex ≤ NumberOfVertices − 1)
   };

   class Output {
   public:
      std::vector<pmi_float> k[12]; // transition rates
   };

   PMI_eNMPTransitionRates_Base (const PMI_Environment& env);

   virtual ~PMI_eNMPTransitionRates_Base ();

   virtual void compute(const Input& input, Output& output) = 0;

   // random number generators
   double UnifRanNum (int &idum);
   double GausRanNum (int &idum);
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_eNMPTransitionRates_Base*
   new_PMI_eNMPTransitionRates_Base_func
      (const PMI_Environment& env);
extern "C" new_PMI_eNMPTransitionRates_Base_func
   new_PMI_eNMPTransitionRates_Base;
```

Example: eNMP Model Transition Rates

This example illustrates the implementation of the eNMP model transition rates using the standard C++ interface:

```
#include "PMI.h"
#include <cmath>
#include <vector>

// Implementation of transitions rates for the eNMP model.

class eNMPRates : public PMI_eNMPTransitionRates {

protected:
   int NumberOfSamples, NumberOfVertices;
   double Xsec, Vth, x0, nu0;
   std::vector<double> Eti;
   std::vector<double> Etpi;
   std::vector<double> Ri;
   std::vector<double> Rpi;
   std::vector<double> ESi; Model
   std::vector<double> ESpi;
   std::vector<double> ET2pi;
   std::vector<double> E1p1i;
   std::vector<double> E2p2i;
   std::vector<double> xti;

public:
   eNMPRates (const PMI_Environment& env);
   ~eNMPRates ();
   void compute (const Input& input, Output& output);
};

eNMPRates::
eNMPRates (const PMI_Environment& env) : PMI_eNMPTransitionRates (env)
{
   NumberOfSamples = InitParameter ("NumberOfSamples", 1000); // 1
   NumberOfVertices = InitParameter ("NumberOfVertices", 1);  // 1
   Xsec = InitParameter ("Xsec", 1.0e-15);  // cm^2
```

```
        Vth  = InitParameter ("Vth" , 1.2e+07);  // cm/s
        x0   = InitParameter ("x0"  ,     0.5);  // A
        nu0  = InitParameter ("nu0" , 1.0e+13);  // s^-1

        double Et0   = InitParameter ("Et"   , -0.5);  // eV
        double Etp0  = InitParameter ("Etp"  ,  0.5);  // eV
        double R0    = InitParameter ("R"    ,  0.6);  // 1
        double Rp0   = InitParameter ("Rp"   ,  0.6);  // 1
        double ES0   = InitParameter ("ES"   ,  1.0);  // eV
        double ESp0  = InitParameter ("ESp"  ,  1.0);  // eV
        double ET2p0 = InitParameter ("ET2p" ,  0.5);  // eV
        double E1p10 = InitParameter ("E1p1" ,  1.0);  // eV
        double E2p20 = InitParameter ("E2p2" ,  0.5);  // eV
        double xtmin = InitParameter ("xtmin",  0.0);  // A

        double Etsig   = InitParameter ("Etsig"  , 0.1);  // eV
        double Etpsig  = InitParameter ("Etpsig" , 0.1);  // eV
        double Rsig    = InitParameter ("Rsig"   , 0.1);  // 1
        double Rpsig   = InitParameter ("Rpsig"  , 0.1);  // 1
        double ESsig   = InitParameter ("ESsig"  , 0.1);  // eV
        double ESpsig  = InitParameter ("ESpsig" , 0.1);  // eV
        double ET2psig = InitParameter ("ET2psig", 0.1);  // eV
        double E1p1sig = InitParameter ("E1p1sig", 0.1);  // eV
        double E2p2sig = InitParameter ("E2p2sig", 0.1);  // eV
        double xtmax   = InitParameter ("xtmax"  , 0.0);  // A

        int idum = -1;
        for (int i = 0; i < NumberOfSamples*NumberOfVertices; ++i) {
          double Et   = Et0   + Etsig  *GausRanNum(idum);
          double Etp  = Etp0  + Etpsig *GausRanNum(idum);
          double R    = R0    + Rsig   *GausRanNum(idum);
          double Rp   = Rp0   + Rpsig  *GausRanNum(idum);
          double ES   = ES0   + ESsig  *GausRanNum(idum);
          double ESp  = ESp0  + ESpsig *GausRanNum(idum);
          double ET2p = ET2p0 + ET2psig*GausRanNum(idum);
          double E1p1 = E1p10 + E1p1sig*GausRanNum(idum);
          double E2p2 = E2p20 + E2p2sig*GausRanNum(idum);
          double xt = xtmin + (xtmax - xtmin)*UnifRanNum(idum);
          if (R   < 1.0e-10) R   = 1.0e-10;
          if (Rp  < 1.0e-10) Rp  = 1.0e-10;
          if (ES  < 1.0e-10) ES  = 1.0e-10;
          if (ESp < 1.0e-10) ESp = 1.0e-10;
          Eti.push_back(Et);
          Etpi.push_back(Etp);
          Ri.push_back(R);
          Rpi.push_back(Rp);
          ESi.push_back(ES);
          ESpi.push_back(ESp);
```

```
            ET2pi.push_back(ET2p);
            E1p1i.push_back(E1p1);
            E2p2i.push_back(E2p2);
            xti.push_back(xt);
        }
    }


    eNMPRates::
    ~eNMPRates ()
    {
    }


    void eNMPRates::
    compute (const Input& input, Output& output)
    {
        // Compute NBTI transition rates .
        // The order of transition rates and derivatives are:
        // k14h, k14e, k41h, k41e (k14 = k14h + k14e; k41 = k41h + k41e)
        // k23h, k23e, k32h, k32e (k23 = k23h + k23e; k32 = k32h + k32e)
        // k13, k31, k24, k42

        // Get the input variables.
        const double n  = input.n;   // cm^-3
        const double p  = input.p;   // cm^-3
        const double Nc = input.Nc;  // cm^-3
        const double Nv = input.Nv;  // cm^-3
        const double Eg = input.Eg;  // eV
        const double T  = input.T;    // K
        const double F  = input.F;   // V/cm (this is always |F|)
        const double kT = 8.617331e-5*T;  // kT in eV
        const int vindex = input.vindex;

        // Initialize the output variables.
        for (int i = 0; i < 12; ++i) {
            output.k[i].resize(NumberOfSamples, 0.0);
            output.dkdn[i].resize(NumberOfSamples, 0.0);
            output.dkdp[i].resize(NumberOfSamples, 0.0);
            output.dkdNc[i].resize(NumberOfSamples, 0.0);
            output.dkdNv[i].resize(NumberOfSamples, 0.0);
            output.dkdEg[i].resize(NumberOfSamples, 0.0);
            output.dkdT[i].resize(NumberOfSamples, 0.0);
            output.dkdF[i].resize(NumberOfSamples, 0.0);
        }

        // Calculate the rates for each sample.
        for (int is = 0; is < NumberOfSamples; ++is) {
            int ii = is + vindex*NumberOfSamples;
            const double Et = Eti[ii];
```

```
                const double Etp = Etpi[ii];
                const double R = Ri[ii];
                const double Rp = Rpi[ii];
                const double ES = ESi[ii];
                const double ESp = ESpi[ii];
                const double ET2p = ET2pi[ii];
                const double E1p1 = E1p1i[ii];
                const double E2p2 = E2p2i[ii];
                const double xt = xti[ii];
                const double sigma = Xsec * exp(-xt/x0);
                const double xtcm = xt*1.0e-8;
                const double R1p1 = R  + 1.0;
                const double R3p1 = Rp + 1.0;
                const double R1fac = R1p1*sqrt(R1p1)*sigma*Vth;
                const double R3fac = R3p1*sqrt(R3p1)*sigma*Vth;

                // Trap energies relative to valence band.
                const double Etv  = Et  + xtcm * F;
                const double Etpv = Etp + xtcm * F;

                // Get transition energies and derivatives.
                const double E14 = (ES/R1p1 - R*(Etv - ET2p))/R1p1;
                const double E41 = E14 + Etv - ET2p;
                const double E32 = (ESp/R3p1 - Rp*Etpv)/R3p1;
                const double E23 = E32 + Etpv;
                const double dE14dF = -R/R1p1*xtcm;
                const double dE41dF = dE14dF + xtcm;
                const double dE32dF = -Rp/R3p1*xtcm;
                const double dE23dF = dE32dF + xtcm;
                const double E13 = E1p1 + Etp - Et;
                const double E31 = E1p1;
                const double E24 = E2p2 + ET2p;
                const double E42 = E2p2;

                // Get transition rates and derivatives.
                const double k14 = R1fac*p*exp(-E14/kT);
                const double dk14dp = k14/p;
                const double dk14dT = k14*(E14/kT)/T;
                const double dk14dF = k14*(-dE14dF/kT);
                const double k41 = R1fac*Nv*exp(-E41/kT);
                const double dk41dNv = k41/Nv;
                const double dk41dT  = k41*(E41/kT)/T;
                const double dk41dF  = k41*(-dE41dF/kT);
                const double k23 = R3fac*Nv*exp(-E23/kT);
                const double dk23dNv = k23/Nv;
                const double dk23dT  = k23*(E23/kT)/T;
                const double dk23dF  = k23*(-dE23dF/kT);
                const double k32 = R3fac*p*exp(-E32/kT);
```

```
        const double dk32dp = k32/p;
        const double dk32dT = k32*(E32/kT)/T;
        const double dk32dF = k32*(-dE32dF/kT);
        const double k13 = nu0*exp(-E13/kT);
        const double dk13dT = k13*(E13/kT)/T;
        const double k31 = nu0*exp(-E31/kT);
        const double dk31dT = k31*(E31/kT)/T;
        const double k24 = nu0*exp(-E24/kT);
        const double dk24dT = k24*(E24/kT)/T;
        const double k42 = nu0*exp(-E42/kT);
        const double dk42dT = k42*(E42/kT)/T;

        // Fill the output variables.
        output.k[0][is]=k14;
        output.dkdp[0][is]=dk14dp;
        output.dkdT[0][is]=dk14dT;
        output.dkdF[0][is]=dk14dF;
        output.k[2][is]=k41;
        output.dkdNv[2][is]=dk41dNv;
        output.dkdT[2][is]=dk41dT;
        output.dkdF[2][is]=dk41dF;
        output.k[4][is]=k23;
        output.dkdNv[4][is]=dk23dNv;
        output.dkdT[4][is]=dk23dT;
        output.dkdF[4][is]=dk23dF;
        output.k[6][is]=k32;
        output.dkdp[6][is]=dk32dp;
        output.dkdT[6][is]=dk32dT;
        output.dkdF[6][is]=dk32dF;
        output.k[8][is]=k13;
        output.dkdT[8][is]=dk13dT;
        output.k[9][is]=k31;
        output.dkdT[9][is]=dk31dT;
        output.k[10][is]=k24;
        output.dkdT[10][is]=dk24dT;
        output.k[11][is]=k42;
        output.dkdT[11][is]=dk42dT;
    }
}

extern "C"
PMI_eNMPTransitionRates*
   new_PMI_eNMPTransitionRates (const PMI_Environment& env)
{ return new eNMPRates (env);
}
```

Piezoelectric Polarization

The effects of piezoelectric polarization can be modeled by adding the divergence of the piezoelectric polarization vector as an additional charge term:

$$q_{PE} = -\nabla P_{PE} \tag{1276}$$

to the right-hand side of the Poisson equation (see Eq. 37, p. 173):

$$\nabla \varepsilon \cdot \nabla \phi = -q(p - n + N_D - N_A + q_{PE}) \tag{1277}$$

The quantity P_{PE} denotes the piezoelectric polarization vector, which may defined by a PMI. The built-in models for piezoelectric polarization are discussed in Dependency of Saturation Velocity on Stress on page 879.

The name of the PMI is specified in the `Physics` section of the command file as follows:

```
Physics {
   Piezoelectric_Polarization (pmi_polarization)
}
```

The piezoelectric polarization vector and the piezoelectric charge may be plotted by:

```
Plot {
   PE_Polarization/vector
   PE_Charge
}
```

Sentaurus Device assumes that the piezoelectric polarization vector P_{PE} is zero outside of the device. This boundary condition may lead to an unexpectedly large charge density if P_{PE} has a nonzero component orthogonal to the boundary (discontinuity in ∇P_{PE}).

Dependencies

The piezoelectric polarization model does not have explicit dependencies. However, it can use the runtime support. In particular, it has access to the stress fields.

The model must compute:

`pol`   Piezoelectric polarization vector $[\text{Ccm}^{-2}]$

The resulting vector `pol` has the dimension 3. However, only the first *dim* components need to be defined, where *dim* is equal to the dimension of the problem.

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_Polarization : public PMI_Vertex_Interface {

public:
   PMI_Polarization (const PMI_Environment& env);
   virtual ~PMI_Polarization ();

   virtual void Compute_pol
      (double pol [3]) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_Polarization* new_PMI_Polarization_func
   (const PMI_Environment& env);
extern "C" new_PMI_Polarization_func new_PMI_Polarization;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_Polarization_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
   };

   class Output {
   public:
     pmi_float pol [3];  // piezoelectric polarization
   };

   PMI_Polarization_Base (const PMI_Environment& env);
   virtual ~PMI_Polarization_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_Polarization_Base* new_PMI_Polarization_Base_func
   (const PMI_Environment& env);
extern "C" new_PMI_Polarization_Base_func new_PMI_Polarization_Base;
```

Example: Gaussian Polarization Model

In this example, the piezoelectric polarization vector P_{PE} has a simple Gaussian shape in the x-direction:

```
#include "PMIModels.h"

class Gauss_Polarization : public PMI_Polarization {
private:
  double x0, c, a;

public:
  Gauss_Polarization (const PMI_Environment& env);
  ~Gauss_Polarization ();

  void Compute_pol (double pol [3]);
};

Gauss_Polarization::
Gauss_Polarization (const PMI_Environment& env) :
  PMI_Polarization (env)
{ x0 = InitParameter ("x0", 0.0);
  c = InitParameter ("c", 1.0);
  a = InitParameter ("a", 1e-5);
}

Gauss_Polarization::
~Gauss_Polarization ()
{
}

void Gauss_Polarization::
Compute_pol (double pol [3])
{ double x, y, z;
  ReadCoordinate (x, y, z);
  pol [0] = a * exp (-c * (x-x0) * (x-x0));
  pol [1] = 0.0;
  pol [2] = 0.0;
}

extern "C"
```

```
    PMI_Polarization* new_PMI_Polarization
      (const PMI_Environment& env)
    { return new Gauss_Polarization (env);
    }
```

Incomplete Ionization

The ionization factors $G_D(T)$ and $G_A(T)$ (see Incomplete Ionization Model on page 279) can be defined by a PMI.

The name of the PMI should be specified in the Physics section of the command file as follows:

```
Physics {
   IncompleteIonization( Model( PMI_model_name("Species_name1
      Species_name2 ...") ) )
}
```

In addition, it is possible to have a PMI for each species separately:

```
Physics {
   IncompleteIonization(
      Model(
         PMI_model_name1("Species_name1")
         PMI_model_name2("Species_name2")
      )
   )
}
```

The species PMI parameters should be defined in the parameter file (see Parameter File of Sentaurus Device on page 1088).

Dependencies

The ionization factors $G_D(T)$ and $G_A(T)$ may depend on the variable:

t   Lattice temperature [K]

The PMI model must compute the following results:

g   Ionization factor $G(T)$

In the case of the standard interface, the following derivative must be computed as well:

dgdt   Derivative of $G(T)$ with respect to T

Standard C++ Interface

The following base class is declared in the file PMIModels.h:

```
enum PMI_SpeciesType {
  PMI_acceptor,
  PMI_donor
};

class PMI_DistributionFunction : public PMI_Vertex_Interface {

private:
  const PMI_SpeciesType speciesType;
  const char* speciesName;

public:
  PMI_DistributionFunction (const PMI_Environment& env,
                            const char* name
                            const PMI_SpeciesType type = PMI_acceptor);

  virtual ~PMI_DistributionFunction ();

  PMI_SpeciesType SpeciesType () const { return speciesType; }
  const char* SpeciesName () const { return speciesName; }

  // read parameter from Sentaurus Device parameter file
  // (override for PMI_Vertex_Interface::ReadParameter)
  const PMIBaseParam* ReadParameter (const char* name) const;

  // initialize parameter from Sentaurus Device parameter file or from default
  // value (override for PMI_Vertex_Interface::InitParameter)
  double InitParameter (const char* name, double defaultvalue) const;

  virtual void Compute_g
    (const double T,        // lattice temperature
     double& g) = 0;        // g = G(T)

  virtual void Compute_dgdt
    (const double T,        // lattice temperature
     double& dgdt) = 0;     // dgdt = G'(T)

};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_DistributionFunction* new_PMI_DistributionFunction_func
   (const PMI_Environment& env);
extern "C" new_PMI_DistributionFunction_func new_PMI_DistributionFunction;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_DistributionFunction_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      pmi_float t;   // lattice temperature
   };

   class Output {
   public:
      pmi_float g;   // ionization factor
   };

   PMI_DistributionFunction_Base (const PMI_Environment& env,
                                  const char* name,
                                  const PMI_SpeciesType type = PMI_acceptor);
   virtual ~PMI_DistributionFunction_Base ();

   PMI_SpeciesType SpeciesType () const;
   const char* SpeciesName () const;

   const PMIBaseParam* ReadParameter (const char* name) const;
   double InitParameter (const char* name, double defaultvalue) const;

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_DistributionFunction_Base* new_PMI_DistributionFunction_Base_func
   (const PMI_Environment& env, const char* name, const PMI_SpeciesType type);
extern "C" new_PMI_DistributionFunction_Base_func
   new_PMI_DistributionFunction_Base;
```

Example: Matsuura Incomplete Ionization Model

The following C++ code implements the Matsuura model [1] for dopant Al in SiC material:

$$G_A(T) = 4\exp\left(\frac{\Delta E_A - E_{ex}}{kT}\right) \cdot \left(g_1 + \sum_{r=2} g_r \exp\left(\frac{\Delta E_r - \Delta E_A}{kT}\right)\right) \tag{1278}$$

where g_1 is the ground-state degeneracy factor, g_r is the $(r-1)$-th excited state degeneracy factor, and ΔE_r is the difference in energy between the $(r-1)$-th excited state level and E_V. ΔE_r is given by the hydrogenic dopant model [2]:

$$\Delta E_r = 13.6 \cdot \frac{m^*}{m_0 \cdot \varepsilon_s^2} \cdot \frac{1}{r^2} \qquad [\text{eV}] \tag{1279}$$

where m^* is the hole effective mass in SiC, and ε_s is the dielectric constant of SiC.

The acceptor level is described as [2]:

$$\Delta E_A = \Delta E_1 + E_{CCC} \tag{1280}$$

where E_{CCC} is the energy induced due to central cell corrections.

The ensemble average E_{ex} of the ground and excited state levels of the acceptor is given by [3]:

$$E_{ex} = \frac{\displaystyle\sum_{r=2} (\Delta E_A - \Delta E_r) g_r \exp\left(-\frac{\Delta E_A - \Delta E_r}{kT}\right)}{g_1 + \displaystyle\sum_{r=2} g_r \exp\left(-\frac{\Delta E_A - \Delta E_r}{kT}\right)} \tag{1281}$$

The Matsuura model can be implemented as follows:

```
class Matsuura_DistributionFunction : public PMI_DistributionFunction {

protected:
  const double kB_300; //  Boltzmann constant * 300   [eV]
  int   nb_item;   //  number of item in sum
  double *gr, *dEr;
  double Eex, dEA, Eccc;

public:
  Matsuura_DistributionFunction (const PMI_Environment& env,
                                 const char* name,
                                 const PMI_SpeciesType type = PMI_acceptor);

  ~Matsuura_DistributionFunction ();
```

```
   void Compute_g
     (const double T,        // lattice temperature
      double& g);            // g = G(T)


   void Compute_dgdt
     (const double T,        // lattice temperature
      double& dgdt);         // dgdt = G'(T)

    double Compute_Eex(double T);// compute Eex(T) Eq. 1281, p. 1225
    double Compute_dEexdT(double T);// compute dEex/dT

};

Matsuura_DistributionFunction::
Matsuura_DistributionFunction (const PMI_Environment& env,
                               const char* name,
                               const PMI_SpeciesType type) :
  PMI_DistributionFunction (env, name, type),
  kB_300(1.380662e-23*300./1.602192e-19),  //  kB*T0/e0 = 0.02585199527 [eV]
  Eex(0.)
{
  nb_item  = InitParameter ("NumberOfItem", 1);
  Eccc     = InitParameter ("Eccc", 0);

  if(nb_item < 1) {
    printf("ERROR; PMI model Matsuura_DistributionFunction: parameter
NumberOfItem < 1 \n");
   exit(1);
  }
  gr  = new double[nb_item];
  dEr = new double[nb_item];

  char str_r[6], name_gr[6];

  int r;
  for(r=0; r<nb_item; ++r) {
    name_gr[0] = 'g';  name_gr[1] = '\0';
    sprintf(str_r, "%d\0", r+1);
    strcat(name_gr, str_r);
    const PMIBaseParam* par = ReadParameter(name_gr);
    if(!par) {
      printf("ERROR; PMI model Matsuura_DistributionFunction: cannot read
parameter %s \n", name_gr);
    gr[r] = 2;
} else
      gr[r] = *par;
```

```
      }

        const PMIBaseParam* par = ReadParameter("dE1");
        if(!par) {
       //  dE[r] = 13.6 * m_eff/m0/eps/eps/r/r
          Compute_dEr(nb_item, dEr);
        } else {
          char name_dEr[6];
          for(r=0; r<nb_item; ++r) {
            strcpy(name_dEr, "dE");
            sprintf(str_r, "%d\0", r+1);
            strcat(name_dEr, str_r);
            const PMIBaseParam* par = ReadParameter(name_dEr);
            if(!par) {
              printf("ERROR; PMI model Matsuura_DistributionFunction: cannot read
parameter %s \n", name_dEr);
              exit(1);
            }
            dEr[r] = *par;
          }
        }
      dEA = dEr[0] + Eccc;
    }

     Matsuura_DistributionFunction::
    ~Matsuura_DistributionFunction ()
    {
      delete[] gr;
      delete[] dEr;
    }

    void Matsuura_DistributionFunction::Compute_g
        (const double T,                    // lattice temperature
         double& g)                         // g = G(T)
    {
      const double kT = kB_300*T/300;

      Eex = Compute_Eex(T);
      g = gr[0];

      for(int r=1; r<nb_item; ++r) {
        double delta = dEA - dEr[r];
        g += gr[r]*exp( -delta/kT );
      }
      g *= 4.*exp( (dEA-Eex)/kT );
    }

    void Matsuura_DistributionFunction::Compute_dgdt
```

```
      (const double T,         // lattice temperature
       double& dgdt)           // dgdt = G'(T)
{
  const double kT = kB_300*T/300;

  Eex = Compute_Eex(T);
  double s1, s2 = gr[0], s3, s4 = 0., delta, tmp;

  for(int r=1; r<nb_item; ++r) {
    delta = dEA - dEr[r];
    tmp   = gr[r]*exp( -delta/kT );
    s2   += tmp;
    s4   += tmp*delta/kT/T;                // s4 = ds2/dT
  }

  delta = dEA - Eex;
  s1 = 4.*exp( delta/kT );
  double dEex_dT = Compute_dEexdT(T);
  s3 = s1*( -dEex_dT/kT - delta/kT/T );    // s3 = ds1/dT

  dgdt = s3*s2 + s1*s4;        // dgdt = d(s1*s2)/dT

  return;
}

// Eex is given by Eq. 1281, p. 1225
double Matsuura_DistributionFunction::Compute_Eex(double T)
{
  const double kT = kB_300*T/300;

  double s1 = 0., s2 = gr[0];

  for(int r=1; r<nb_item; ++r) {
    double delta = dEA - dEr[r];
    double tmp   = gr[r]*exp( -delta/kT );
    s1 += delta*tmp;
    s2 += tmp;
  }

  return s1/s2;

}

double Matsuura_DistributionFunction::Compute_dEexdT(double T)
{
  const double kT = kB_300*T/300;

  double s1 = 0., s2 = gr[0], s3 = 0., s4 = 0.;
```

```
      for(int r=1; r<nb_item; ++r) {
        double delta = dEA - dEr[r];
        double tmp   = gr[r]*exp( -delta/kT );
        s1 += delta*tmp;
        s2 += tmp;
        s3 += delta*tmp*delta/kT/T;  //  s3 = ds1/dT
        s4 += tmp*delta/kT/T;        //  s4 = ds2/dT
      }

      return (s3*s2 - s1*s4)/s2/s2;

  }

  extern "C"
  PMI_DistributionFunction* new_PMI_DistributionFunction
    (const PMI_Environment& env,
     const char* name,
     const PMI_SpeciesType type)
  {
    return new Matsuura_DistributionFunction (env, name, type);
  }

  void Compute_dEr(int nb_item, double* dEr)
  {
    // dEr is given by Eq. 1279, p. 1225

    // data from file: 6H-SiC.par
    const double epsilon = 9.66;                       //  dielectric constant
    const double mh      = 1;                          //  hole effective mass in SiC

    const double E0 = 13.6*mh/epsilon/epsilon;

    for(int r=1; r<=nb_item; ++r) {
      dEr[r-1] = E0/r/r;
    }
  }
```

Hot-Carrier Injection

Sentaurus Device provides a PMI for implementing hot-carrier injection models and computing the injection currents defined by the model. It is activated in the `Physics` interface section of the command file, `GateCurrent` subsection:

```
Physics(MaterialInterface="Silicon/Oxide"){
   GateCurrent( PMI_model(electron) )
}
```

The model can be used for both carrier types with either `PMI_model(electron hole)` or `PMI_model()`. The interface has access to the device mesh and device data (see Vertex-Based Runtime Support for Multistate Configuration–Dependent Models on page 1075).

Dependencies

A hot-carrier PMI model has no explicit dependencies. However, it can depend on any field at runtime using the access to device data. The model must compute:

gCurr   Vector of region/interface arrays with hot-carrier injection current densities; each region/interface array consists of the current density in each vertex of a region interface.

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_HotCarrierInjection : public PMI_Device_Interface {

protected:
   const PMI_CarrierType cType;

public:
   PMI_HotCarrierInjection (const PMI_Device_Environment& env,
      const PMI_CarrierType cType);
   virtual ~PMI_HotCarrierInjection ();

   virtual void Compute_gCurr
      (const des_regioninterface_vector& regioninterfaces,
                           // region interfaces associated with the model
```

```
        des_array_vector& gCurr) = 0; // gate injection current in each vertex
                                      // of specified region interfaces
};
```

Two virtual constructors are required for electron and hole hot injection:

```
typedef PMI_HotCarrierInjection* new_PMI_HotCarrierInjection_func
   (const PMI_Device_Environment& env, const PMI_CarrierType carType);
extern "C" new_PMI_HotCarrierInjection_func new_PMI_e_HotCarrierInjection;
extern "C" new_PMI_HotCarrierInjection_func new_PMI_h_HotCarrierInjection;
```

Simplified C++ Interface

The following base class is declared in the file PMI.h:

```
class PMI_HotCarrierInjection_Base : public PMI_Device_Base {

public:
   class Input : public PMI_Device_Input_Base {
   public:
      des_regioninterface_vector regioninterfaces; // region interfaces
                                                   // associated with model
                                                   // name
   };

   class Output {
   public:
      sdevice_array_vector gCurr;  // gate injection current in each vertex
                                   // of specified region interfaces
   };

   PMI_HotCarrierInjection_Base (const PMI_Device_Environment& env);
   virtual ~PMI_HotCarrierInjection_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_HotCarrierInjection_Base* new_PMI_HotCarrierInjection_Base_func
   (const PMI_Device_Environment& env);
extern "C" new_PMI_HotCarrierInjection_Base_func
   new_PMI_e_HotCarrierInjection_Base;
extern "C" new_PMI_HotCarrierInjection_Base_func
   new_PMI_h_HotCarrierInjection_Base;
```

Example: Lucky Model

The following example reimplements the built-in lucky injection model for electrons using the hot-carrier injection PMI:

```
#include <math.h>
#include "PMIModels.h"

class PMI_LuckyModel : public PMI_HotCarrierInjection {
private:
  const des_mesh* mesh;  //device mesh
  des_data* data;  //device data
  const double*const* measure;
  const double*const* surface_measure;
public:
  PMI_LuckyModel(const PMI_Device_Environment& env,
                 const PMI_CarrierType carType);
  ~PMI_LuckyModel();
  void Compute_gCurr(const des_regioninterface_vector& regioninterfaces,
                     des_array_vector& gCurr);
};

PMI_LuckyModel::
PMI_LuckyModel(const PMI_Device_Environment& env,
               const PMI_CarrierType carType) :
  PMI_HotCarrierInjection(env, carType)
{
  mesh = Mesh();
  data = Data();
  measure = data->ReadMeasure();
  surface_measure = data->ReadSurfaceMeasure();
}

PMI_LuckyModel::
~PMI_LuckyModel()
{
}

void PMI_LuckyModel::
Compute_gCurr(const des_regioninterface_vector& regioninterfaces,
              des_array_vector& gCurr)
{
  //compute current for each des_regioninterface associated with model
  for(int inter=0; inter < regioninterfaces.size(); inter++) {
    for(int k=0; k < regioninterfaces.at(inter)->size_vertex(); k++)
      gCurr[inter][k] = 0.0;
```

```
des_regioninterface* ri = regioninterfaces.at(inter);
des_bulk* b1 = ri->bulk1();
des_bulk* b2 = ri->bulk2();

//recognize regioninterface or regioninterface category
if(((b1->material() == "Silicon") && (b2->material() == "Oxide")) ||
   ((b1->material() == "Oxide") && (b2->material() == "Silicon"))) {

  des_bulk* semReg;
  des_bulk* insReg;
  if((b1->material() == "Silicon") && (b2->material() == "Oxide")) {
    semReg = b1;
    insReg = b2;
  }
  if((b2->material() == "Silicon") && (b1->material() == "Oxide")) {
    semReg = b2;
    insReg = b1;
  }

  //read region interface constants
  double eLambd = 8.9000e-07;//eLsem
  double eLambdR = 6.2000e-06;//eLsemR
  double eOxLambd = 3.2000e-07;//eLins
  double eBarrierHeight = 3.1;//eBar0
  double eAlfa = 2.6000e-04;//eBL12
  double eBeta = 3.0000e-05;//eBL23

  //read DataEntries used in computation
  const double* pot =
    data->ReadScalar(des_data::vertex, "ElectrostaticPotential");
  const double* OxField =
    data->ReadScalar(des_data::vertex,"InsulatorElectricField");
  const double* Epsilon =
    data->ReadScalar(des_data::element, "DielectricConstant");
  const double* eCurrent = NULL;
  const double* eField = NULL;
  if(cType == PMI_Electron) {
    eCurrent = data->ReadScalar(des_data::vertex, "eCurrentDensity");
    eField = data->ReadScalar(des_data::vertex,"eEparallel");
  }

  //integrate over the corresponding semiconductor region
  for(size_t vi = 0; vi < semReg->size_vertex(); vi++) {
    des_vertex* rv = semReg->vertex(vi);

    //find the nearest interface vertex
    //(distance to interface)
    des_vertex* NearestInterVertex;
```

```
int NearestInterVertexRIind;
double NearestDistance = 1.0e50;
for(size_t k=0; k < ri->size_vertex(); k++) {
  des_vertex* interVert = ri->vertex(k);
  bool isSemiconductor = false;
  for(size_t i = 0; i < interVert->size_region(); i++) {
    des_bulk* b = dynamic_cast<des_bulk*>(interVert->region(i));
    if(b->material() == "Silicon") {
      isSemiconductor = true;
    }
  }
  if(isSemiconductor) {
    double dist = 0.0;
    for(int kk=0; kk < mesh->dim(); kk++)
      dist += (interVert->coord()[kk] - rv->coord()[kk])*
        (interVert->coord()[kk] - rv->coord()[kk]);
    dist = sqrt(dist);
    if(dist < NearestDistance) {
      NearestDistance = dist;
      NearestInterVertex = interVert;
      NearestInterVertexRIind = k;
    }
  }
}//nearest interface vertex

//find the nearest gate contact vertex
//(distance from NearestIntVertex to gate contact)
des_vertex* NearestContVertex;
double NearestContDistance = 1.0e50;
for(size_t k=0; k < insReg->size_vertex(); k++) {
  des_vertex* vins = insReg->vertex(k);
  if(vins->size_region() > 1) {
    for(size_t vvr = 0; vvr < vins->size_region(); vvr++) {
      des_region* rr = vins->region(vvr);
      if(rr->type() == des_region::contact) {
        //contact vertex
        double dist = 0.0;
        for(int kk=0; kk < mesh->dim(); kk++)
         dist += (vins->coord()[kk] - NearestInterVertex->coord()[kk])*
            (vins->coord()[kk] - NearestInterVertex->coord()[kk]);
        dist = sqrt(dist);
        if(dist < NearestContDistance) {
          NearestContDistance = dist;
          NearestContVertex = vins;
        }
      }//contact vertex
    }
  }
```

```
                  }//nearest gate contact vertex

                  //coordinates and distances are in um
                  //transform to cm
                  double OxThickn = NearestContDistance*1.0e-4;
                  double DistToSurf = NearestDistance*1.0e-4;

                  double xEps[3] = {0.0, 0.0, 0.0};
                  for(int k = 0; k < mesh->dim(); k++)
                    xEps[k] = 0.5*(NearestInterVertex->coord()[k]
                                 + NearestContVertex->coord()[k]);
                  des_element* xEl;
                  //find the oxide element
                  for(size_t ei = 0; ei < insReg->size_element(); ei++) {
                    des_element* e = insReg->element(ei);
                    for(size_t evi = 0; evi < e->size_vertex(); evi++) {
                      double minCoord[3] = {1.0e50, 1.0e50, 1.0e50};
                      double maxCoord[3] = {-1.0e50, -1.0e50, -1.0e50};
                      des_vertex* ev = e->vertex(evi);
                      for(int i = 0; i < mesh->dim(); i++) {
                        if(ev->coord()[i] < minCoord[i])
                          minCoord[i] = ev->coord()[i];
                        if(ev->coord()[i] > maxCoord[i])
                          maxCoord[i] = ev->coord()[i];
                      }
                      for(int i = 0; i < mesh->dim(); i++) {
                        if( (xEps[i] >= minCoord[i]) && (xEps[i] >= minCoord[i]) ) {
                          xEl = e;
                        }
                      }
                    }
                  }
                  double OxConst = Epsilon[xEl->index()];
                  double OxImage0 = 1.6e-19/16/3.1452/8.85e-14/OxConst;

                  //for electrons
                  if(cType == PMI_Electron) {
                    double eCur = 0.0;
                    double eOxField = pot[NearestContVertex->index()]
                      -pot[NearestInterVertex->index()];
                    eOxField = eOxField > 0
                      ? OxField[NearestInterVertex->index()]
                      : -OxField[NearestInterVertex->index()];
                    double barrier;
                    if(pot[NearestInterVertex->index()]
                         < pot[NearestContVertex->index()])
                      barrier = eBarrierHeight
                        - eAlfa*sqrt(fabs(eOxField))
```

```
              - eBeta*pow(fabs(eOxField),2.0/3.0);
          else
            barrier = eBarrierHeight
              + (pot[NearestInterVertex->index()] -
                pot[NearestContVertex->index()])
              - eAlfa*sqrt(fabs(eOxField))
              - eBeta*pow(fabs(eOxField),2.0/3.0);
          if(barrier < 0) barrier = 0.0;
          double eBarrierLoc = barrier;
          double p1 = 0.0;
          double eEnergy = eField[rv->index()]*eLambd;
          if(eEnergy > 1.0e-30) {
            p1 = 0.25;
            if (eBarrierLoc > 1.0e-30)
              p1 = 0.25*eEnergy/eBarrierLoc*exp(-eBarrierLoc/eEnergy);
          }
          double p2 = exp(-DistToSurf/eLambd);
          double eDistFromSurf = 1.0e30;
          if (eOxField > 1.0e-30) eDistFromSurf = sqrt(OxImage0/eOxField);
          double p3 = exp(-eDistFromSurf/eOxLambd);

          //find the node measure
          double node_measure = 0.0;
          for(size_t ei = 0; ei < rv->size_element(); ei++) {
            des_element* e = rv->element(ei);
            des_bulk* bulk = e->bulk();
            if(bulk->material() == "Silicon") {
              for(size_t evi = 0; evi < e->size_vertex(); evi++) {
                des_vertex* ev = e->vertex(evi);
                if(ev->index() == rv->index()) {
                  node_measure += measure[e->index()][evi];
                }
              }
            }//semiconductor element
          }//node measure

          //convert measure in cm^dim
          node_measure = node_measure*pow(1.0e-4,mesh->dim());

          eCur = eCurrent[rv->index()]*p1*p2*p3*node_measure/eLambdR;
          double risurface =
            surface_measure[ri->index()][NearestInterVertexRIind];
          //convert to cm^(dim-1)
          risurface = risurface*pow(1.0e-4,(mesh->dim()-1));
          gCurr[inter][NearestInterVertexRIind] += eCur/risurface;
        }

        //for holes
```

```
        if(cType == PMI_Hole) {
          }
        }//end integration on semiconductor region
      }//end model implementation
    }//end loop over "PMI_HotCarrierInjection" model regioninterfaces
}

extern "C" {
  PMI_HotCarrierInjection* new_PMI_e_HotCarrierInjection
          (const PMI_Device_Environment& env, const PMI_CarrierType carType)
  {
    return new PMI_LuckyModel(env, carType);
  }
}

extern "C" {
  PMI_HotCarrierInjection* new_PMI_h_HotCarrierInjection
          (const PMI_Device_Environment& env, const PMI_CarrierType carType)
  {
    return new PMI_LuckyModel(env, carType);
  }
}
```

Piezoresistive Coefficients

Sentaurus Device provides a PMI for implementing the dependencies of the piezoresistive prefactors over the normal electric field (see Enormal- and MoleFraction-Dependent Piezo Coefficients on page 863). It is activated in the `Piezo` section of the command file, in the `Tensor` subsection:

```
Physics {
   ...
   Piezo(
      Model(Mobility(Tensor("pmi_model")))
   )
}
```

Dependencies

The piezoresistive prefactors `ePij` and `hPij` may depend on the following variable:

`Enormal`   Normal to interface semiconductor–dielectric electric field $[\mathrm{Vcm}^{-1}]$

The PMI model must compute the following results:

p11, p12, p44   Piezoresistive prefactors [1]

In the case of the standard interface, the following derivatives must be computed as well:

dp11, dp12, dp44   Derivatives of pij with respect to Enormal $[\mathrm{V}^{-1}\mathrm{cm}]$

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_PiezoresistanceFactor : public PMI_Vertex_Interface {

public:
   PMI_PiezoresistanceFactor (const PMI_Environment& env);
   virtual ~PMI_PiezoresistanceFactor ();

   virtual void Compute_Pij(const double Enormal,
      double& p11, double& p12, double& p44) = 0;

   virtual void Compute_DerPij(const double Enormal,
      double& dp11, double& dp12, double& dp44) = 0;
};
```

Two virtual constructors are required for the calculation of the piezoresistive prefactors.

```
typedef PMI_PiezoresistanceFactor* new_PMI_PiezoresistanceFactor_func
   (const PMI_Environment& env);
extern "C" new_PMI_PiezoresistanceFactor_func new_PMI_ePiezoresistanceFactor;
extern "C" new_PMI_PiezoresistanceFactor_func new_PMI_hPiezoresistanceFactor;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_PiezoresistanceFactor_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      pmi_float Enormal;  // normal to interface electric field
   };
```

```
class Output {
public:
   pmi_float p11;  // piezoresistive prefactor
   pmi_float p12;  // piezoresistive prefactor
   pmi_float p44;  // piezoresistive prefactor
};

PMI_PiezoresistanceFactor_Base (const PMI_Environment& env);
virtual ~PMI_PiezoresistanceFactor_Base ();

virtual bool IsPrefactor () = 0;

virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_PiezoresistanceFactor_Base*
   new_PMI_PiezoresistanceFactor_Base_func (const PMI_Environment& env);
extern "C" new_PMI_PiezoresistanceFactor_Base_func
   new_PMI_ePiezoresistanceFactor_Base;
extern "C" new_PMI_PiezoresistanceFactor_Base_func
   new_PMI_hPiezoresistanceFactor_Base;
```

Current Plot File of Sentaurus Device

The current plot PMI allows user-computed entries to be added to the current plot file. It is specified in the `CurrentPlot` section of the command file, for example:

```
CurrentPlot {
   pmi_CurrentPlot
}
```

The interface has access to the device mesh and device data (see Mesh-Based Runtime Support on page 1076).

See Current Plot File on page 1317 for a Tcl-based alternative to the current plot PMI.

Structure of Current Plot File

A current plot file consists of a header section and a data section. For each function, the structure can be described as follows:

```
dataset name
function name
value₀
value₁
...
```

A dataset name denotes a dataset, for example:

```
time
Tmin
```

If a dataset corresponds to a region or contact, it is customary to add the region or contact name:

```
gate Charge
```

The function name describes the function, for example:

```
ElectrostaticPotential
Temperature
```

Afterwards, a function value is added to the current plot file for each plot time point.

Standard C++ Interface

The following base class is declared in the file PMIModels.h:

```cpp
class PMI_CurrentPlot : public PMI_Device_Interface {

public:
   PMI_CurrentPlot (const PMI_Device_Environment& env);
   virtual ~PMI_CurrentPlot ();

   virtual void Compute_Dataset_Names
      (des_string_vector& dataset) = 0;

   virtual void Compute_Function_Names
      (des_string_vector& function) = 0;

   virtual void Compute_Plot_Values
      (des_double_vector& value) = 0;
};
```

The methods `Compute_Dataset_Names()` and `Compute_Function_Names()` are used to generate the header in the current plot file (see Structure of Current Plot File on page 1240). `Compute_Plot_Values()` is called for each plot time point to compute the plot values. Use the `push_back()` function to add values to the arrays `dataset`, `function`, or `value`.

> **NOTE**   All three methods `Compute_Dataset_Names()`,
> `Compute_Function_Names()`,   and   `Compute_Plot_Values()`
> must always compute the same number of values. Otherwise, an
> inconsistent current plot file will be generated.

The prototype for the virtual constructor is given as:

```
typedef PMI_CurrentPlot* new_PMI_CurrentPlot_func
   (const PMI_Device_Environment& env);
extern "C" new_PMI_CurrentPlot_func new_PMI_CurrentPlot;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_CurrentPlot_Base : public PMI_Device_Base {

public:
   class Input : public PMI_Device_Input_Base {
   public:
   };

   class Output_Header {
   public:
      des_string_vector dataset;   // array of dataset names
      des_string_vector function;  // array of function names
   };

   class Output_Body {
   public:
      sdevice_pmi_float_vector value;  // array of plot values
   };

   PMI_CurrentPlot_Base (const PMI_Device_Environment& env);
   virtual ~PMI_CurrentPlot_Base ();

   virtual void compute_header (Output_Header& output) = 0;
   virtual void compute_body (const Input& input, Output_Body& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_CurrentPlot_Base* new_PMI_CurrentPlot_Base_func
   (const PMI_Device_Environment& env);
extern "C" new_PMI_CurrentPlot_Base_func new_PMI_CurrentPlot_Base;
```

Example: Average Electrostatic Potential

The following example computes regionwise averages for the electrostatic potential. This is the same functionality as provided by the built-in current plot command (see Tracking Additional Data in the Current File on page 110):

```
class CurrentPlot : public PMI_CurrentPlot {
private:
  typedef std::vector<des_bulk*> des_bulk_vector;

  const des_mesh* mesh;      // device mesh
  des_bulk_vector regions;   // list of semiconductor bulk regions
  double scale;              // scaling factor

public:
  CurrentPlot (const PMI_Device_Environment& env);
  ~CurrentPlot ();

  void Compute_Dataset_Names (des_string_vector& dataset);
  void Compute_Function_Names (des_string_vector& function);
  void Compute_Plot_Values (des_double_vector& value);
};


CurrentPlot::
CurrentPlot (const PMI_Device_Environment& env) :
  PMI_CurrentPlot (env)
{ mesh = Mesh ();
  // determine regions to process
  for (size_t ri = 0; ri < mesh->size_region (); ri++) {
    des_region* r = mesh->region (ri);
    if (r->type () == des_region::bulk) {
      des_bulk* b = dynamic_cast <des_bulk*> (r);
      if (b->material () != "Oxide") {
        // we found a semiconductor bulk region
        regions.push_back (b);
      }
    }
  }

  // read parameters
```

```
      scale = InitParameter ("scale", 0.0);
}

CurrentPlot::
~CurrentPlot ()
{
}

void CurrentPlot::
Compute_Dataset_Names (des_string_vector& dataset)
{ for (size_t ri = 0; ri < regions.size (); ri++) {
    des_bulk* b = regions [ri];
    std::string name = "Average_";
    name += b->name ();
    name += "ElectrostaticPotential";
    dataset.push_back (name);
  }
}

void CurrentPlot::
Compute_Function_Names (des_string_vector& function)
{ for (size_t ri = 0; ri < regions.size (); ri++) {
    function.push_back ("ElectrostaticPotential");
  }
}

void CurrentPlot::
Compute_Plot_Values (des_double_vector& value)
{ des_data* data = Data ();
  const double*const* measure = data->ReadMeasure ();
  const double* pot = data->ReadScalar (des_data::vertex,
                                        "ElectrostaticPotential");
  for (size_t ri = 0; ri < regions.size (); ri++) {
    des_bulk* b = regions [ri];

    double sum_pot = 0.0;
    double sum_measure = 0.0;

    for (size_t ei = 0; ei < b->size_element (); ei++) {
      des_element* e = b->element (ei);
      for (size_t vi = 0; vi < e->size_vertex (); vi++) {
        des_vertex* v = e->vertex (vi);
        const double m = measure [e->index ()][vi];
        const double p = pot [v->index ()];
        sum_pot += m * p;
        sum_measure += m;
      }
    }
```

```
      value.push_back (scale * (sum_pot / sum_measure));
    }
  }

extern "C" {
PMI_CurrentPlot* new_PMI_CurrentPlot (const PMI_Device_Environment& env)
{ return new CurrentPlot (env);
}
}
```

Postprocess for Transient Simulation

The postprocess PMI allows you to post-compute data during a transient simulation. The PMI is called after a transient time step has succeeded. It is specified in the Math section of the command file, for example:

```
Math {
    PostProcess (
        Transient = "pmi_postprocess"
    )
}
```

The interface provides access to the device mesh and device data (see Mesh-Based Runtime Support on page 1076).

Standard C++ Interface

The following base class is declared in the file PMIModels.h:

```
class PMI_PostProcess : public PMI_Device_Interface {

public:
    PMI_PostProcess (const PMI_Device_Environment& env);
    virtual ~PMI_PostProcess ();

    virtual void Compute_PostProcess () = 0;
}
```

The method Compute_PostProcess() is called after the transient time step has successfully completed.

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_PostProcess_Base : public PMI_Device_Base {

public:
   class Input : public PMI_Device_Input_Base {
   public:
   };

   class Output {
   public:
   };

   PMI_PostProcess_Base (const PMI_Device_Environment& env);
   virtual ~PMI_PostProcess_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_PostProcess_Base* new_PMI_PostProcess_Base_func
   (const PMI_Device_Environment& env);
extern "C" new_PMI_PostProcess_Base_func new_PMI_PostProcess_Base;
```

The method `compute()` is called after the transient time step has successfully completed.

Example: Postprocess User-Field

The following code modifies the user-field depending on the current temperature change and transient step size after the transient time step has succeeded:

```
#include "PMIModels.h"

class PostProcess : public PMI_PostProcess {

private:
   const des_mesh* mesh;

public:
   PostProcess (const PMI_Device_Environment& env);
   ~PostProcess ();
   void Compute_PostProcess ();
};
```

```
PostProcess::
PostProcess (const PMI_Device_Environment& env) :
   PMI_PostProcess (env)
{
   mesh = Mesh();
}

PostProcess::
~PostProcess ()
{
}

void PostProcess::
Compute_PostProcess ()
{
   des_data* data = Data();

   const double* T = data->ReadScalar(des_data::vertex,
      "LatticeTemperature");
   const double* T0 = data->ReadScalar(des_data::vertex, "PMIUserField0");

   double* delta_T = new double [mesh->size_vertex ()];
   for (int vi=0; vi<mesh->size_vertex (); vi++) {
      delta_T[vi] = (T[vi]-T0[vi])/ReadTransientStepSize();
   }
   data->WriteScalar(des_data::vertex, "PMIUserField0", T);
   data->WriteScalar(des_data::vertex, "PMIUserField1", delta_T);
   if (delta_T!=NULL) { delete [] delta_T; }
}
```

Preprocessing for Newton Iterations and Newton Step Control

The Newton step PMI allows you to precompute data during Newton iterations (using a nonlinear solver). This PMI is called after each Newton iteration. The interface provides access to the device mesh and device data (see). This PMI is specified in the `Coupled` section (subsection `PMI_NewtonStep`) of the command file, for example:

```
Coupled( PMI_NewtonStep( pmiNewtonStep(<parameter_list>) ) )
   { Poisson Electron Hole }
```

Here, `pmiNewtonStep` is the name of the PMI model. Different `Coupled` sections can use different PMI models.

For example:

```
Solve {
   # "pmi_Newton1" is name the first PMI function
   Coupled( PMI_NewtonStep(pmi_Newton1) )
   { Poisson electron hole }

   Transient (
      InitialTime = 0.0 Finaltime = 1.0
      InitialStep = 0.01 MaxStep = 0.1 MinStep = 1.0e-06
   ) {# "pmi_Newton2" is name the second PMI function
      Coupled( PMI_NewtonStep( PMI_NewtonStep(pmi_Newton2(parameter_list)) ) )
      { Poisson Electron Hole Temperature }
   }

   Quasistationary (
      InitialStep=0.1 MaxStep=0.5 MinStep=0.001
      Increment=1.3
      Goal {name="drain" Voltage=0.6}
   )
   {# same PMI function
      Coupled( PMI_NewtonStep(pmi_Newton2(parameter_list)...) )
      { poisson electron hole }
   }
}
```

Standard C++ Interface

The following base class is declared in the file PMIModels.h:

```
class PMI_NewtonStep : public PMI_Device_Interface
{

protected:
   PMI_Newton::Info *info;

public:
   PMI_NewtonStep (const PMI_Device_Environment& env, PMI_Newton::Info *i=0);
      virtual ~PMI_NewtonStep ();
   PMI_Newton::Info* getNewtonInfo() {
      return info;
   }

// methods to be implemented by user
   virtual PMI_Result Compute (char* err_msg) = 0;
};
```

The method `Compute()` is called after each Newton iteration. The enumerator `PMI_Result` is defined in the file `PMIModels.h`:

```
enum PMI_Result {
   PMI_NextStep  = 0,
   PMI_Converged = 1,
   PMI_Diverged  = 2,
   PMI_Undefined
};
```

Function PMI_Newton::GetLogFile() and Class PMI_Newton::Info

The `PMIModels.h` file contains the function `FILE* PMI_Newton::GetLogFile()`. It returns a pointer to the log file and, therefore, the PMI function can print messages to the log file. See the relevant files of the following example:

```
$STROOT/tcad/$STRELEASE/lib/sdevice/src/pmi_NewtonStep
```

The `PMI_Newton::Info` class is an interface class between Sentaurus Device and `PMI_NewtonStep`, and it contains information about the Newton process. The function `getNewtonInfo()` returns the corresponding pointer. The important functions of this class are as follows (see Standard C++ Interface on page 1247):

- `IsTrans()`, `IsQstat()`, and `IsContin()` return a value equal to `true` if the `Coupled` statement is a subsection of the corresponding section: `Transient`, `Quasistationary`, or `Continuation`.

- `InitialStep()`, `MaxStep()`, `MinStep()`, `Decrement()`, `Increment()`, `InitialTime()`, `FinalTime()`, and `MaxIters()` return the corresponding values as in the command file.

- `UsedIters()`, `RHS()`, `NewtonStep()`, `Error()`, `TimeFrom()`, and `TimeTo()` return the corresponding values as in the log file.

- `std::vector<std::string> pdeName` contains the PDE name as in the log file.

- `ChangeTimeTo(double t)` performs PMI time-step control (see PMI_NewtonStep Iterations: Flowchart of Computation on page 1249).

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_NewtonStep_Base : public PMI_Device_Base
{
protected:
   PMI_Newton::Info *info;
```

```
public:
   class Input : public PMI_Device_Input_Base {
   public:
      Input (const PMI_NewtonStep_Base* newtonstep_base);
   };

   class Output {
   public:
      char err_msg[256];
   };

   PMI_NewtonStep_Base(
      const PMI_Device_Environment& env, PMI_Newton::Info *i=0);
      virtual ~PMI_NewtonStep_Base ();

   PMI_Newton::Info* getNewtonInfo() {
      return info;
   }

   virtual PMI_Result compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_NewtonStep_Base* new_PMI_NewtonStep_Base_func
   (const PMI_Device_Environment& env, PMI_Newton::Info *i);
extern "C" new_PMI_NewtonStep_Base_func new_PMI_NewtonStep_Base;
```

The method `compute()` is called after each Newton iteration.

PMI_NewtonStep Iterations: Flowchart of Computation

The following example shows the `Quasistationary` command (see previous example):

```
Starting solve of next problem:
Quasistationary (
   Initial step in t: 0.1, Minimum step in t: 0.001, Maximum step in t: 0.5,
   ...
) { Coupled ( PMI_NewtonStep(pmi_Newton2(parameter_list)) )
   { Poisson Electron Hole }
}
   // call constructor PMI_NewtonStep
   PMI_NewtonStep *pmi_Newton = new PMI_NewtonStep (. . .)
   bool Is_pmiConverged = false, Is_pmiDiverged = false;

Computing step from t=0.4 to t=0.5
// for this case PMI_Newton::Info functions return the following values:
```

```
// TimeFrom()==0.4 and TimeTo()==0.5
Iteration   |Rhs|        |step|        error
----------------------------------------------------------------
0           3.89e+08
1           1.21e+07     1.25e-03     3.12e+02
    ...
m           6.62e+06     3.36e-05     5.85e+00
      int pmiResult = pmi_Newton->Compute();
      if( pmiResult != pmiNextStep){
        if(pmiResult == PMI_Converged) Is_pmiConverged = true;
        if(pmiResult == PMI_Diverged)  Is_pmiDinverged = true;
      }
      if(Is_sdeviceDiverged || Is_pmiDiverged) {
         // If pmiResult==PMI_Diverged, then user have to use
         // function ChangeTimeTo(new_t) (new_t <= TimeTo())
         // In this case sdevice reduces the time step.
         // It is PMI time step control
         goto Iteration#0;  // sdevice decrease step
      } else if(Is_sdeviceConverged && Is_pmiConverged)
        goto Finish;
      } else {
        goto NextNewtonStep
      }
    ...
Finished, because...
Error smaller than 1 ( 7.3461E-02 ) and  Is_pmiConverged == true
   // call destructor ~PMI_NewtonStep
```

Special Contact PMI for Raytracing

The PMI for raytracing allows you to access and change the parameters of a ray at special contacts. These contacts are drawn in the same manner as electrodes and thermodes (see Boundary Condition for Raytracing on page 605). The raytrace PMI is specified in the RayTraceBC section of the command file:

```
RayTraceBC {...
   { Name = "pmi_contact"
     PMIModel = "pmi_modelname"
   }
}
```

The name of "pmi_contact" must match the contact name in the device. Any ray that hits this special contact invokes a call to this PMI. This raytrace PMI works only with the raytracer (see Raytracer on page 593) and the complex refractive index model (see Complex Refractive Index Model on page 578).

NOTE   When using multithreading of the raytracer, you must carefully design
the PMI code to be thread safe. This means that global variables should
not be used since multiple threads may change the global variables at the
same time, leading to confusion in the user PMI code at runtime.

Dependencies

The raytrace PMI depends on the following variables:

wavelength	Wavelength [cm]
incident_angle	Incident angle [radian]
*incident_dirvec	Direction vector of incident ray
*polarvec	Polarization vector of incident ray
*normalvec	Normal vector to surface of impingement from region 1 to region 2
*intersectpoint	Intersection position vector [cm]
*region1_name	Name of region 1 (string)
*region2_name	Name of region 2 (string)
n1_real	Real part of refractive index 1
n1_imag	Imaginary part of refractive index 1
n2_real	Real part of refractive index 2
n2_imag	Imaginary part of refractive index 2
reflected_angle	Reflected angle [radian]
transmitted_angle	Transmitted angle [radian]
*reflected_dirvec	Direction vector of reflected ray
*transmitted_dirvec	Direction vector of transmitted ray
*reflected_startposition	Starting position vector of reflected ray [cm]
*transmitted_startposition	Starting position vector of transmitted ray [cm]
R_TE	Power TE reflection coefficient
T_TE	Power TE transmission coefficient

| R_TM | Power TM reflection coefficient |
| T_TM | Power TM transmission coefficient |

To obtain the rate intensity (units of s^{-1}) carried by the ray, you need to compute the square of the length of *polarvec. This rate intensity includes all previous absorptions sustained by the ray when it traversed absorptive regions of the device, and it can be used directly to compute the amount of optical generation (with units of s^{-1}). However, for raytracing used in LED simulations, the square of the length of *polarvec gives only a relative intensity value because the polarization vector of the head ray of the raytree is initialized to a length of 1.0.

If the reflection or transmission coefficients are equal to zero, no reflected or transmitted rays are created in the raytracing process.

With this PMI model, you can change the following variables:

reflected_angle	Reflected angle [radian]
transmitted_angle	Transmitted angle [radian]
*reflected_dirvec	Direction vector of reflected ray
*transmitted_dirvec	Direction vector of transmitted ray
*reflected_startposition	Starting position vector of reflected ray [cm]
*transmitted_startposition	Starting position vector of transmitted ray [cm]
R_TE	Power TE reflection coefficient
T_TE	Power TE transmission coefficient
R_TM	Power TM reflection coefficient
T_TM	Power TM transmission coefficient

If you want to change the direction vector, angle, or position vector of the reflected or transmitted ray, the respective flags must be set to TRUE:

- is_reflectedangle_changed
- is_reflecteddirvec_changed
- is_transmittedangle_changed
- is_transmitteddirvec_changed
- is_reflected_new_startposition
- is_transmitted_new_startposition

However, no flags are needed if you want to change the power reflection or transmission coefficients.

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_RayTraceBoundary : public PMI_Vertex_Interface {
public:
   PMI_RayTraceBoundary (const PMI_Environment& env);
   virtual ~PMI_RayTraceBoundary();

   // methods to be implemented by user
   virtual void Compute_BoundaryParameters
      (// Non-changeable quantities
      const double wavelength,                  // wavelength [cm]
      const double incident_angle,              // incident angle
      const double* incident_dirvec,            // dir vector of incident ray
      const double* polarvec,                   // polar vec of incident ray
      const double* normalvec,                  // normal to impingement
      const double* intersectpoint,             // intersection point
      const char* region1_name,                 // name of region 1
      const char* region2_name,                 // name of region 2
      const double n1_real,                     // real part of refr index 1
      const double n1_imag,                     // imag part of refr index 1
      const double n2_real,                     // real part of refr index 2
      const double n2_imag,                     // imag part of refr index 2
      // User changeable quantities
      bool& is_reflectedangle_changed,          // is refl angle changed?
      bool& is_reflecteddirvec_changed,         // is reflected dir changed?
      bool& is_transmittedangle_changed,        // is transm angle changed?
      bool& is_transmitteddirvec_changed,       // is transm dir changed?
      bool& is_reflected_new_startposition,     // is refl pos changed?
      bool& is_transmitted_new_startposition,   // is transm pos changed?
      double& reflected_angle,                  // reflected angle
      double& transmitted_angle,                // transmitted angle
      double* reflected_dirvec,                 // dir vec of reflected ray
      double* transmitted_dirvec,               // dir vec of transmitted ray
      double* reflected_startposition,          // start pos of reflected ray
      double* transmitted_startposition,        // start pos of transm ray
      double& R_TE,                             // power TE reflection coeff.
      double& T_TE,                             // power TE transmission coeff.
      double& R_TM,                             // power TM reflection coeff.
      double& T_TM                              // power TM transmission coeff.
      ) = 0;

   // Auxiliary functions for users
```

```
        void ReadComplexRefractiveIndex(std::string location_name,
           double wavelength,     // in microns
           double& n,
           double& k,
           PMI_RayTraceBoundary::LocationType location_type =
           PMI_RayTraceBoundary::Material);
        private:
        const PMI_Environment* thisenv;
     };
```

An internal auxiliary function called `ReadComplexRefractiveIndex(...)` has been
implemented to allow you to compute the complex refractive index of any material or region
at a particular wavelength. The constraint is that, if a requested material does not exist in the
device structure, it must at least be defined in the parameter file. The complex refractive index
specification (for example, wavelength dependency for the real part or imaginary part or both)
is taken from the command file. For materials that do not exist in the device structure, the
specification from the default `Physics` section is used unless it is explicitly given in a
corresponding separate material `Physics` section.

Example: Assessing and Modifying a Ray

The following example shows how to access the information about a ray that intersects the
special raytrace PMI contact, and how you can change the information of the ray:

```
   class Dummy_RayTraceBoundary : public PMI_RayTraceBoundary {
   private:
      // short ind_field; // field index for optical generation
      //      double shape; // transient curve shape
      //      double G1, G2, G3, T1, T2, T3, T4; // const for shapes
      int count;
      double d1;
   public:
      Dummy_RayTraceBoundary (const PMI_Environment& env);
      ~Dummy_RayTraceBoundary ();

      void Compute_BoundaryParameters
        (const double wavelength,                // wavelength [cm]
        const double incident_angle,          // incident angle
        const double* incident_dirvec,        // dir vec of incident ray
        const double* polarvec,               // polar vec of incident ray
        const double* normalvec,              // normal to impingement
        const double* intersectpoint,         // intersection point
        const char* region1_name,             // name of region 1
        const char* region2_name,             // name of region 2
        const double n1_real,                 // real part of refr index 1
        const double n1_imag,                 // imag part of refr index 1
```

```
        const double n2_real,                   // real part of refr index 2
        const double n2_imag,                   // imag part of refr index 2
        // User changeable quantities
        bool& is_reflectedangle_changed,        // is refl angle changed?
        bool& is_reflecteddirvec_changed,       // is refl dir changed?
        bool& is_transmittedangle_changed,      // is transm angle changed?
        bool& is_transmitteddirvec_changed,     // is transm dir changed?
        bool& is_reflected_new_startposition,   // is refl pos changed?
        bool& is_transmitted_new_startposition, // is transm pos changed?
        double& reflected_angle,                // reflected angle
        double& transmitted_angle,              // transmitted angle
        double* reflected_dirvec,               // dir vec of reflected ray
        double* transmitted_dirvec,             // dir vec of transmitted ray
        double* reflected_startposition,        // start pos of reflected ray
        double* transmitted_startposition,      // start pos of transm ray
        double& R_TE,                           // power TE reflection coeff.
        double& T_TE,                           // power TE transmission coeff.
        double& R_TM,                           // power TM reflection coeff.
        double& T_TM                            // power TM transmission coeff.
        );
};

Dummy_RayTraceBoundary::
Dummy_RayTraceBoundary (const PMI_Environment& env) :
    PMI_RayTraceBoundary (env)
{
    printf("PMI: initializing ray trace PMI\n");
}

Dummy_RayTraceBoundary::
~Dummy_RayTraceBoundary ()
{
}

void Dummy_RayTraceBoundary::
Compute_BoundaryParameters (
        const double wavelength,
        const double incident_angle,
        const double* incident_dirvec,
        const double* polarvec,
        const double* normalvec,
        const double* intersectpoint,
        const char* region1_name,
        const char* region2_name,
        const double n1_real,
        const double n1_imag,
        const double n2_real,
        const double n2_imag,
```

```
        // User changeable quantities
        bool& is_reflectedangle_changed,
        bool& is_reflecteddirvec_changed,
        bool& is_transmittedangle_changed,
        bool& is_transmitteddirvec_changed,
        bool& is_reflected_new_startposition,
        bool& is_transmitted_new_startposition,
        double& reflected_angle,
        double& transmitted_angle,
        double* reflected_dirvec,
        double* transmitted_dirvec,
        double* reflected_startposition,
        double* transmitted_startposition,
        double& R_TE,
        double& T_TE,
        double& R_TM,
        double& T_TM
    )
    {
        // Ray goes from region 1 to region 2.
        // PMI contact is the interface between regions 1 and 2.
        printf("Region 1: Name=%s, Refractive Index = %e + i%e\n",
            region1_name, n1_real, n1_imag);
        printf("Angles: Incident=%lf, Reflected=%lf, Transmitted=%lf\n",
            incident_angle, reflected_angle, transmitted_angle);
        printf("Wavelength = %e [cm]\n", wavelength);
        printf("Incident Ray Direction=(%e,%e,%e)\n",
            incident_dirvec[0], incident_dirvec[1], incident_dirvec[2]);
        printf("Power Coefficients: R_TE=%e, T_TE=%e, R_TM=%e, T_TM=%e\n",
            R_TE, T_TE, R_TM, T_TM);

        // For example, change reflected direction to (1,2,3)
        is_reflecteddirvec_changed = TRUE;
        reflected_dirvec[0] = 1.0;
        reflected_dirvec[1] = 2.0;
        reflected_dirvec[2] = 3.0;
    }
    extern "C" {
        PMI_RayTraceBoundary* new_PMI_RayTraceBoundary (const PMI_Environment& env)
        { return new Dummy_RayTraceBoundary (env);
        }
    }
}
```

Spatial Distribution Function

The spatial distribution function $R(w, l, E)$ can be defined by a PMI (see Heavy Ions on page 668).

The name of the PMI must be specified in the `Physics` section of the command file as follows:

```
Physics {
  HeavyIon(
    SpatialShape = PMI_shape_name
  )
}
```

or:

```
Physics {
  HeavyIon(
    SpatialShape = PMI_shape_name(Energy = value) # [eV]
  )
}
```

Dependencies

The spatial distribution function $R(w, l, E)$ depends on the following variables:

`w`	Radius defined as the perpendicular distance from the track [cm]
`l`	Coordinate along the track [cm]
`E`	Energy of heavy ion [eV]

The PMI model must compute the following result:

`R`	The value of the spatial distribution $R(w, l, E)$ [1]

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_SpatialDistributionFunction: public PMI_Vertex_Interface {
//  * The spatial distribution function:
//  *
//  *   R(w,l,E)
//  *
//  * where
//  *   - l is the coordinate along the particle path [um];
//  *   - w is radial coordinate orthogonal to l [um];
//  *   - E is energy of heavy ion [eV];

public:
  PMI_SpatialDistributionFunction (const PMI_Environment& env,
                                   const char* IonType);

  virtual ~PMI_SpatialDistributionFunction ();

// user-defined name of heavy ion (see Using Alpha Particle Model on page 666)
const char* GetHeavyIonType () const;

// methods to be implemented by user
  virtual void Compute_R (double& R, const double w, const double l = -1.,
                          const double E = -1.) = 0;

};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_SpatialDistributionFunction*
  new_PMI_SpatialDistributionFunction_func
     (const PMI_Environment& env, const char* HeavyIonName);
new_PMI_SpatialDistributionFunction_func new_PMI_SpatialDistributionFunction;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_SpatialDistributionFunction_Base : public PMI_Vertex_Base {

public:
  class Input : public PMI_Vertex_Input_Base {
  public:
     pmi_float w;  // radius (perpendicular distance from track)
```

```
    pmi_float l;  // coordinate along track
    pmi_float E;  // energy of heavy ion
};

class Output {
public:
    pmi_float R;  // spatial distribution
};

PMI_SpatialDistributionFunction_Base (const PMI_Environment& env,
                                      const char* name);
virtual ~PMI_SpatialDistributionFunction_Base ();

const char* GetHeavyIonType () const;

virtual void compute (const Input& input, Output& output) = 0;
};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_SpatialDistributionFunction_Base*
   new_PMI_SpatialDistributionFunction_Base_func
      (const PMI_Environment& env, const char* HeavyIonName);
extern "C" new_PMI_SpatialDistributionFunction_Base_func
   new_PMI_SpatialDistributionFunction_Base;
```

Example: Gaussian Spatial Distribution Function

The built-in Gaussian spatial distribution function (see Heavy Ions on page 668) can also be implemented as a PMI model:

```
#include "PMIModels.h"

class Gaussian_SpatialDistributionFunction : public
PMI_SpatialDistributionFunction {

public:
   Gaussian_SpatialDistributionFunction (const PMI_Environment& env,
      const char* HeavyIonName);
   ~Gaussian_SpatialDistributionFunction ();

   void Compute_R
      (double& R, const double w, const double l, const double E);
};

Gaussian_SpatialDistributionFunction::
Gaussian_SpatialDistributionFunction (const PMI_Environment& env, const char*
```

```
HeavyIonName) :
   PMI_SpatialDistributionFunction (env, HeavyIonName)
{}

 Gaussian_SpatialDistributionFunction::
~Gaussian_SpatialDistributionFunction ()
{}

void Gaussian_SpatialDistributionFunction::
Compute_R(double& R, const double w, const double l, const double E)
{
   //   the unit w,l is [cm]
   //   the unit E is [eV] (in this implementation not used)
   //   R(w,l,E) = exp( -(w/wt(l))^2 )

   double wt = 1.e-4; // scaling factor 1um = 1.e-4cm
   double x = w/wt;

   R = exp(-x*x);

}

extern "C"
PMI_SpatialDistributionFunction* new_PMI_SpatialDistributionFunction
   (const PMI_Environment& env, const char* HeavyIonName)
{
  return new Gaussian_SpatialDistributionFunction (env, HeavyIonName);
}
```

Metal Resistivity

The metal resistivity $\rho = 1/\sigma$ can be defined by a PMI (see Transport in Metals on page 239).

The name of the PMI must be specified in the `Physics` section of the command file as follows:

```
Physics {
   MetalResistivity (pmi_model)
}
```

The simplified interface PMI_MetalResistivity_Base supports the diffusion-reaction species interface (see Reaction–Diffusion Species Interface (Compute Scope) on page 1074).

Dependencies

The metal resistivity depends on the variables:

t   Lattice temperature [K]

f   Absolute value of the electric field [$V cm^{-1}$]

The PMI model must compute the following result:

Resist   Metal resistivity [Ωcm]

In the case of the standard interface, the following derivatives must be computed as well:

dResistdt   Derivative of Resist with respect to t [$\Omega K^{-1} cm$]

dResistdf   Derivative of Resist with respect to f [$\Omega V^{-1} cm^2$]

Standard C++ Interface

The following base class is declared in the file PMIModels.h:

```
class MetalResistivity : public PMI_MetalResistivity {

public:
   MetalResistivity (const PMI_Environment& env);
   virtual ~MetalResistivity ();

   virtual void Compute_Resist
      (const double t,     // lattice temperature
       const double f,     // absolute value of electric field
      double& Resist);     // metal resistivity

   virtual void Compute_dResistdt
      (const double t,     // lattice temperature
       const double f,     // absolute value of electric field
      double& dResistdt);  // derivative of metal resistivity
                           // with respect to lattice temperature

   virtual void Compute_dResistdf
      (const double t,     // lattice temperature
       const double f,     // absolute value of electric field
      double& dResistdf);  // derivative of metal resistivity
```

```
                                        // with respect to electric field
    };
```

The following virtual constructor must be implemented:

```
    typedef PMI_MetalResistivity* new_PMI_MetalResistivity_func
       (const PMI_Environment& env);
    extern "C" new_PMI_MetalResistivity_func new_PMI_MetalResistivity;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
    class PMI_MetalResistivity_Base : public PMI_Vertex_Base {

    public:
       class Input : public PMI_Vertex_Input_Base {
       public:
         pmi_float t;    // lattice temperature
         pmi_float f;    // absolute value of the electric field
       };

       class Output {
       public:
         pmi_float Resist;  // metal resistivity
       };

       PMI_MetalResistivity_Base (const PMI_Environment& env);
       virtual ~PMI_MetalResistivity_Base ();

       virtual void compute (const Input& input, Output& output) = 0;
    };
```

The following virtual constructor must be implemented:

```
    extern "C"
    PMI_MetalResistivity_Base* new_PMI_MetalResistivity_Base
       (const PMI_Environment& env);
```

Example: Linear Metal Resistivity

The following C++ code implements linear metal resistivity:

```cpp
#include "PMIModels.h"

class MetalResistivity : public PMI_MetalResistivity
{
   private:
      double R0, AlphaT;

   public:
      MetalResistivity (const PMI_Environment& env);
      ~MetalResistivity ();

      void Compute_Resist
         (const double t,      // lattice temperature
          const double f,      // absolute value of electric field
          double& Resist);     // metal resistivity

      void Compute_dResistdt
         (const double t,      // lattice temperature
          const double f,      // absolute value of electric field
          double& dResistdt);  // derivative of metal resistivity
                               // with respect to lattice temperature

      void Compute_dResistdf
         (const double t,      // lattice temperature
          const double f,      // absolute value of electric field
          double& dResistdf);  // derivative of metal resistivity
                               // with respect to electric field
};

MetalResistivity::
MetalResistivity (const PMI_Environment& env) :
   PMI_MetalResistivity (env)
{ // Gold values
   R0    = InitParameter ("R0",    2.0400e-06);  // [ohm*cm]
   AlphaT = InitParameter ("AlphaT", 4.0000e-03);  // [1/K]
}

MetalResistivity::
~MetalResistivity ()
{}

void MetalResistivity::
Compute_Resist (const double t, const double f, double& Resist)
```

```
{
   Resist = R0*( 1 + AlphaT*( t - 273 ) );
}

void MetalResistivity::
Compute_dResistdt (const double t, const double f, double& dResistdt)
{
   dResistdt = R0*AlphaT;
}

void MetalResistivity::
Compute_dResistdf (const double t, const double f, double& dResistdf)
{
   dResistdf = 0;
}

extern "C"
PMI_MetalResistivity* new_PMI_MetalResistivity
   (const PMI_Environment& env)
{
   return new MetalResistivity(env);
}
```

Heat Generation Rate

The total heat generation rate is the term on the right-hand side of Eq. 69, p. 193. You can specify an additional term `pmi_Heat` for a given material or region:

```
Total_Heat = existing_Heat + pmi_Heat
```

The name of the PMI must be specified in the new subsection `HeatSource(pmi_model)` in the `Physics` section of the command file as follows:

```
Physics (Material = "Silicon") {
   HeatSource (pmi_Heat_Si)
}
```

To plot the `pmi_Heat` values, specify the keyword `pmiHeat` in the `Plot` section of the command file.

Dependencies

The heat generation depends on the variables:

n	Electron density [cm^{-3}]
p	Hole density [cm^{-3}]
t	Lattice temperature [K]
f	Electric field vector [Vcm^{-1}]
g	Gradient temperature [Kcm^{-1}]

The PMI model must compute the following results:

Heat	Heat generation rate [Wcm^{-3}]

In the case of the standard interface, the following derivatives must be computed as well:

dHeat_dn	Derivative of `Heat` with respect to `n` [W]
dHeat_dp	Derivative of `Heat` with respect to `p` [W]
dHeat_dt	Derivative of `Heat` with respect to `t` [$\text{Wcm}^{-3}\text{K}^{-1}$]
dHeat_df	Derivative of `Heat` with respect to each component `f` [$\text{Wcm}^{-2}\text{V}^{-1}$]
dHeat_dg	Derivative of `Heat` with respect to each component `g` [$\text{Wcm}^{-2}\text{K}^{-1}$]

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_Heat_Generation : public PMI_Vertex_Interface {

public:
   PMI_Heat_Generation (const PMI_Environment& env);
   virtual ~PMI_Heat_Generation ();

   // methods to be implemented by user
   virtual void Compute_Heat
     (const double n,              // electron density
      const double p,              // hole density
      const double t,              // lattice temperature
```

```
          const double f[3],            // electric field vector
          const double g[3],            // gradient of temperature
          double& heat) = 0;            // heat generation rate

       virtual void Compute_dHeat_dn
         (const double n,               // electron density
          const double p,               // hole density
          const double t,               // lattice temperature
          const double f[3],            // electric field vector
          const double g[3],            // gradient of temperature
          double& dHeat_dn) = 0;        // derivative of heat with respect to n

       virtual void Compute_dHeat_dp
         (const double n,               // electron density
          const double p,               // hole density
          const double t,               // lattice temperature
          const double f[3],            // electric field vector
          const double g[3],            // gradient of temperature
          double& dHeat_dp) = 0;        // derivative of heat with respect to p

       virtual void Compute_dHeat_dt
         (const double n,               // electron density
          const double p,               // hole density
          const double t,               // lattice temperature
          const double f[3],            // electric field vector
          const double g[3],            // gradient of temperature
          double& dHeat_dt) = 0;        // derivative of heat with respect to t

       virtual void Compute_dHeat_df
         (const double n,               // electron density
          const double p,               // hole density
          const double t,               // lattice temperature
          const double f[3],            // electric field vector
          const double g[3],            // gradient of temperature
          double dHeat_df[3]) = 0;      // derivative of heat with respect to f

       virtual void Compute_dHeat_dg
         (const double n,               // electron density
          const double p,               // hole density
          const double t,               // lattice temperature
          const double f[3],            // electric field vector
          const double g[3],            // gradient of temperature
          double dHeat_dg[3]) = 0;      // derivative of heat with respect to g
    };
```

The following virtual constructor must be implemented:

```
typedef PMI_Heat_Generation* new_PMI_Heat_Generation_func
   (const PMI_Environment& env);
extern "C" new_PMI_Heat_Generation_func new_PMI_HeatGeneration;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_HeatGeneration_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
    pmi_float n;      // electron density
    pmi_float p;      // hole density
    pmi_float t;      // lattice temperature
    pmi_float f[3];   // electric field vector
    pmi_float g[3];   // gradient of temperature
   };

   class Output {
   public:
    pmi_float heat;  // heat generation rate
   };

   PMI_HeatGeneration_Base (const PMI_Environment& env);
   virtual ~PMI_HeatGeneration_Base ();

   virtual void compute (const Input& input, Output& output) = 0;

};
```

The prototype for the virtual constructor is given as:

```
typedef PMI_HeatGenerationFunction_Base*
   new_PMI_HeatGenerationFunction_Base_func
      (const PMI_Environment& env);
extern "C" new_PMI_HeatGenerationFunction_Base_func
   new_PMI_HeatGenerationFunction_Base;
```

Example: Dependency on Electric Field and Gradient of Temperature

In the following example, heat generation has a linear dependency on the electric field and the gradient of temperature:

```
// Heat = kappa*(E,gratT)*1[1/V]
//    where
//    E - electric field vector,
//    gradT - gradient of temperature.
//
// The 1D equation
//     -div(kappa*grad(T(x))) = Heat, 0 <= x <= L
//       T(0) = T0,
//       T(L) = T1,
// has the exact solution:
//       T(x) = (T1-T0)*(exp(-E*x)-1)/(exp(-E*L)-1) + T0

class HeatGeneration : public PMI_HeatGeneration_Base
{
private:
   double kappa;

public:
   HeatGeneration (const PMI_Environment& env);
   ~HeatGeneration ();
   void compute (const Input& input, Output& output);
};

HeatGeneration::HeatGeneration (const PMI_Environment& env) :
   PMI_HeatGeneration_Base (env)
{
   kappa = InitParameter("kappa", 0.01);  //  [W/(K*cm)]
}

HeatGeneration::~HeatGeneration () {}

void HeatGeneration::compute (const Input& input, Output& output)
{
   const pmi_float (&f)[3] = input.f;
   const pmi_float (&g)[3] = input.g;

   output.heat = kappa*(f[0]*g[0] + f[1]*g[1] + f[2]*g[2]);
}
```

```
extern "C"
PMI_HeatGeneration_Base* new_PMI_HeatGeneration_Base
   (const PMI_Environment& env)
{ return new HeatGeneration (env);}
```

Thermoelectric Power

The thermoelectric powers P_n and P_p in semiconductors can be defined by a PMI (see Thermoelectric Power (TEP) on page 913).

The name of the PMI can be specified regionwise, materialwise, or globally in the `Physics` section of the command file as follows:

```
Physics(Material="Silicon") {
   TEPower(pmi_model)
}
```

Dependencies

The semiconductor TEPs may depend on the following variables:

t   Lattice temperature [K]

dens   Carrier density $[\text{cm}^{-3}]$

The PMI model must compute the following results:

power   Thermoelectric power $[\text{V K}^{-1}]$

In the case of the standard interface, the following derivatives must be computed as well:

dpowerdt   Derivative of `power` with respect to `t` $[\text{V K}^{-2}]$

dpowerddens   Derivative of `power` with respect to `dens` $[\text{V K}^{-1}\text{cm}^{-3}]$

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_ThermoElectricPower : public PMI_Vertex_Interface {

public:
   PMI_ThermoElectricPower(const PMI_Environment& env);
   virtual ~PMI_ThermoElectricPower ();

   virtual void Compute_power(
      const double t,         // lattice temperature
      const double dens,      // carrier density
      double& power);         // thermoelectric power

   virtual void Compute_dpowerdt(
      const double t,         // lattice temperature
      const double dens,      // carrier density
      double& dpowerdt);      // derivative of thermoelectric power
                              // with respect to lattice temperature

   virtual void Compute_dpowerddens(
      const double t,         // lattice temperature
      const double dens,      // carrier density
      double& dpowerddens);   // derivative of thermoelectric power
                              // with respect to carrier density
};
```

The following virtual constructor must be implemented:

```
typedef PMI_ThermoElectricPower* new_PMI_ThermoElectricPower_func
   (const PMI_Environment& env);
extern "C" new_PMI_ThermoElectricPower_func new_PMI_e_ThermoElectricPower;
extern "C" new_PMI_ThermoElectricPower_func new_PMI_h_ThermoElectricPower;
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_ThermoElectricPower_Base : public PMI_Vertex_Base {

public:
   class Input : public PMI_Vertex_Input_Base {
   public:
      pmi_float t;      // lattice temperature
      pmi_float dens;   // carrier density
```

```
   };

   class Output {
   public:
      pmi_float power;  // thermoelectric power
   };

   PMI_ThermoElectricPower_Base (const PMI_Environment& env);
   virtual ~PMI_ThermoElectricPower_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
};
```

The following virtual constructor must be implemented:

```
extern "C"
PMI_ThermoElectricPower_Base* new_PMI_ThermoElectricPower_Base
   (const PMI_Environment& env);
```

Example: Analytic TEP

The following C++ code implements an analytic TEP model (see Thermoelectric Power (TEP) on page 913):

```
#include "PMIModels.h"

namespace {
   // pi
   double pi = 3.141592654;
   // electron mass in kg
   double m0 = 9.109534e-31;
   // Planck's constant in J*s
   double h_planck = 6.626176e-34;
   // Boltzmann constant in J/K
   double kB = 1.380662e-23;
   // electron charge in C
   double e0 = 1.602192e-19;

   double pow_1_5 (double x) {
      return (x==1) ? 1 : x * sqrt (x);
   }

   double Compute_NB_By3_2 (double m_r) {
      double val = 2 * pow_1_5(2 * pi * (kB/h_planck) * (m0/h_planck)) / 1e6;
      val *= pow_1_5(m_r);
      return val;
   }
```

```
      }

      class AnalyticalTEP_ThermoElectricPower : public PMI_ThermoElectricPower
      {
         protected:
            double k_c, s_c;
            // relative effective mass
            double m_r;
            int sign;

         public:
            AnalyticalTEP_ThermoElectricPower(const PMI_Environment& env);
            ~AnalyticalTEP_ThermoElectricPower ();

            void Compute_power
               (const double t,        // lattice temperature
                const double dens,     // carrier density
                double& power);        // thermoelectric power

            void Compute_dpowerdt
               (const double t,        // lattice temperature
                const double dens,     // carrier density
                double& dpowerdt);     // derivative of thermoelectric power
                                       // with respect to lattice temperature

            void Compute_dpowerddens
               (const double t,        // lattice temperature
                const double dens,     // carrier density
                double& dpowerddens);  // derivative of thermoelectric power
                                       // with respect to carrier density
      };

      AnalyticalTEP_ThermoElectricPower::
      AnalyticalTEP_ThermoElectricPower (const PMI_Environment& env) :
         PMI_ThermoElectricPower (env)
      {
      }

      AnalyticalTEP_ThermoElectricPower::
      ~AnalyticalTEP_ThermoElectricPower ()
      {
      }

      void AnalyticalTEP_ThermoElectricPower::
      Compute_power (const double t, const double dens, double& power)
      {
         double NB = Compute_NB_By3_2(m_r) * pow_1_5(t);
         if(sign < 0)
```

```
        power = k_c * (log(dens/NB) + s_c - 2.5);
    else
        power = k_c * (log(NB/dens) - s_c + 2.5);
    power *= (kB/e0);
}


void AnalyticalTEP_ThermoElectricPower::
Compute_dpowerdt (const double t, const double dens, double& dpowerdt)
{
    dpowerdt = sign * (kB/e0) * k_c * 1.5 / t;
}


void AnalyticalTEP_ThermoElectricPower::
Compute_dpowerddens (const double t, const double dens, double& dpowerddens)
{
    dpowerddens = -sign * (kB/e0) * k_c / dens;
}


class AnalyticalTEP_e_ThermoElectricPower :
public AnalyticalTEP_ThermoElectricPower
{
  public:
   AnalyticalTEP_e_ThermoElectricPower(const PMI_Environment& env);
   ~AnalyticalTEP_e_ThermoElectricPower () {}
};


AnalyticalTEP_e_ThermoElectricPower::
AnalyticalTEP_e_ThermoElectricPower(const PMI_Environment& env) :
AnalyticalTEP_ThermoElectricPower(env) {
    // default values
    k_c = InitParameter("k_c_e", 1);
    s_c = InitParameter("s_c_e", 1);
    m_r = InitParameter("m_r_e", 1);
    sign = -1;
}


class AnalyticalTEP_h_ThermoElectricPower :
public AnalyticalTEP_ThermoElectricPower
{
  public:
   AnalyticalTEP_h_ThermoElectricPower(const PMI_Environment& env);
   ~AnalyticalTEP_h_ThermoElectricPower () {}
};


AnalyticalTEP_h_ThermoElectricPower::
AnalyticalTEP_h_ThermoElectricPower(const PMI_Environment& env) :
AnalyticalTEP_ThermoElectricPower(env) {
    // default values
```

```
      k_c = InitParameter("k_c_h", 1);
      s_c = InitParameter("s_c_h", 1);
      m_r = InitParameter("m_r_h", 1);
      sign = 1;
   }

   extern "C"
   PMI_ThermoElectricPower* new_PMI_e_ThermoElectricPower
      (const PMI_Environment& env)
   {
      return new AnalyticalTEP_e_ThermoElectricPower(env);
   }

   extern "C"
   PMI_ThermoElectricPower* new_PMI_h_ThermoElectricPower
      (const PMI_Environment& env)
   {
      return new AnalyticalTEP_h_ThermoElectricPower(env);
   }
```

Metal Thermoelectric Power

The metal thermoelectric power P in metals can be defined by a PMI (see Thermoelectric Power (TEP) on page 913).

The name of the PMI can be specified regionwise, materialwise, or globally in the `Physics` section of the command file as follows:

```
Physics(Material="Copper") {
   MetalTEPower(pmi_model)
}
```

Dependencies

The metal thermoelectric power may depend on the following variables:

t	Lattice temperature [K]
qf	Quasi-Fermi potential [V]
f	Electric field vector [Vcm^{-1}]

The PMI model must compute the following result:

power   Thermoelectric power $[\text{V}\,\text{K}^{-1}]$

In the case of the standard interface, the following derivatives must be computed as well:

dpowerdt   Derivative of power with respect to t $[\text{V}\,\text{K}^{-2}]$

dpowerdqf   Derivative of power with respect to qf $[\text{K}^{-1}]$

dpowerdf   Derivative of power with respect to each component of f $[\text{cm}\,\text{K}^{-1}]$,
               a vector with up to three entries

Standard C++ Interface

The following base class is declared in the file PMIModels.h:

```
class PMI_MetalThermoElectricPower : public PMI_Vertex_Interface {

public:
    PMI_MetalThermoElectricPower(const PMI_Environment& env);
    virtual ~MetalPMI_ThermoElectricPower ();

    virtual void Compute_power(
        const double t,         // lattice temperature
        const double qf,        // quasi-Fermi potential
        const double f[3]       // electric field vector
        double& power);         // thermoelectric power

    virtual void Compute_dpowerdt(
        const double t,         // lattice temperature
        const double qf,        // quasi-Fermi potential
        const double f[3]       // electric field vector
        double& dpowerdt);      // derivative of thermoelectric power
                                // with respect to lattice temperature

    virtual void Compute_dpowerdqf(
        const double t,         // lattice temperature
        const double qf,        // quasi-Fermi potential
        const double f[3]       // electric field vector
        double& dpowerdqf);     // derivative of thermoelectric power
                                // with respect to quasi-Fermi potential
    virtual void Compute_dpowerdf(
        const double t,         // lattice temperature
        const double qf,        // quasi-Fermi potential
```

```
            const double f[3]        // electric field vector
            double& dpowerdf[3]);    // derivative of thermoelectric power
                                     // with respect to electric field
    };
```

The following virtual constructor must be implemented:

```
typedef PMI_MetalThermoElectricPower* new_PMI_MetalThermoElectricPower_func
    (const PMI_Environment& env);
extern "C" new_PMI_MetalThermoElectricPower_func
                                    new_PMI_MetalThermoElectricPower;
```

Simplified C++ Interface

The following base class is declared in the file PMI.h:

```
class PMI_MetalThermoElectricPower_Base : public PMI_Vertex_Base {

public:
    class Input : public PMI_Vertex_Input_Base {
    public:
        pmi_float t;        // lattice temperature
        pmi_float qf;       // quasi-Fermi potential
        pmi_float f[3];     // electric field vector
    };

    class Output {
    public:
        pmi_float power;  // thermoelectric power
    };

    PMI_MetalThermoElectricPower_Base (const PMI_Environment& env);
    virtual ~PMI_MetalThermoElectricPower_Base ();

    virtual void compute (const Input& input, Output& output) = 0;
};
```

The following virtual constructor must be implemented:

```
extern "C"
PMI_MetalThermoElectricPower_Base* new_PMI_MetalThermoElectricPower_Base
    (const PMI_Environment& env);
```

Example: Linear Field Dependency of Metal TEP

The following C++ code implements a metal TEP PMI depending linearly on two of the electric field components:

```cpp
#include "PMIModels.h"

namespace {
   // Boltzmann constant in J/K
   double kB = 1.380662e-23;
   // electron charge in C
   double e0 = 1.602192e-19;
}

class MetalThermoElectricPower : public PMI_MetalThermoElectricPower
{
   private:
      double alpha, beta;

   public:
      MetalThermoElectricPower(const PMI_Environment& env);
      ~MetalThermoElectricPower ();

      void Compute_power
         (const double t,         // lattice temperature
          const double qf,        // quasi-Fermi potential
          const double f[3],      // electric field vector
          double& power);         // thermoelectric power

      void Compute_dpowerdt
         (const double t,         // lattice temperature
          const double qf,        // quasi-Fermi potential
          const double f[3],      // electric field vector
          double& dpowerdt);      // derivative of thermoelectric power
                                  // with respect to lattice temperature

      void Compute_dpowerdqf
         (const double t,         // lattice temperature
          const double qf,        // quasi-Fermi potential
          const double f[3],      // electric field vector
          double& dpowerdqf);     // derivative of thermoelectric power
                                  // with respect to quasi-Fermi potential

      void Compute_dpowerdf
         (const double t,         // lattice temperature
          const double qf,        // quasi-Fermi potential
          const double f[3],      // electric field vector
```

```
              double dpowerdf[3]);    // derivative of thermoelectric power
                                      // with respect to electric field
};

MetalThermoElectricPower::
MetalThermoElectricPower (const PMI_Environment& env) :
   PMI_MetalThermoElectricPower (env)
{
   // default values
   alpha = InitParameter("alpha",1);
   beta = InitParameter("beta",1e-2);
}

MetalThermoElectricPower::
~MetalThermoElectricPower ()
{
}

void MetalThermoElectricPower::
Compute_power (const double t, const double qf, const double f[3],
               double& power)
{
   power = 1e-6 * 1e-2 * (f[0] + f[1]);
}

void MetalThermoElectricPower::
Compute_dpowerdt (const double t, const double qf, const double f[3],
                  double& dpowerdt)
{
   dpowerdt = 0;
}

void MetalThermoElectricPower::
Compute_dpowerdqf (const double t, const double qf, const double f[3],
                   double& dpowerdqf)
{
   dpowerdqf = 0;
}

void MetalThermoElectricPower::
Compute_dpowerdf (const double t, const double qf, const double f[3],
                  double dpowerdf[3])
{
   dpowerdf[0] = 1e-6 * 1e-2;
   dpowerdf[1] = 1e-6 * 1e-2;
   dpowerdf[2] = 0;
}
```

```
extern "C"
PMI_MetalThermoElectricPower* new_PMI_MetalThermoElectricPower
   (const PMI_Environment& env)
{
   return new MetalThermoElectricPower(env);
}
```

Diffusivity

The diffusivity $D_i \exp(-E_{\mathrm{d}i}/(kT))$ and the prefactor of the thermal diffusion term α_{td} can be defined by a PMI (see Hydrogen Transport on page 500).

The name of the PMI can be specified regionwise, materialwise, or globally in the `Physics` section of the command file as follows:

```
Physics ( Material = "Oxide" ) {
   HydrogenDiffusion(
      HydrogenAtom (
         Diffusivity = pmi_model
         Alpha = pmi_otherModel
      )
      ...
   )
}
```

Dependencies

The diffusivity and the prefactor of the thermal diffusion term may depend on the following variables:

f	Modulus of electric field $[\mathrm{V\,cm^{-1}}]$
h	Density of hydrogen species (atom, molecule, ion) $[\mathrm{cm^{-3}}]$
t	Lattice temperature [K]

The PMI model must compute the following result:

d	Diffusivity $D_i \exp(-E_{\mathrm{d}i}/(kT))$ $[\mathrm{cm^2\,s^{-1}}]$ (PMI model for `Diffusivity`) or prefactor of thermal diffusion term α_{td} [1] (PMI model for `Alpha`)

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```cpp
class PMI_HydrogenDiffusivity_Base : public PMI_Vertex_Base {

public:
   const PMI_HydrogenType hydrogen_type;
   class Input : public PMI_Vertex_Input_Base {
   public:
      Input (const PMI_HydrogenDiffusivity_Base* hydrogendiffusivity_base,
               const int vertex);
      pmi_float h; // density of hydrogen atoms, molecules, or ions
                   //           (depending on type) [/cm^3]
      pmi_float t; // lattice temperature [K]
      pmi_float f; // absolute value of electric field [V/cm]
   };

   class Output {
   public:
      pmi_float d; // diffusivity [cm^2*s^-1] or prefactor of the thermal
                   //           diffusion term [1]
   };

   PMI_HydrogenDiffusivity_Base (const PMI_Environment& env, const
      PMI_HydrogenType type);
   virtual ~PMI_HydrogenDiffusivity_Base ();

   virtual void compute (const Input& input, Output& output) = 0;
}
```

The following virtual constructor must be implemented:

```cpp
extern "C"
PMI_HydrogenDiffusivity_Base* new_PMI_HydrogenDiffusivity_Base
   (const PMI_Environment& env, const PMI_HydrogenType type);
```

Example: Field-Dependent Hydrogen Diffusivity

The following C++ code implements a field-dependent hydrogen diffusivity:

```cpp
#include "PMIModels.h"

class pmi_HydrogenDiffusivity : public PMI_HydrogenDiffusivity_Base {
   private:
      double d0; // [cm^2*s^-1]
      double f0; // [eV]
```

```
      double fe; // [1]
      double ed; // [eV]

   public:
      pmi_HydrogenDiffusivity (const PMI_Environment& env,
         const PMI_HydrogenType type);
      ~pmi_HydrogenDiffusivity ();

      void compute (const Input& input, Output& output);
};

pmi_HydrogenDiffusivity::
pmi_HydrogenDiffusivity (const PMI_Environment& env,
   const PMI_HydrogenType type) :
PMI_HydrogenDiffusivity_Base (env, type)
{
   // for hydrogen atom
   double d0_a = InitParameter ("d0_a", 1.0e-5);
   double f0_a = InitParameter ("f0_a", 1.0e-5);
   double fe_a = InitParameter ("fe_a", 0.5);
   double ed_a = InitParameter ("ed_a", 0.5);

   // for hydrogen molecule
   double d0_m = InitParameter ("d0_m", 1.0e-5);
   double f0_m = InitParameter ("f0_m", 1.0e-5);
   double fe_m = InitParameter ("fe_m", 0.5);
   double ed_m = InitParameter ("ed_m", 0.5);

   // for hydrogen ion
   double d0_i = InitParameter ("d0_i", 1.0e-5);
   double f0_i = InitParameter ("f0_i", 1.0e-5);
   double fe_i = InitParameter ("fe_i", 0.5);
   double ed_i = InitParameter ("ed_i", 0.5);

   if (hydrogen_type == PMI_HydrogenAtom)
   {
      d0 = d0_a;
      f0 = f0_a;
      fe = fe_a;
      ed = ed_a;
   }
   else if(hydrogen_type == PMI_HydrogenMolecule)
   {
      d0 = d0_m;
      f0 = f0_m;
      fe = fe_m;
      ed = ed_m;
   }
```

```
      else if(hydrogen_type == PMI_HydrogenIon)
      {
         d0 = d0_i;
         f0 = f0_i;
         fe = fe_i;
         ed = ed_i;
      }
      else
      {
         std::cout << "unexpected hydrogen type!\n";
         exit(-1);
      }
}
pmi_HydrogenDiffusivity::
~pmi_HydrogenDiffusivity ()
{
}

void pmi_HydrogenDiffusivity::
compute (const Input& input, Output& output)
{
   pmi_float kt = 0.0258519952664849131 * (input.t/300.0); // [eV]
   // field-induced activation energy lowering
   pmi_float ea = ed - f0*pow(input.f, fe); // ed - f0*(f/(1[V/cm])^fe

   // set activation energy equal to zero if it is negative
   if(ea<0.0) ea = 0.0;
   ea /= kt;

   output.d = d0*exp(-ea);
}

extern "C"
PMI_HydrogenDiffusivity_Base* new_PMI_HydrogenDiffusivity_Base
(const PMI_Environment& env, const PMI_HydrogenType type)
{
   return new pmi_HydrogenDiffusivity (env, type);
}
```

Gamma Factor for Density Gradient Model

The density-gradient quantization model (see Density Gradient Model on page 294) contains the fit factor:

$$\gamma = \gamma_0 \cdot \gamma_{\mathrm{pmi}} \tag{1282}$$

where γ_0 is the solution-independent value, and γ_{pmi} is dependent on the solution [4].

The name of the PMI can be specified regionwise, materialwise, or globally in the `Physics` section of the command file as follows:

```
Physics ( Material = "Silicon" ) {
   eQuantumPotential( Gamma(name=pmi_eGamma -EffectiveMass)
   hQuantumPotential( Gamma(name=pmi_hGamma)
}
```

This model has the optional flag `EffectiveMass` (default) or `-EffectiveMass`. If the option `-EffectiveMass` is activated, the DOS mass that is used as the prefactor of the density gradient equation is replaced with the free electron mass (only in the quantum potential model).

Dependencies

The γ_{pmi} may depend on the following variables:

$$\gamma_{\mathrm{pmi}} = \gamma_{\mathrm{pmi}}(c, T_c, E_{\mathrm{normal}}, h) \tag{1283}$$

where:

`c=n,p`	Carrier density $[\mathrm{cm}^{-3}]$ for `eQuantumPotential`, `hQuantumPotential` models
T_c	Carrier temperature [K]
E_{normal}	Electric field perpendicular to interface $[\mathrm{Vcm}^{-1}]$
`h`	Layer thickness $[\mu\mathrm{m}]$

The PMI model must compute the following result:

`Gamma`	[unitless]

In the case of the standard interface, the following derivatives must be computed as well:

dGamma_dc	Derivative of Gamma with respect to n, p $[\text{cm}^3]$
dGamma_dt	Derivative of Gamma with respect to T_c $[\text{K}^{-1}]$
dGamma_df	Derivative of Gamma with respect to E_{per} $[\text{cmV}^{-1}]$
dGamma_dh	Derivative of Gamma with respect to h $[\text{cmV}^{-1}]$

Standard C++ Interface

The following base class is declared in the file PMIModels.h:

```
class PMI_QDDGamma : public PMI_Vertex_Interface {

public:
   PMI_QDDGamma(const PMI_Environment& env);
   virtual ~PMI_QDDGamma ();

   virtual void Compute_gamma(
      const double c,          // carrier density
      const double t,          // carrier temperature
      const double f,          // Enormal to interface
      const double h,          // layer thickness
      double& gamma) = 0;      // gamma

   virtual void Compute_dgamma_dc
      (const double c,          // carrier density
       const double t,          // carrier temperature
       const double f,          // Enormal to interface
       const double h,          // layer thickness
       double& dgammadc) = 0;   // derivative of gamma with respect to
                                // carrier density

   virtual void Compute_dgamma_dt
      (const double c,          // carrier density
       const double t,          // carrier temperature
       const double f,          // Enormal to interface
       const double h,          // layer thickness
       double& dgammadt) = 0;   // derivative with respect to carrier
                                // temperature

   virtual void Compute_dgamma_df
      (const double c,          // carrier density
       const double t,          // carrier temperature
       const double f,          // Enormal to interface
```

```
      const double h,           // layer thickness
      double& dgammadf) = 0;    // derivative with respect to Enormal to
                                // interface

  virtual void Compute_dgamma_dh
    (const double c,            // carrier density
     const double t,            // carrier temperature
     const double f,            // Enormal to interface
     const double h,            // layer thickness
     double& dgammadh) = 0;     // derivative with respect to layer thickness
};
```

The following virtual constructor must be implemented:

```
typedef PMI_QDDGamma* new_PMI_QDDGamma_func
   (const PMI_Environment& env);
extern "C" new_PMI_QDDGamma_func    new_PMI_QDDGamma;
```

Simplified C++ Interface

The following base class is declared in the file PMI.h:

```
class PMI_MSC_QDDGamma_Base : public PMI_MSC_Vertex_Base {
   public:
     class Input : public PMI_Vertex_Input_Base {
     public:
       Input (const PMI_MSC_QDDGamma_Base* msc_qddgamma_base,
              const int vertex);

       pmi_float n;   // electron density
       pmi_float p;   // hole density
       pmi_float T;   // lattice temperature
       pmi_float eT;  // electron temperature
       pmi_float hT;  // hole temperature
       std::vector<pmi_float> s;  // phase fraction
     };
   class Output {
     public:
       pmi_float val;  // solution-dependent gamma value
     };

     PMI_MSC_QDDGamma_Base (const PMI_Environment& env,
                                      const std::string& msconfig_name,
                                      const int model_index);

     virtual ~PMI_MSC_QDDGamma_Base ();
```

```
        virtual void compute (const Input& input, Output& output) = 0;

    };
```

The following virtual constructor must be implemented:

```
extern "C"
PMI_QDDGamma_Base* new_PMI_QDDGamma_Base (const PMI_Environment& env);
```

Example: Solution-Dependent Gamma Factor

The following C++ code implements a solution-dependent `Gamma` factor (simplified C++ interface):

```
#include <math.h>
#include "PMI.h"

//   gamma = gxy*gc*gt*gf*gh
//     where:
//     gxy = g0 + ax*x/x0 + ay*y/y0;
//     gc = exp(xc/(1+xc));   xc = Sqr(log(c/c0))
//     gt = exp(xt);          xt = (t-300)/cT0
//     gf = 1 + af*xf*xf;     xf = (f-f1)/f0
//     gh = 1 + ah*(xh - 1);  xh = h/h0

class eQDDGamma : public PMI_QDDGamma_Base{
private:
  // see above
  double g0, x0, y0, ax, ay;
  double c0, cT0;
  double h0, ah;
  double f0, f1, af;

  int formula;
  enum {is_c=1, is_t=2, is_f=4, is_h=8};

public:
  eQDDGamma (const PMI_Environment& env);
  ~eQDDGamma ();
void compute (const Input& input, Output& output);
};

eQDDGamma::
eQDDGamma (const PMI_Environment& env) :
  PMI_QDDGamma_Base (env)
{
  g0 = InitParameter("g0",  1.);      //  [1]
```

```
      c0 = InitParameter("c0",  1e10);    //  [cm-3]
     cT0 = InitParameter("cT0", 300.);    //  [K]
      x0 = InitParameter("x0", 1.);       //  [um]
      ax = InitParameter("ax", 0.);       //  [1]
      y0 = InitParameter("y0", 1.);       //  [um]
      ay = InitParameter("ay", 0.);       //  [1]
      h0 = InitParameter("h0", 1.);       //  [um]
      ah = InitParameter("ah", 0.);       //  [1]
      f0 = InitParameter("f0", 1e7);      //  [V/cm]
      f1 = InitParameter("f1", 1e7);      //  [V/cm]
      af = InitParameter("af", 0.);       //  [1]

  formula = InitParameter("formula", 0);  //  [1]
  if(formula < 0)  formula = 0;
  if(formula > 15) formula = 15;


}
eQDDGamma::~eQDDGamma (){}

void eQDDGamma::
compute (const Input& input, Output& output)
{
  const pmi_float& c = input.c;  // carrier density
  const pmi_float& t = input.t;  // carrier temperature
  const pmi_float& f = input.f;  // Enormal to interface
  const pmi_float& h = input.h;  // layer thickness

  double x, y, z;
  input.ReadCoordinate (x, y, z);
  pmi_float gxy = g0 + ax*x/x0 + ay*y/y0;

  pmi_float gc = 1.;
  pmi_float gt = 1.;
  pmi_float gf = 1.;
  pmi_float gh = 1.;

  if(formula & is_c) {
    const pmi_float n  = (c < 1e-4 ? 1e-4 : c);
    const pmi_float xc = log(n/c0)*log(n/c0);
    gc = exp(xc/(1.+xc));
  }
  if(formula & is_t) {
    const pmi_float xt = (t-300)/cT0;
    gt = exp(xt);
  }
  if(formula & is_f) {
    const pmi_float xf = (f - f1)/f0;
    gf = 1. + af*xf*xf;
```

```
    }
    if(formula & is_h) {
      const pmi_float xh = h/h0;
      gh = 1. + ah*(xh - 1.);
    }

    output.gamma = gxy*gc*gt*gf*gh;
  }

  extern "C"
  PMI_QDDGamma_Base* new_PMI_QDDGamma_Base
    (const PMI_Environment& env)
  {
    return new eQDDGamma(env);}
```

Schottky Resistance Model

The Schottky resistance model (see Resistive Contacts on page 213 and Resistive Interfaces on page 219) emulates the behavior of a Schottky contact or interface. The Schottky resistance PMI allows users to define the contact- or interface-distributed Schottky resistance as an arbitrary function of lattice temperature, electron temperature, hole temperature, electron affinity, band gap, bandgap narrowing, conduction-band effective density-of-states, valence-band effective density-of-states, and effective intrinsic density.

The name of the PMI can be specified interface-wise or electrode-wise in the `Physics` section of the command file as follows:

```
Physics ( Electrode = "top2" ) {
   DistResist=SchottkyResist(pmi_schottkyresist1)
}

Physics(RegionInterface="r1/r5") {
   DistResist=SchottkyResist(pmi_schottkyresist2)
}
```

Dependencies

The Schottky resistance R_d may depend on the following variables:

$$R_d = R_d(T, T_n, T_p, \chi, E_g, E_{bgn}, N_C, N_V, n_{i, eff}) \tag{1284}$$

where:

T	Lattice temperatures [K]
T_n, T_p	Carrier temperatures [K]
χ	Electron affinity [eV]
E_g	Band gap [eV]
E_{bgn}	Bandgap narrowing [eV]
N_C, N_V	Conduction and valence band density-of-states [cm^{-3}]
$n_{i, eff}$	Effective intrinsic density cm^{-3}]

The PMI model must compute the following result:

`Rd`	[Ωcm^2]

In the case of the standard interface, the following derivatives must be computed as well:

`dRd_dT`	Derivative of `Rd` with respect to T [$\Omega cm^2 K^{-1}$]
`dRd_dTn`	Derivative of `Rd` with respect to T_n [$\Omega cm^2 K^{-1}$]
`dRd_dTp`	Derivative of `Rd` with respect to T_p [$\Omega cm^2 K^{-1}$]
`dRd_dChi`	Derivative of `Rd` with respect to χ [$\Omega cm^2 eV^{-1}$]
`dRd_dEg`	Derivative of `Rd` with respect to E_g [$\Omega cm^2 eV^{-1}$]
`dRd_dEbgn`	Derivative of `Rd` with respect to E_{bgn} [$\Omega cm^2 eV^{-1}$]
`dRd_dNc`	Derivative of `Rd` with respect to N_C [$\Omega cm^{-1} eV^{-1}$]
`dRd_dNv`	Derivative of `Rd` with respect to N_V [$\Omega cm^{-1} eV^{-1}$]
`dRd_dnieff`	Derivative of `Rd` with respect to $n_{i, eff}$ [$\Omega cm^{-1} eV^{-1}$]

Standard C++ Interface

The following base class is declared in the file `PMIModels.h`:

```
class PMI_SchottkyResistanc : public PMI_Vertex_Interface {
public:
   class Input {
      public:
         double t; // lattice temperature
         double tn; // electron temperature
         double tp; // hole temperature
         double affin; // electron affinity
         double Eg; // bandgap
         double Ebgn; // bandgap narrowing
         double nc; // conduction-band effective density of states
         double nv; // valence-band effective density of states
         double nie;  // effective intrinsic density
   };

   class Output {
      public:
         double resist; // Schottky resistance
         double dresistdt; // temperature derivative
         double dresistdtn; // electron temperature derivative
         double dresistdtp; // hole temperature derivative
         double dresistdaffin; // electron affinity derivative
         double dresistdEg; // bandgap derivative
         double dresistdEbgn; // bandgap narrowing derivative
         double dresistdnc; // conduction-band effective state dens derivative
         double dresistdnv; // valence-band effective state dens derivative
         double dresistdnie; // intrinsic carrier density derivative
   };

   PMI_SchottkyResistance (const PMI_Environment& env);
   virtual ~PMI_SchottkyResistance ();

   virtual void compute(const Input& input, Output& output) = 0;
};
```

The following virtual constructor must be implemented:

```
virtual extern "C"
PMI_SchottkyResistance* new_PMI_SchottkyResistance(const PMI_Environment& env)
```

Simplified C++ Interface

The following base class is declared in the file `PMI.h`:

```
class PMI_SchottkyResistance_Base : public PMI_Vertex_Base {
  public:
    class Input : public PMI_Vertex_Input_Base {
    public:
      Input (const PMI_SchottkyResistance_Base* schottkyresist_base,
             const int vertex);
      pmi_float t;  // lattice temperature
      pmi_float tn; // electron temperature
      pmi_float tp; // hole temperature
      pmi_float affin; // electron affinity
      pmi_float Eg; // bandgap
      pmi_float Ebgn; // bandgap narrowing
      pmi_float nc; // conduction-band effective density of states
      pmi_float nv; // valence-band effective density of states
      pmi_float nie;  // effective intrinsic density
    };
    class Output {
      public:
        pmi_float resist;  // Schottky resistance
    };

    PMI_SchottkyResistance_Base (const PMI_Environment& env);

    virtual ~PMI_SchottkyResistance_Base ();

    virtual void compute (const Input& input, Output& output) = 0;
};
```

The following virtual constructor must be implemented:
```
extern "C"
PMI_SchottkyResistance_Base* new_PMI_SchottkyResistance_Base(const
PMI_Environment& env);
```

Example: Built-in Schottky Resistance Model

The following C++ code reimplements the built-in Schottky resistance model (simplified C++ interface):

```
#include <math.h>
#include "PMI.h"

class Builtin_SchottkyResistance: public PMI_SchottkyResistance_Base {
private:
   pmi_float ComputeSchottkyResistance(const Input& input);

public:
   Builtin_SchottkyResistance(const PMI_Environment& env);
   ~Builtin_SchottkyResistance();
   void compute(const Input& input, Output& output);
};

Builtin_SchottkyResistance::
Builtin_SchottkyResistance(const PMI_Environment& env) :
          PMI_SchottkyResistance_Base (env) {}

Builtin_SchottkyResistance::
~Builtin_SchottkyResistance() {}

pmi_float Builtin_SchottkyResistance::
ComputeSchottkyResistance(const Input& input) {
   // Planck's constant divided by 2pi in J*s
   const double h_bar = 1.0545886641968826638371913965e-34;
   // Epsilon 0 in As/Vcm
   const double eps0 = 8.8542e-14;
   // electron charge in C
   const double e0 = 1.602192e-19;
   // electron mass in kg
   const double m0 = 9.109534e-31;
   // Boltzmann constant in J/K
   const double kB = 1.380662e-23;

   pmi_float tempDEV = 300; // K
   pmi_float kT = kB*tempDEV/e0; // energy in eV

   pmi_float dop = input.ReadDoping(PMI_Donor) -
                   input.ReadDoping(PMI_Acceptor);
   pmi_float epsSEM = input.InitModelParameter("epsilon", "Epsilon", 1);
   pmi_float N = (dop > 0) ? dop : -dop;

   double rinf = 0;
```

```
      double PhiB = 0;
      double M = 0;

      if(dop > 0) { // q = -1
         rinf = input.InitModelParameter("Rinf_e","SchottkyResistance",
                                         2.4000e-09);
         PhiB = input.InitModelParameter("PhiB_e", "SchottkyResistance", 0.6);
         M = input.InitModelParameter("mt_e", "SchottkyResistance", 0.19);
      } else { // q = 1
         rinf = input.InitModelParameter("Rinf_h", "SchottkyResistance",
                                         5.2000e-09);
         PhiB = input.InitModelParameter("PhiB_h", "SchottkyResistance", 0.51);
         M = input.InitModelParameter("mt_h", "SchottkyResistance", 0.16);
      }

      pmi_float Rinf = rinf*300/tempDEV;
      pmi_float E00 = h_bar/2.0*100.0*sqrt(N/eps0/epsSEM/M/m0); // eV

      pmi_float E0 = 0;
      if(E00 < kT/100)
         E0 = kT;
      else if(E00 > kT*100)
         E0 = E00;
      else
         E0 = E00*cosh(E00/kT)/sinh(E00/kT);

      return Rinf*exp(PhiB/E0);
}

void Builtin_SchottkyResistance::
compute(const Input& input, Output& output) {
   output.resist = ComputeSchottkyResistance(input);
}


extern "C"
PMI_SchottkyResistance_Base* new_PMI_SchottkyResistance_Base(
    const PMI_Environment& env) {
  return new Builtin_SchottkyResistance(env);
}
```

Ferromagnetism and Spin Transport

The following PMI models for ferromagnetism and spin transport are supported:

- User-Defined Interlayer Exchange Coupling
- User-Defined Bulk or Interface Contributions to the Effective Magnetic Field on page 1298
- User-Defined Magnetostatic Potential Calculation on page 1307

All PMI models for ferromagnetism and spin transport are based on the simplified C++ interface.

User-Defined Interlayer Exchange Coupling

Interfaces of ferromagnetic regions separated by thin paramagnetic layers lead to an interlayer coupling energy density $U_{\text{interlayer}}$ [5]. As usual, the derivative of this energy density with respect to the local magnetization contributes to the effective magnetic field of the LLG equation. In contrast to Eq. 920, p. 810, $U_{\text{interlayer}}$ in this case is a surface energy density, not a volume energy density. The resulting effective magnetic field contribution has units of A rather than A/m; with the observation that $(J/T)/m^2 = A$, this is seen to correspond simply to a surface density of magnetic dipoles.

The theory of interlayer exchange is well developed (for example, [6]). It explains why interlayer exchange oscillates between ferromagnetic and anti-ferromagnetic behavior as a function of the paramagnetic spacer thickness, and it establishes a clear link between oscillation periods present in this thickness dependency and *critical spanning vectors* of the Fermi surface of the spacer material. Despite this, the quantitative prediction of the interaction remains difficult even in ideal thin film stacks. Structural non-idealities (such as surface roughness) can cause additional complexity such as the emergence of bi-quadratic terms in the coupling energy, which favor orthogonal alignment of the magnetization directions in the ferromagnetic regions. Therefore, the most appropriate functional form for describing the coupling strength may depend on the particular use case. For this reason, it was decided to provide a generic infrastructure for assembling interlayer exchange contributions into the LLG equation, but to leave the choice of the particular expression to assemble on the *interlayer exchange edges* to users.

Syntax of Command File and Parameter File

An interlayer exchange PMI is activated for a particular interface by adding the following line to the corresponding interface `Physics` section of the command file:

```
Magnetism(InterlayerExchange(PMImodel=<name>))
```

If the PMI model uses named model parameters (for example, by calling `InitParameter()`), the parameters are read from the interface-specific section of the parameter file.

Base Class for Interlayer Exchange PMIs

PMI models for the interlayer exchange terms of the LLG equation are derived from the base class `PMI_LLGInterlayerExchange_Base`, which has the following definition:

```
//! Base-class for interlayer exchange terms the LLG equation
class PMI_LLGInterlayerExchange_Base : public PMI_Device_Base {
public:
   class Input : public PMI_Device_Input_Base {
   public:
      //! Constructor
      Input(const PMI_Device_Base*);
      pmi_float m_loc[3]; ///< magnetization dir. at the local end of the edge
      pmi_float m_rem[3]; ///< magnetization dir. at the remote end of the edge
      pmi_float length;   ///< the length of the interlayer exchange edge [m]
   };
   class Output {
   public:
      Output(const PMI_Device_Base *base);

      //! Derivative of surface energy density w.r.t. to local magnetization
      pmi_float dU_by_dmloc[3];
   };

   PMI_LLGInterlayerExchange_Base (const PMI_Device_Environment& env);
   virtual ~PMI_LLGInterlayerExchange_Base ();
   virtual void compute (const Input& input, Output& output) = 0;
};
```

The PMI implementer must provide the function:

```
compute(const Input& input, Output& output)
```

Here, `compute()` is called once for each interlayer exchange edge, and the `input` object contains the magnetization directions at the local and remote ends of the edge (as Cartesian unit vectors) as well as the layer thickness (in meter).

The function writes the gradient of the interlayer-exchange energy density with respect to the local magnetization direction into the `dU_by_dmloc` field of the `output` object (unit: J/m^2).

Example: ILE Model With a Simple Oscillatory Thickness Dependency

This model implements an interlayer exchange (ILE) surface energy density of the form $U_{\text{interlayer}} = J_1(t)\vec{m}_{\text{loc}} \cdot \vec{m}_{\text{rem}}$.

For the thickness-dependent coupling strength $J_1(t)$, a phase-shifted sine function with a t^{-2} envelope is assumed:

$$J_1(t) = J_0 \sin\left(\frac{2\pi t}{\Lambda} + \delta\right)/t^2 \tag{1285}$$

Here, t (in Å) is the spacer thickness, and Λ (in Å) is the oscillation period. Instead of the rather inconvenient parameters J_0 and δ, users are expected to supply the coupling strength J_{max} (in mJ/m^2) at the first anti-ferromagnetic peak of $J_1(t)$ and the thickness t_{max} (in Å) at which this maximum occurs.

Implementation of the Simple Interlayer Exchange PMI

To implement the simple interlayer exchange PMI model, you must declare a derived class:

```
#include "PMI.h"
#include <cmath>

class InterlayerExchange_sinD_over_D2 : public PMI_LLGInterlayerExchange_Base
{
public:
    InterlayerExchange_sinD_over_D2(const PMI_Device_Environment &env);
    void compute(const Input &input, Output &output);

    // Auxiliary function for thickness dependence of coupling strength
    inline pmi_float func(const pmi_float &x, const pmi_float &shift) {
        return sin(x + shift) / (x * x);
    }
private:
    double Jmax;        ///< Coupling strength at first AF peak [mJ/m^2]
    double tmax;        ///< Position of first peak [Aangstroem]
    double Lambda;      ///< Period of oscillation [Aangstroem]
    pmi_float delta;    ///< Phase shift to move first AF peak to tmax
    pmi_float scale;    ///< Scaling factor to scale first AF peak to Jmax
};
```

The constructor of the derived class reads the model parameters from the .par file and determines the phase shift and the prefactor in $J_1(t)$ from J_{max} and t_{max}.

```
InterlayerExchange_sinD_over_D2::
InterlayerExchange_sinD_over_D2(const PMI_Device_Environment &env)
: PMI_LLGInterlayerExchange_Base(env)
{
```

```
Jmax   = InitParameter("Jmax", 0.0);   // unit: [mJ/m^2]
Lambda = InitParameter("Lambda", 0.0); // unit: [Aangstroem]
tmax   = InitParameter("tmax", 0.0);   // unit: [Aangstroem]

// adjust delta and scale to position the first peak at (tmax, Jmax)
pmi_float tmax_scaled = tmax * 2 * M_PI / Lambda;
delta = M_PI - tmax_scaled + atan(0.5 * tmax_scaled);
scale = 1.0 / func(tmax_scaled, delta);
}
```

The `compute()` function computes $\vec{\nabla}_{\vec{m}_{\mathrm{loc}}} U_{\mathrm{interlayer}} = J_1(t)\vec{m}_{\mathrm{rem}}$ for a single interlayer exchange edge (note the unit conversion factors):

```
compute(const Input &input, Output &output) {
   pmi_float scaled_distance = 1e10 * input.length * 2*M_PI / Lambda;
   pmi_float f = -1e-3 * scale * Jmax * func(scaled_distance, delta);
   output.dU_by_dmloc[0] = f * input.m_rem[0];
   output.dU_by_dmloc[1] = f * input.m_rem[1];
   output.dU_by_dmloc[2] = f * input.m_rem[2];
}
```

Finally, you must provide a so-called virtual constructor function that allocates a variable of the new class:

```
extern "C"
PMI_LLGInterlayerExchange_Base*
new_PMI_LLGInterlayerExchange_Base(const PMI_Device_Environment& env) {
   return new InterlayerExchange_sinD_over_D2(env);
}
```

NOTE   This function must have C linkage and exactly the same name as declared in the `PMI.h` header file.

NOTE   If `Magnetism(InterlayerExchange)` is specified in the `.cmd` file without providing a PMI model name, Sentaurus Device loads an implementation of the above model as the default ILE model. For the purpose of reading parameters from the `.par` file, the model name `InterlayerExchange` is used.

User-Defined Bulk or Interface Contributions to the Effective Magnetic Field

The base class `PMI_LLGHeff_Base` has been provided for assembling extra generic contributions to the effective magnetic field in bulk regions (unit: A/m) or on interfaces (unit: A).

Syntax of Command File and Parameter File

PMIs for generic bulk or interface $\vec{H}_{\text{eff}}$ contributions are activated by adding the following line to the corresponding region or interface `Physics` sections of the command file:

```
LLG(HEff("<name1>" ["<name2>" ...]))
```

Contributions from all selected models are added during assembly.

Model parameters (if any) are taken from the appropriate region-specific or interface-specific sections of the `.par` file.

Base Class for Generic Bulk or Interface for Effective Magnetic Field PMIs

PMI models for generic bulk or interface $\vec{H}_{\text{eff}}$ contributions are derived from the base class `PMI_LLGHeff_Base`:

```
//! Base-class for local contributions to H_eff in the LLG equation
class PMI_LLGHeff_Base : public PMI_Device_Base {
public:
   class Input : public PMI_Device_Input_Base {
   public:
      //! Constructor
      Input(const PMI_Device_Base*);
      //! Location types for PMI_LLGHeff_Base
      enum locT {
         UNDEFINED_LOCATION, ///< Nothing (only used as initial value)
         DOMAIN_INTERFACE,   ///< Subset of a mesh interface (METIS domain)
         MESH_INTERFACE,     ///< Full mesh interface
         DOMAIN_BULK,        ///< Subset of a mesh bulk region (METIS domain)
         BULK                ///< Full mesh bulk region
      };
      locT locationType;   ///< Specifies how to interpret the vertex list
      int interfaceIndex;  ///< Mesh interface index (or -1 if called for bulk)
```

```
      //! Bulk region index; valid both during bulk and interface assembly.
      /**
       * For interface terms, this can be used to distinguish between
       * interior and exterior normal vectors: if \a regionIndex is equal to
       * region1 of the mesh interface, the vector returned by
       * ReadAveragedNormalVectorAtInterfaceVertex points away from region
       * \a regionIndex; otherwise it points into region \a regionIndex.
       */
      int regionIndex;

      //! \a vertexList is only used for DOMAIN_INTERFACE and DOMAIN_BULK
      /**
       * \a locationType determines how bulk vertex indices for assembly are
       * obtained:
       *
       * DOMAIN_INTERFACE:
       *   Mesh()->regioninterface((interfaceIndex)
       *         ->vertex([vertexList[i])->index()
       *   i = 0, ..., vertexList->size())-1
       * MESH_INTERFACE:
       *   Mesh()->regioninterface(interfaceIndex)->vertex(i)->index()
       *   i = 0, ..., Mesh()->regioninterface(locationIndex)->size_vertex()-1
       * DOMAIN_BULK:
       *   Mesh()->region(locationIndex)->vertex(vertexList[i])->index()
       *   i = 0, ..., vertexList->size())-1
       * BULK:
       *   Mesh()->region(locationIndex)->vertex(i)->index()
       *   i = 0, ..., Mesh()->region(locationIndex)->size_vertex()-1
       */
    const std::vector<int> *vertexList;
}; //end of class PMI_LLGHeffBase::Input

class Output {
public:
    Output(const PMI_Device_Base *base);
    sdevice_pmi_float_vector Hx;  // x-component of Heff at each vertex
    sdevice_pmi_float_vector Hy;  // y-component of Heff at each vertex
    sdevice_pmi_float_vector Hz;  // z-component of Heff at each vertex
};

PMI_LLGHeff_Base (const PMI_Device_Environment& env);
virtual ~PMI_LLGHeff_Base ();
virtual void compute (const Input& input, Output& output) = 0;
```

```
      //! Get averaged normal vector for interface vertex
      /**
       *  @param[in] i - interface index
       *  @param[in] v - interface vertex index on \a i
       *  @returns pointer to the coordinates of the normal vector
       */
      const double *
         ReadAveragedNormalVectorAtInterfaceVertex(int i, int v);
      //! Read SaturationMagnetization for region ri
      double ReadSaturationMagnetization(int ri);
   };
```

The PMI implementer must provide the function:

```
compute(const Input& input, Output& output)
```

This function is called once per parallel (bulk or interface) domain of the device, and the `compute()` function is expected to provide values for the `Hx`, `Hy`, and `Hz` fields of the `output` object at each global vertex in the current domain.

Example: Exchange Bias

Typical anisotropy models do not distinguish between $\vec{m}$ and $-\vec{m}$. Interfaces between ferromagnetic and anti-ferromagnetic layers, however, may break the symmetry between parallel and anti-parallel alignment of the magnetization directions on either side of the interface. This effect is known as *exchange bias*, which can be described by an interface contribution to $\vec{H}_{\text{eff}}$ of the form $I_{\text{bias}}\vec{d}_{\text{bias}}$, where:

- I_{bias} (`I_bias` in the .par file) describes the strength of the exchange bias (unit: A, corresponding to an interface density of magnetic dipoles as discussed above).
- $\vec{d}_{\text{bias}}$ (`biasDir` in the .par file) is the bias direction.

Positive values of I_{bias} correspond to the case that favors alignment of the magnetization at the surface of the ferromagnetic layer parallel to $\vec{d}_{\text{bias}}$.

Implementation of the Exchange Bias PMI

To implement the exchange bias model, you must declare a derived class:

```
#include <PMI.h>
#include <cmath>
class PMI_ExchangeBias : public PMI_LLGHeff_Base {
public:
   PMI_ExchangeBias(const PMI_Device_Environment& env);
   void computeForInterfaceVertex(int ii, int ivi,
                                  PMI_LLGHeff_Base::Output &out);
```

```
      void compute(const PMI_LLGHeff_Base::Input &in,
                   PMI_LLGHeff_Base::Output &out);
  private:
     std::vector<double> biasDir;  ///< direction of the bias field (normalized)
     double Ibias; ///< J/T / m^2 = A (surface density of magnetic dipoles)
};
```

The constructor of the derived class reads the model parameters from the .par file:

```
PMI_ExchangeBias::PMI_ExchangeBias(const PMI_Device_Environment& env)
: PMI_LLGHeff_Base(env), biasDir(3)
{
   Ibias = InitParameter("I_bias", 0.0);
   InitParameter("biasDir", biasDir);
   if (biasDir.size() != 3) {
      printf("PMI model ExchangeBias --- biasDir must be a 3D vector!\n");
      exit(1);
   }
   // convert biasDir to unit vector
   double length = std::sqrt(biasDir[0] * biasDir[0] +
                             biasDir[1] * biasDir[1] +
                             biasDir[2] * biasDir[2]);
   if (length == 0) {
      printf("PMI model ExchangeBias --- "
             "biasDir must be a non-zero 3D vector!\n");
      exit(1);
   }
   biasDir[0] /= length;
   biasDir[1] /= length;
   biasDir[2] /= length;
}
```

During model evaluation, Sentaurus Device calls the compute() function. Exchange bias is an interface effect. Therefore, in.locationType must refer to an interface; other location types are rejected:

```
void PMI_ExchangeBias::compute(const PMI_LLGHeff_Base::Input &in,
                               PMI_LLGHeff_Base::Output &out)
{
  switch(in.locationType) {
  case PMI_LLGHeff_Base::Input::DOMAIN_INTERFACE:
     if (!in.vertexList) {
       printf("PMI_ExchangeBias on DOMAIN_INTERFACE needs a vertexList!\n");
       exit(1);
     }
     for (int i = 0; i < in.vertexList->size(); i++) {
       computeForInterfaceVertex(in.interfaceIndex,(*in.vertexList)[i], out);
     }
     break;
```

```
    case PMI_LLGHeff_Base::Input::MESH_INTERFACE:
      {
        size_t n = Mesh()->regioninterface(in.interfaceIndex)->size_vertex();
        for (size_t i = 0; i < n; i++) {
            computeForInterfaceVertex(in.interfaceIndex, i, out);
        }
      }
      break;
    default:
      printf("PMI_ExchangeBias does not support locationType=%d\n",
             in.locationType);
      exit(1);
    }
  }
```

The calculation for each selected interface vertex is performed by the function `computeForInterfaceVertex(ii, vi, &out)`, where `ii` denotes the index of the current mesh interface, and `vi` is the vertex index relative to this interface. The `out` object provides storage for the resulting effective magnetic field:

```
  void PMI_ExchangeBias::computeForInterfaceVertex(int ii, int ivi,
                                                      PMI_LLGHeff_Base::Output &out)
  {
     const des_mesh *mesh = Mesh();
     const des_regioninterface* interface = Mesh()->regioninterface(ii);
     size_t bulk_vi = interface->vertex(ivi)->index();
     // Unit of surface effective magnetic field: A (not A/m as in bulk)
     out.Hx[bulk_vi] = Ibias * biasDir[0];
     out.Hy[bulk_vi] = Ibias * biasDir[1];
     out.Hz[bulk_vi] = Ibias * biasDir[2];
  }
```

Finally, you must provide a so-called virtual constructor function, which allocates a variable of the new class:

```
  extern "C"
  PMI_LLGHeff_Base* new_PMI_LLGHeff_Base(const PMI_Device_Environment& env) {
     return new PMI_ExchangeBias(env);
  }
```

NOTE   This function must have C linkage and exactly the same name as declared in the `PMI.h` header file.

NOTE   This model is included in the installation of Sentaurus Device under the PMI model name `ExchangeBias`, which corresponds to the C++ file name `ExchangeBias.C`.

Example: Interface Anisotropy

Frequently, an interface between a ferromagnetic material and adjacent materials gives rise to a contribution to the energy density of the magnetic system that favors perpendicular alignment of the magnetization over in-plane alignment. The interface anisotropy model describes this effect in terms of a surface energy density proportional to the square of the scalar product of the magnetization direction $\vec{m}$ and the surface normal direction $\vec{n}$. The resulting effective magnetic field contribution takes the form $-I_{\text{aniso}}\vec{n}(\vec{n} \cdot \vec{m})$ (unit: A, corresponding to an interface density of magnetic dipoles as discussed above). Positive values of I_{aniso} favor an out-of-plane magnetization direction; negative values favor in-plane magnetization.

The interface anisotropy model can describe the transition from in-plane magnetic alignment in magnetic thin films of moderate thickness to perpendicular magnetic alignment in very thin films. For positive I_{aniso} (I_aniso in the .par file, unit: A). there is competition between an effective bulk anisotropy term due to the geometry, which favors in-plane magnetic alignment, and the interface anisotropy, which favors out-of-plane alignment. With decreasing film thickness, the relative importance of the interface term grows. For very thin films, the interface term dominates, resulting in perpendicular magnetic alignment.

Implementation of the Interface Anisotropy PMI

Like the exchange bias model, the interface anisotropy model is derived from `PMI_LLGHeff_Base`:

```
#include <PMI.h>
#include <cmath>

class PMI_InterfaceAnisotropy : public PMI_LLGHeff_Base {
public:
    PMI_InterfaceAnisotropy(const PMI_Device_Environment& env);
    void computeForInterfaceVertex(int ii, int ivi,
                                   PMI_LLGHeff_Base::Output &out);
    void compute(const PMI_LLGHeff_Base::Input &in,
                 PMI_LLGHeff_Base::Output &out);
private:
    double I_aniso;       ///< J/T/m^2 = A (surface density of magnetic dipoles)
    const pmi_float* mx; ///< x-component of magnetization direction
    const pmi_float* my; ///< y-component of magnetization direction
    const pmi_float* mz; ///< z-component of magnetization direction
};
```

Again, the constructor reads the model parameter:

```
PMI_InterfaceAnisotropy::
PMI_InterfaceAnisotropy(const PMI_Device_Environment& env)
: PMI_LLGHeff_Base(env)
{ I_aniso = InitParameter("I_aniso", 0.0); }
```

For the most part, the `compute()` function of the interface anisotropy model is identical to that of the exchange bias model. However, there is one important difference: The effective field of the interface anisotropy model depends on the magnetization density.

Therefore, the `compute()` function of `PMI_InterfaceAnisotropy` must read the magnetization data:

```
void PMI_InterfaceAnisotropy::compute(const PMI_LLGHeff_Base::Input &in,
                                      PMI_LLGHeff_Base::Output &out)
{
    sdevice_data *data = Data();
    mx = data->ReadScalar(sdevice_data::vertex, "MagnetizationDir_x");
    my = data->ReadScalar(sdevice_data::vertex, "MagnetizationDir_y");
    mz = data->ReadScalar(sdevice_data::vertex, "MagnetizationDir_z");
    switch(in.locationType) {
        ... THE REST OF THE FUNCTION AS IN PMI_ExchangeBias ...
    }
}
```

The `computeForInterfaceVertex()` function handles the calculation of the scalar product between the surface normal vector and the magnetization direction. Note how the components of the magnetization vector `m[]` are set from the `mx`, `my`, and `mz` components. This provides the correct (local) derivatives of the effective field contribution to the LLG equation:

```
void
PMI_InterfaceAnisotropy::
computeForInterfaceVertex(int ii, int ivi, PMI_LLGHeff_Base::Output &out)
{
    const des_mesh *mesh = Mesh();
    const des_regioninterface* interface = Mesh()->regioninterface(ii);
    size_t bulk_vi = interface->vertex(ivi)->index();
    const double *n = ReadAveragedNormalVectorAtInterfaceVertex(ii, ivi);

    pmi_float m[3];
    m[0] = pmi_float(mx[bulk_vi].get_value<double>(), 3, 0);
    m[1] = pmi_float(my[bulk_vi].get_value<double>(), 3, 1);
    m[2] = pmi_float(mz[bulk_vi].get_value<double>(), 3, 2);

    pmi_float dot_prod = n[0] * m[0] + n[1] * m[1] + n[2] * m[2];

    // Unit of surface effective magnetic field: A (not A/m as in bulk)
    out.Hx[bulk_vi] = -I_aniso * dot_prod * n[0];
    out.Hy[bulk_vi] = -I_aniso * dot_prod * n[1];
    out.Hz[bulk_vi] = -I_aniso * dot_prod * n[2];
}
```

The implementation is completed by the definition of the virtual constructor:

```
extern "C"
PMI_LLGHeff_Base* new_PMI_LLGHeff_Base(const PMI_Device_Environment& env) {
   return new PMI_InterfaceAnisotropy(env);
}
```

NOTE   This model is included in the installation of Sentaurus Device under the
PMI model name `InterfaceAnisotropy`.

Example: Local Demagnetizing Field

This model implements a local expression for the demagnetizing field in terms of a diagonal
demagnetizing tensor $\underline{N} = \mathrm{diag}(N_x, N_y, N_z)$: $\vec{H}_{\mathrm{eff,\,demag}} = -\underline{N}\vec{M} = -M_{\mathrm{sat}}\underline{N}\vec{m}$.

Implementation of the Local Demagnetizing Field PMI

The model is derived from the base class `PMI_LLGHeff_Base`:

```
#include <PMI.h>
class LocalDemagnetizingField : public PMI_LLGHeff_Base {
public:
   LocalDemagnetizingField(const PMI_Device_Environment& env);
   void computeForBulkVertex(int ri, int vi, PMI_LLGHeff_Base::Output &out);
   void compute(const PMI_LLGHeff_Base::Input &in,
                PMI_LLGHeff_Base::Output &out);
private:
   const pmi_float* mx; ///< x-component of magnetization direction
   const pmi_float* my; ///< y-component of magnetization direction
   const pmi_float* mz; ///< z-component of magnetization direction
   double Nx; /// demagnetizing factor along x-axis
   double Ny; /// demagnetizing factor along y-axis
   double Nz; /// demagnetizing factor along z-axis
};
```

As usual, the constructor of the derived class reads the model parameters from the `.par` file:

```
LocalDemagnetizingField::
LocalDemagnetizingField(const PMI_Device_Environment& env)
: PMI_LLGHeff_Base(env)
{
   Nx = InitParameter("Nx", 0.0);
   Ny = InitParameter("Ny", 0.0);
   Nz = InitParameter("Nz", 0.0);
}
```

In contrast to the exchange bias model and the interface anisotropy model, the local demagnetizing field model implements a bulk contribution to the effective magnetic field. Consequently, the `compute()` function now requires `in.locationType` to refer to a bulk region or domain:

```
void LocalDemagnetizingField::compute(const PMI_LLGHeff_Base::Input &in,
                                             PMI_LLGHeff_Base::Output &out)
{
    // Get magnetization direction
    sdevice_data *data = Data();
    mx = data->ReadScalar(sdevice_data::vertex, "MagnetizationDir_x");
    my = data->ReadScalar(sdevice_data::vertex, "MagnetizationDir_y");
    mz = data->ReadScalar(sdevice_data::vertex, "MagnetizationDir_z");

    switch(in.locationType) {
    case PMI_LLGHeff_Base::Input::DOMAIN_BULK:
      if (!in.vertexList) {
       printf("LocalDemagnetizingField on DOMAIN_BULK needs a vertexList!\n");
       exit(1);
      }
      for (size_t i = 0; i < (*in.vertexList).size(); i++) {
          computeForBulkVertex(in.regionIndex, (*in.vertexList)[i], out);
      }
      break;
    default:
      printf("LocalDemagnetizingField does not support locationType=%d\n",
              in.locationType);
      exit(1);
    }
}
```

The evaluation of the effective magnetic field contribution at each bulk node is handled by the `computeForBulkVertex(ri, vi, &out)` function. The argument `ri` is the region index, and the argument `vi` is the global vertex index of the evaluation point. The region index is needed to query the saturation magnetization:

```
void
LocalDemagnetizingField::computeForBulkVertex(int ri, int vi,
                                                PMI_LLGHeff_Base::Output &out)
{
    pmi_float m[3];
    m[0] = pmi_float(mx[vi].get_value<double>(), 3, 0);
    m[1] = pmi_float(my[vi].get_value<double>(), 3, 1);
    m[2] = pmi_float(mz[vi].get_value<double>(), 3, 2);

    double Msat = ReadSaturationMagnetization(ri);
```

```
    // Effective magnetic field A/m
    out.Hx[vi] = -Nx * Msat * m[0];
    out.Hy[vi] = -Ny * Msat * m[1];
    out.Hz[vi] = -Nz * Msat * m[2];
}
```

Finally, the virtual constructor must be defined:

```
extern "C"
PMI_LLGHeff_Base* new_PMI_LLGHeff_Base(const PMI_Device_Environment& env) {
    return new LocalDemagnetizingField(env);
}
```

> **NOTE**   This model is included in the installation of Sentaurus Device under the
> PMI model name `LocalDemagnetizingField`.

User-Defined Magnetostatic Potential Calculation

For the special case of an effective magnetic field contribution that can be written as the gradient of a magnetostatic potential, $\vec{H}_{\text{longitudinal}} = -\vec{\nabla}\varphi_{\text{max}}$, you can reuse the base class `PMI_LLGHeff_Base` to calculate a magnetostatic potential instead of a magnetic field (see Base Class for Generic Bulk or Interface for Effective Magnetic Field PMIs on page 1298).

In this mode of operation, the `compute()` function does not populate the fields of the `output` object with magnetic field values. Instead, it prepares an array containing the magnetostatic potential for each vertex (unit: $\mu\text{m} \cdot \text{A/m}$) and uses this to set the value of the `MagnetostaticPotential` field by calling the `sdevice_data::WriteScalar()` function.

The resulting magnetostatic potential and the corresponding magnetic field can be plotted like other fields in Sentaurus Device:

```
Plot {
    MagnetostaticPotential
    LongitudinalMagneticField/Element/Vector
}
```

Syntax of Command File and Parameter File

This special mode is activated by adding the following statement to the global `Physics` section of the command file:

```
Magnetism(MagnetostaticPotentialPMI=<name>)
```

Parameters (if any) are read from the global section of the `.par` file, and the `locationType` in the `input` object is set to zero. Instead of being called in parallel for each parallel domain of the device, for the magnetostatic potential calculation, there is only one global call for the entire device. User-defined parallelization, for example, using OpenMP, can be used to accelerate this call.

References

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[2]   P. Y. Yu and M. Cardona, *Fundamentals of Semiconductors: Physics and Materials Properties*, Berlin: Springer, 2nd ed., 1999.

[3]   K. F. Brennan, *The Physics of Semiconductors: With applications to optoelectronic devices*, Cambridge: Cambridge University Press, 1999.

[4]   M. G. Ancona, "Density-gradient theory: a macroscopic approach to quantum confinement and tunneling in semiconductor devices," *Journal of Computational Electronics*, vol. 10, no. 1–2, pp. 65–97, 2011.

[5]   P. Bruno, "Interlayer Exchange Interactions in Magnetic Multilayers," *Magnetism: Molecules to Materials III*, J. S. Miller and M. Drillon (eds.), Wiley-VCH: Weinheim, pp. 329–353, 2002.

[6]   M. D. Stiles, "Interlayer Exchange Coupling," *Ultrathin Magnetic Structures III: Fundamentals of Nanomagnetism*, J. A. C. Bland and B. Heinrich (eds.), Springer: Berlin, pp. 99–142, 2005.

CHAPTER 39 Tcl Interfaces

This chapter discusses the Tcl interfaces that can be used to customize device simulations in Sentaurus Device.

Overview

You can use Tcl scripts to control various aspects of a Sentaurus Device simulation. Tcl scripts can be used in the following circumstances:

- You can use the Tcl interpreter to execute a command file (see Tcl Command File on page 159).

- Tcl expressions are recognized in the context of enhanced spectrum control to compute optical generation (see Enhanced Spectrum Control on page 538).

- A Tcl formula can be used to add data to the current plot file (see Tcl Formulas on page 115).

- The Tcl current plot interface (see Current Plot File on page 1317) represents an alternative to the current plot PMI described in Current Plot File of Sentaurus Device on page 1239.

Mesh-based Tcl interfaces, such as the current plot interface, need access to Sentaurus Device mesh and data. This runtime support is described in Mesh-Based Runtime Support on page 1309.

Mesh-Based Runtime Support

The Tcl runtime environment is accessed through a Tcl pointer `tcl_cp_adr`:

```
upvar #1 tcl_cp_adr tcl_cp_adr
```

When the Tcl pointer `tcl_cp_adr` to the runtime environment has been obtained, you can perform the following operations:

- Read a parameter from the command file:

```
$tcl_cp_adr InitParameter $name $defaultvalue
```

- Read a string parameter from the command file:

```
$tcl_cp_adr InitStringParameter $name $defaultvalue
```

- Read the time in seconds during transient simulations:

      $tcl_cp_adr ReadTime

- Read the step size in seconds during transient simulations:

      $tcl_cp_adr ReadTransientStepSize

- Read the step type during transient simulations:

      $tcl_cp_adr ReadTransientStepType

  Returns either $::PMI_UndefStepType, $::PMI_TR, $::PMI_BDF, or $::PMI_BE.

- Read pointer to the Sentaurus Device mesh (see Device Mesh on page 1310):

      set mesh [$tcl_cp_adr Mesh]

- Read pointer to the Sentaurus Device data (see Device Data on page 1315):

      set data [$tcl_cp_adr Data]

Device Mesh

Use a pointer to the Sentaurus Device mesh for the following operations:

- Dimension of mesh:

      $mesh dim

- Read element (i, j) of reference coordinate system, where $0 \le i, j < \dim$:

      $mesh ref_coordinates $i $j

- Number of vertices:

      $mesh size_vertex

- Number of element vertices:

      $mesh size_element_vertex

- Read pointer to vertex i :

      set vertex [$mesh vertex $i]

- Number of edges:

      $mesh size_edge

- Read pointer to edge i :

      set edge [$mesh edge $i]

- Number of elements:

      $mesh size_element

■ Read pointer to element i:

    set element [$mesh element $i]

■ Number of regions:

    $mesh size_region

■ Read pointer to region i:

    set region [$mesh region $i]

■ Number of region interfaces:

    $mesh size_regioninterface

■ Read pointer to region interface i:

    set regioninterface [$mesh regioninterface $i]

Vertex

Use a pointer to a vertex for the following operations:

■ Read index to access vertex data:

    $vertex index

■ Read index to access element–vertex data:

    $vertex element_vertex_index $element

■ Read coordinates:

    $vertex coord $d

The value of d determines the component, $0 \le d < \dim$.

■ Determine whether this vertex has the same coordinates as vertex v:

    $vertex equal_coord $v

■ Number of edges connected to this vertex:

    $vertex size_edge

■ Read pointer to edge i:

    set edge [$vertex edge $i]

■ Number of elements connected to this vertex:

    $vertex size_element

■ Read pointer to element i:

    set element [$vertex element $i]

■ Number of regions connected to this vertex:

    $vertex size_region

- Read pointer to region *i*:

  ```
  set region [$vertex region $i]
  ```

- Number of region interfaces connected to this vertex:

  ```
  $vertex size_regioninterface
  ```

- Read pointer to region interface *i*:

  ```
  set regioninterface [$vertex regioninterface $i]
  ```

Edge

Use a pointer to an edge for the following operations:

- Read index to access edge data:

  ```
  $edge index
  ```

- Read pointer to first vertex of edge:

  ```
  set vertex [$edge start]
  ```

- Read pointer to second vertex of edge:

  ```
  set vertex [$edge end]
  ```

- Number of elements connected to this edge:

  ```
  $edge size_element
  ```

- Read pointer to element *i*:

  ```
  set element [$edge element $i]
  ```

- Number of regions containing edge:

  ```
  $edge size_region
  ```

- Read pointer to region *i*:

  ```
  set region [$edge region $i]
  ```

Element

Use a pointer to an element for the following operations:

- Read index to access element data:

  ```
  $element index
  ```

- Read type of element:

  ```
  $element type
  ```

  Returns one of the following values:

  ```
  $::des_element_point
  $::des_element_line
  $::des_element_triangle
  $::des_element_rectangle
  $::des_element_tetrahedron
  $::des_element_pyramid
  $::des_element_prism
  $::des_element_cuboid
  $::des_element_tetrabrick
  ```

- Number of vertices in element:

  ```
  $element size_vertex
  ```

- Read pointer to vertex i:

  ```
  set vertex [$element vertex $i]
  ```

- Number of edges connected to this element:

  ```
  $element size_edge
  ```

- Read pointer to edge i:

  ```
  set edge [$element edge $i]
  ```

- Read pointer to bulk region containing element:

  ```
  set bulk [$element bulk]
  ```

- Start index for element–vertex data in element:

  ```
  $element element_vertex_offset
  ```

Region

Use a pointer to a region for the following operations:

- Read index:

  ```
  $region index
  ```

- Read type of region:

  ```
  $region type
  ```

  Returns either `$::des_region_bulk` or `$::des_region_contact`.

- Read name of region:

  ```
  $region name
  ```

- Number of vertices in region:

      $region size_vertex

- Read pointer to vertex *i* :

      set vertex [$region vertex $i]

- Number of edges in region:

      $region size_edge

- Read pointer to edge *i* :

      set edge [$region edge $i]

Use the following functions to convert a pointer to a region into a pointer to a bulk region or a contact:

    set bulk [tcl_cp_region2bulk $region]
    set contact [tcl_cp_region2contact $region]

A pointer to a bulk region supports the following additional operations:

- Read material of region:

      $bulk material

- Number of elements in region:

      $bulk size_element

- Read pointer to element *i* :

      set element [$bulk element $i]

- Number of region interfaces in region:

      $bulk size_regioninterface

- Read pointer to region interface *i* :

      set regioninterface [$bulk regioninterface $i]

Region Interface

Use a pointer to a region interface for the following operations:

- Read index:

      $regioninterface index

- Read pointer to first bulk region connected to region interface:

      set bulk [$regioninterface bulk1]

- Read pointer to second bulk region connected to region interface:

      set bulk [$regioninterface bulk2]

- Determine whether this region interface is a heterointerface:

  ```
  $regioninterface is_heterointerface
  ```

- Number of vertices in region interface:

  ```
  $regioninterface size_vertex
  ```

- Read pointer to vertex *i*:

  ```
  set vertex [$regioninterface vertex $i]
  ```

- Read index to access data stored on region interface vertex *i*:

  ```
  $regioninterface index $i
  ```

Device Data

Use a pointer to the Sentaurus Device data for the following operations:

- Dimension of mesh:

  ```
  $data dim
  ```

- Read pointer to box method coefficients (2D array, C++ data type `double**`):

  ```
  set coefficient [$data ReadCoefficient]
  ```

- Read pointer to box method measures (2D array, C++ data type `double**`):

  ```
  set measure [$data ReadMeasure]
  ```

- Read pointer to box method surface measures (2D array, C++ data type `double**`):

  ```
  set surfacemeasure [$data ReadSurfaceMeasure]
  ```

- Read pointer to scalar data (1D array, C++ data type `double*`):

  ```
  set scalar [$data ReadScalar $location $name]
  ```

- Read pointer to vector data (2D array, C++ data type `double**`):

  ```
  set vector [$data ReadVector $location $name]
  ```

- Write scalar data (1D array, C++ data type `double*`):

  ```
  $data WriteScalar $location $name $newvalue
  ```

- Read pointer to gradient (2D array, C++ data type `double**`):

  ```
  set gradient [$data ReadGradient $location $name]
  ```

- Read pointer to flux (1D array, C++ data type `double*`):

  ```
  set flux [$data ReadFlux $location $name]
  ```

- Electron distribution from SHE method:

  ```
  $data ReadeSHEDistribution $bulk $vertex $energy
  ```

- Hole distribution from SHE method:

    ```
    $data ReadhSHEDistribution $bulk $vertex $energy
    ```

- Electron density-of-states from SHE method:

    ```
    $data ReadeSHETotalDOS $bulk $energy
    ```

- Hole density-of-states from SHE method:

    ```
    $data ReadhSHETotalDOS $bulk $energy
    ```

- Electron group velocity from SHE method:

    ```
    $data ReadeSHETotalGSV $bulk $energy
    ```

- Hole group velocity from SHE method:

    ```
    $data ReadhSHETotalGSV $bulk $energy
    ```

The following values are recognized for `$location`:

```
$::des_data_vertex
$::des_data_edge
$::des_data_element
$::des_data_rivertex
$::des_data_element_vertex
```

See for the names of scalar and vector data.

One-Dimensional Arrays

Use the following function to allocate a one-dimensional array (C++ data type `double*`):

```
set v1 [tcl_cp_new_double $size]
```

Use the following function to read an element of a one-dimensional array (C++ data type `double*`):

```
set value [tcl_cp_get_double $v1 $index]
```

Use the following function to write an element of a one-dimensional array (C++ data type `double*`):

```
tcl_cp_set_double $v1 $index $value
```

Use the following function to deallocate a one-dimensional array (C++ data type `double*`):

```
tcl_cp_delete_double $v1
```

Two-Dimensional Arrays

Use the following function to read an element of a two-dimensional array (C++ data type `double**`):

```
set value [tcl_cp_get_double2 $v2 $index1 $index2]
```

Current Plot File

The current plot Tcl interface can be used to add new entries to the current plot file. It is functionally equivalent to the current plot PMI described in Current Plot File of Sentaurus Device on page 1239. The required Tcl code must be specified through a `tcl` statement in the `CurrentPlot` section:

```
CurrentPlot {
    Tcl (tcl = "source CurrentPlot.tcl"  par1 = <value>  par2 = <value>)
}
```

In this example, the Tcl code is stored in the file `CurrentPlot.tcl`. If necessary, the model parameters (`par1` and `par2` in this example) can be specified as well.

Tcl Functions

Users must define Tcl functions for the following purposes:

- `tcl_cp_constructor`: Constructor
- `tcl_cp_destructor`: Destructor (optional)
- `tcl_cp_Compute_Dataset_Names`: Compute a list of dataset names for the header of the current plot file
- `tcl_cp_Compute_Function_Names`: Compute a list of function names for the header of the current plot file
- `tcl_cp_Compute_Plot_Values`: Evaluate the current plot values

These Tcl procedures must implement the same functionality as the corresponding methods of the C++ class `PMI_CurrentPlot` (see Current Plot File of Sentaurus Device on page 1239). The Tcl interpreter also has access to runtime support functions and the entire Sentaurus Device mesh and data fields (see Mesh-Based Runtime Support on page 1309).

tcl_cp_constructor

The constructor is invoked once at the beginning of each Tcl current plot statement:

```
proc tcl_cp_constructor {} {
   upvar #1 tcl_cp_adr tcl_cp_adr
   ...
}
```

Note that all the current plot Tcl procedures are executed in their own Tcl namespace. This ensures that multiple Tcl current plot statements can be active simultaneously, and they all operate in their own private namespace. Use the Tcl `upvar` command to access variables in this namespace.

As explained in Mesh-Based Runtime Support on page 1309, the Tcl pointer `tcl_cp_adr` provides access to the Sentaurus Device mesh and data:

```
set mesh [$tcl_cp_adr Mesh]
set data [$tcl_cp_adr Data]
```

The constructor also can be used to precompute data that will be needed later to evaluate the current plot values.

tcl_cp_destructor

This optional procedure can be used to deallocate data structures, or to print statistical output:

```
proc tcl_cp_destructor {} {
}
```

tcl_cp_Compute_Dataset_Names

This procedure must return a Tcl list of dataset names, for example:

```
proc tcl_cp_Compute_Dataset_Names {} {
   lappend result "channel eConductivity"
   return $result
}
```

Multiple dataset names are supported.

tcl_cp_Compute_Function_Names

This procedure must return a Tcl list of function names, for example:

```
proc tcl_cp_Compute_Function_Names {} {
    lappend result "Conductivity"
    return $result
}
```

The number of function names must be identical to the number of dataset names created by `tcl_cp_Compute_Dataset_Names`.

tcl_cp_Compute_Plot_Values

This procedure must return a Tcl list of current plot values. Use the access functions to the Sentaurus Device mesh and data (see Mesh-Based Runtime Support on page 1309) to compute these values:

```
proc tcl_cp_Compute_Plot_Values {} {
    ...
    lappend result 0.0
    return $result
}
```

The number of result values must be identical to the number of dataset names created by `tcl_cp_Compute_Dataset_Names`.

Example

The following example computes the average of the electron conductivity $\sigma_n = qn\mu_n$ in a region. This example also can be found in the directory `$STROOT/tcad/$STRELEASE/lib/sdevice/src/tcl_currentplot`:

```
proc tcl_cp_constructor {} {
    # link to variables in enclosing namespace
    upvar #1 tcl_cp_adr tcl_cp_adr
    upvar #1 Conductivity_Region Conductivity_Region

    set Conductivity_Region \
        [$tcl_cp_adr InitStringParameter "Conductivity_Region" ""]
}

proc tcl_cp_destructor {} {
}
```

```
proc tcl_cp_Compute_Dataset_Names {} {
   upvar #1 Conductivity_Region Conductivity_Region
   lappend result "Tcl_Ave_$Conductivity_Region eConductivity"
   return $result
}

proc tcl_cp_Compute_Function_Names {} {
   lappend result "Conductivity"
   return $result
}

proc tcl_cp_Compute_Plot_Values {} {
   # link to variables in enclosing namespace
   upvar #1 tcl_cp_adr tcl_cp_adr
   upvar #1 Conductivity_Region Conductivity_Region

   set mesh [$tcl_cp_adr Mesh]
   set data [$tcl_cp_adr Data]
   set measure [$data ReadMeasure]

   set q 1.602e-19
   set eDensity [$data ReadScalar $::des_data_vertex "eDensity"]
   set eMobility [$data ReadScalar $::des_data_vertex "eMobility"]

   set sum 0.0
   set sum_m 0.0

   set size_region [$mesh size_region]
   for {set ri 0} {$ri < $size_region} {incr ri} {
      set region [$mesh region $ri]
      if {[$region type] == $::des_region_bulk && \
            [$region name] == $Conductivity_Region} {
         set bulk [tcl_cp_region2bulk $region]
         set size_element [$bulk size_element]
         for {set ei 0} {$ei < $size_element} {incr ei} {
            set element [$bulk element $ei]
            set element_index [$element index]
            set size_vertex [$element size_vertex]
            for {set vi 0} {$vi < $size_vertex} {incr vi} {
               set vertex [$element vertex $vi]
               set vertex_index [$vertex index]

               set n [tcl_cp_get_double $eDensity $vertex_index]
               set mu [tcl_cp_get_double $eMobility $vertex_index]
               set value [expr "$q * $n * $mu"]
```

```
                set m [tcl_cp_get_double2 $measure $element_index $vi]
                set sum [expr "$sum + $m * $value"]
                set sum_m [expr "$sum_m + $m"]
            }
        }
    }
}

if {$sum_m == 0} {
    set average 0
} else {
    set average [expr "$sum / $sum_m"]
}

lappend result $average
}
```

Part VI Appendices

This part of the *Sentaurus™ Device User Guide* contains the following appendices:

APPENDIX A Mathematical Symbols

This appendix contains notational conventions and a list of symbols used in the Sentaurus™ Device User Guide.

They are listed alphabetically. Non-Latin characters are sorted according to their English translation.

$/$	Division, right binding: $a/bc = a/(bc)$
$\hat{a}$	Unit (3D) vector
$\vec{a}$	(3D) vector
$|a|$	Absolute value of a scalar
$|\vec{a}|$	Absolute value of a vector $a = |\vec{a}|$
a^{T}	Transpose of a vector or a matrix
a^{-1}	Inverse of function or matrix, reciprocal of a scalar
$\vec{a} \cdot \vec{b}$	Inner (dot) product
$\vec{a} \times \vec{b}$	Vector (cross) product
$\vec{a}\vec{b}$	Dyadic product: $(\vec{a}\vec{b})_{ij} = \vec{a}_i\vec{b}_j$
$\langle ab\bar{c} \rangle$	Miller indices. a, b, and c are digits; a bar over a digit indicates negation applied to that particular digit.
χ	Electron affinity or thermal resistivity
c_{L}	Lattice heat capacity
e	Base of natural logarithm
$\vec{E}$	Electric field
E_{bgn}	Bandgap narrowing
E_{C}	Conduction band energy

$E_{\mathrm{F},n}$	Electron quasi-Fermi energy
$E_{\mathrm{F},p}$	Hole quasi-Fermi energy
E_{g}	Intrinsic band gap
$E_{\mathrm{g,eff}}$	Effective band gap, $E_{\mathrm{g,eff}} = E_{\mathrm{g}} - E_{\mathrm{bgn}}$
E_{V}	Valence band energy
ε	Absolute dielectric constant of a material
ε_0	Dielectric constant of vacuum
$\vec{F}$	Electric field
F_α	Integral of distribution function; for Fermi statistics, Fermi integral of order α
G	Generation rate (does not include recombination)
γ_n	Degeneracy factor for electrons
γ_p	Degeneracy factor for holes
$\hbar$	Planck's constant divided by 2π
i	Imaginary unit, $\mathrm{i}^2 = -1$
Im	Imaginary part
$\vec{J}_{\mathrm{D}}$	Displacement current density
$\vec{J}_{\mathrm{M}}$	Current density in metals
$\vec{J}_n$	Electron current density
$\vec{J}_p$	Hole current density
k	Boltzmann constant
κ_{L}	Lattice thermal conductivity
κ_n	Electron thermal conductivity
κ_p	Hole thermal conductivity

Λ_n	Electron quantum potential
Λ_p	Hole quantum potential
$\ln$	Natural logarithm
m_0	Free electron mass
m_n	Electron density-of-states mass
m_p	Hole density-of-states mass
μ_n	Electron mobility
μ_p	Hole mobility
n	Electron density
$\hat{n}$	Unit normal vector
$N_{A,0}$	Chemically active acceptor concentration
N_A	Ionized acceptor concentration
N_C	Conduction band density-of-states
$N_{D,0}$	Chemically active donor concentration
N_D	Ionized donor concentration
n_i	Intrinsic density (not accounting for bandgap narrowing)
$n_{i,\text{eff}}$	Effective intrinsic density (accounting for bandgap narrowing)
N_i	Ionized dopant concentration, $N_i = N_A + N_D$
n_{se}	Single exciton density
N_{tot}	Total doping concentration, $N_{\text{tot}} = N_{A,0} + N_{D,0}$
N_V	Valence band density-of-states
p	Hole density
$\vec{P}$	Polarization
P_n	Electron thermoelectric power

P_p	Hole thermoelectric power
Φ_M	Metal Fermi potential
Φ_n	Electron quasi-Fermi potential
Φ_p	Hole quasi-Fermi potential
ϕ	Electrostatic potential
q	Elementary charge
r	Anisotropy factor
R	Recombination rate (does not include generation)
R_{net}	Net recombination rate, $R_{net} = R - G$
Re	Real part
$\vec{S}_L$	Lattice heat flux density
$\vec{S}_n$	Electron heat flux density
$\vec{S}_p$	Hole heat flux density
T	Lattice temperature
T_n	Electron temperature
T_p	Hole temperature
τ_n	Electron lifetime
τ_p	Hole lifetime
Θ	Unit step function (0 for negative arguments, 1 for positive arguments)
$\vec{v}_n$	Electron drift velocity
$\vec{v}_p$	Hole drift velocity
$\vec{v}_{sat,n}$	Electron saturation velocity
$\vec{v}_{sat,p}$	Hole saturation velocity

APPENDIX B Syntax

The syntax of the command file of Sentaurus Device, and the basic syntactical and lexical conventions are described here.

Sentaurus Device has a hierarchical input syntax. At the lowest level, `device`, `system`, and `solve` information is specified as well as the default and global parameters. Inside each `Device` section, the parameters specific to one device type can be specified.

Inside the `System` section, the real devices are specified or 'instantiated.' Here, parameters can be given that are specific to one instantiation of a device. The command file is a collection of specifications used to establish the simulation environment with actions describing which equations must be solved and how they must be solved. The syntax of the command file contains several entry types. All basic command file entries adhere to the syntactical and lexical rules described in Table 176.

Table 176   Entry types in Sentaurus Device

Entry type	Description
Keyword	These are the known names of the command file. They are case insensitive. Therefore, the following keywords are all equivalent: `Quasistationary`, `QuasiStationary`, and `quasistationary`. Most keywords can be abbreviated. The above example can also be written as `QuasiStat`.
Integer	These are (possibly) signed decimal numbers. The following integers are valid: `123`, `-73492`, `0`.
Float	Floating point numbers are compatible with the C language format for floating point numbers. The following floating point numbers are valid: `123`, `123.0`, `1.23e2`, `-1.23E2`.
Vector	Vectors in real space are defined depending on the actual dimension. In 3D, a vector is specified by three floating point numbers; in 2D, by two floating point numbers enclosed in parentheses. The floats are separated by commas or spaces. In 1D, one floating point number without parentheses is sufficient. Valid vectors are `(1,0,2)`, `(1e-4,-1e-3)`, and `1`.
String	Strings are delimited by quotation marks. They are compatible with the C language format for strings. The following strings are valid: `"Vdd"`, `"output/diode"`.
Identifier	These are used to name objects such as nodes, devices, or attributes. They are compatible with the C language format for identifiers. The following identifiers are valid: `Vdd`, `diode`, `bjt_345`.
Assignment	These are used to set values to keywords. Therefore, the following are valid assignments: `Digits=4`, `Save="output/diode"`.

Table 176   Entry types in Sentaurus Device (Continued)

Entry type	Description
Signal	Signals are time dependent, piecewise, linear functions (not to be confused with UNIX signals) that are defined as inputs on the contacts of a device. They are specified as follows: (value0 at time0, value1 at time1, …value_n at time_n). The following signal is valid: `(0 at 0, 1 at 10.0e-9, 1 at 20.0e-9).`

List	Lists are collections of keywords, assignments, and complex entries. They are delimited by "(...)" or "{...}". The following lists are valid:
	`{ Number=0 Voltage=0`
	`  Voltage=( 0 at 0, 0 at 2e-8 ) }`
	`{ Method=Super Digits=6 Numerically }`
	`( MinStep=1e-15 InitialStep=1e-10 Digits=3 )`

Structured entries	These are parameterized definitions or commands that can have the forms: `<keyword> {<keywords>}`, `<keyword> (<keywords>)`, or `<keyword> (<list>) {<list>}`.

APPENDIX C File-Naming Conventions

This appendix describes the file-naming conventions for TCAD tools relevant to Sentaurus Device.

File Extensions

All strings that represent file names containing a dot (.) within their base name are taken literally. Otherwise, Sentaurus Device extends the given strings with the appropriate extension.

Sentaurus Device expands the extensions for output files by its tool extension `_des`, for example, the extension of a saved file is `_des.sav`.

During transient, quasistationary, and continuation simulations, the plot and save files are numbered by a global index.

Table 177   Summary of file extensions used in Sentaurus Device

File	I/O	Extension
Command	I	`_des.cmd, .cmd`
Log	O	`_des.log`
Parameter	I	`.par`
Geometry/Doping	I	`.tdr`
Lifetime	I	`.tdr`
Save	O	`_des.sav`
Load	I	`_des.sav`
Device Plot (grid-based)	O	`_des.tdr`
Current Plot	O	`_des.plt`
AC Extraction	O	`_ac_des.plt`
Montecarlo	I/O	Refer to the *Sentaurus™ Device Monte Carlo User Guide* for more information.

C: File-Naming Conventions
File Extensions

APPENDIX D Command-Line Options

This appendix lists the most useful command-line options available in Sentaurus Device.

Starting Sentaurus Device

To start Sentaurus Device, enter:

```
sdevice [<options>] [<commandfile>]
```

Sentaurus Device appends automatically the corresponding extension to the given command file if necessary. If no command file is specified, Sentaurus Device reads from standard input.

Command-Line Options

Sentaurus Device interprets the following options:

-d	Prints debug information into the `debug` file. The information printed includes the numeric values of the Jacobian and RHS for each equation at each solution step.
-h	Lists these options and exits.
-i	Prints the initial solution in the save file, and print files specified in the `File` section of the command file, and exits without performing further computations.
-L	Writes the silicon model parameters into the file `Silicon.par` and exits.
-L <commandfile>	Writes model parameter files for all the materials, material interfaces, and electrodes used in `<commandfile>` and exits.
-L:<Material>	Writes a model parameter file `<Material>.par` for the specified material and exits.

`-L:<Material>:<x>`	Writes the model parameters for the given material and mole fraction into a file `<Material>.par` and exits.
`-L:<Material>:<x>:<y>`	Writes the model parameters for the given material and mole fractions into a file `<Material>.par` and exits.
`-L:<Material>/<Material>`	Writes a model parameter file `<Material>%<Material>.par` for the specified material interface and exits.
`-L:All`	Writes a separate model parameter file for all materials and exits.
`-M <commandfile>`	Writes a parameter file `models-M.par` for regions with computed mole fraction dependencies.
`-n`	Does not include Newton information in the `log` file.
`-P`	Writes the silicon model parameters into a file `models.par` and exits. This file can be modified and reloaded into Sentaurus Device to make customized changes to physical models and parameters.
`-P <commandfile>`	Writes the model parameters for the materials and interfaces used in `<commandfile>` into a file `models.par` and exits.
`-P:<Material>`	Writes the model parameters for the given material into a file `models.par` and exits.
`-P:<Material>:<x>`	Writes the model parameters for the given material and mole fraction into a file `models.par` and exits.
`-P:<Material>:<x>:<y>`	Writes the model parameters for the given material and mole fractions into a file `models.par` and exits.
`-P:<Material>/<Material>`	Writes the model parameters for the given material interface into a file `models.par` and exits.
`-P:All`	Writes the model parameters for all materials into a file `models.par` and exits.
`-q`	Quiet mode for output.
`-r`	When used with `-L` or `-P`, reads parameters from the material library to generate output.

`-S`	Writes the SiC model parameters into a `models_SiC.par` file and exits. This file can be modified and reloaded into Sentaurus Device to make customized changes to physical models and parameters.
`-v`	Prints header with version number of Sentaurus Device.
`--compiler-version`	Prints the version of the C++ compiler that was used to compile Sentaurus Device.
`--exit-on-failure`	Terminates immediately after a failed solve command.
`--field-names`	Prints fields and their numeric indices for use in the PMI.
`--parameter-names`	Prints the names of the parameters from the parameter file that can be ramped. If a command file is also supplied, Sentaurus Device prints the parameters from the command file that can be ramped.
`--tcl`	Invokes the Tcl interpreter to evaluate the command file.
`--verbose`	Prints additional diagnostic messages (alternatively, set the environment variable `SDEVICE_VERBOSITY` to `high`).
`--xml`	Creates an additional log file with XML tags. The file uses the extension `.xml`.

D: Command-Line Options
Command-Line Options

APPENDIX E Runtime Statistics

This appendix presents information about obtaining runtime statistics from Sentaurus Device.

The sdevicestat Command

The command `sdevicestat` displays some statistics of a previous run of Sentaurus Device based on the information found in its `log` file. For example, the command:

```
sdevicestat test_des.log
```

generates the following statistics:

```
Total number of Newton iterations      : 8
Number of restarts                     : 0
Rhs-time                               : 9.19 % ( 38.80 s )
Jacobian-time                          : 1.43 % ( 6.05 s )
Solve-time                             : 88.76 % ( 374.70 s )
Overhead                               : 0.62 % ( 2.61 s )
Total CPU time (sum of above times)    : 422.16 s
```

The `sdevicestat` command recognizes whether the `WallClock` keyword has been specified in the `Math` section of the Sentaurus Device command file (see Parallelization on page 166). In this case, the same simulation on a dual processor machine may produce the following output:

```
Total number of Newton iterations      : 8
Number of restarts                     : 0
Rhs-time                               : 8.57 % ( 20.68 s )
Jacobian-time                          : 1.96 % ( 4.73 s )
Solve-time                             : 88.33 % ( 213.07 s )
Overhead                               : 1.14 % ( 2.74 s )
Total wallclock time (sum of above times): 241.22 s
```

E: Runtime Statistics
The sdevicestat Command

APPENDIX F Data and Plot Names

This appendix provides information about data and plot names.

Overview

list the plot names that are recognized in a `Plot` section of Sentaurus Device (see) and the data names that are available in the current plot PMI (see). If the plot name is empty, the data name in quotation marks can be used, for example:

```
Plot {
   "eTemperatureRelaxationTime"
}
```

Vector data can be plotted by appending `/Vector` to the corresponding keyword, for example:

```
Plot {
   ElectricField/Vector
}
```

Element-based scalar data can be plotted by appending `/Element` to the corresponding keyword, for example:

```
Plot {
   eMobility/Element
}
```

Special vector data can be plotted by appending `/SpecialVector` to the corresponding keyword, for example:

```
Plot {
   eSHEDistribution/SpecialVector
}
```

Tensor data can be plotted by appending `/Tensor` to the corresponding keyword, for example:

```
Plot {
   Stress/Tensor
}
```

> **NOTE** The location *rivertex* refers to region-interface vertices.

Scalar Data

Table 178   Scalar data

Data name	Plot name	Location	Description	Unit
AbsorbedPhotonDensity	AbsorbedPhotonDensity	vertex	Quantum Yield Models on page 544	$cm^{-3}s^{-1}$
AbsorbedPhotonDensityCoherent	AbsorbedPhotonDensity	vertex	Transfer Matrix Method on page 625	$cm^{-3}s^{-1}$
AbsorbedPhotonDensityFromMonochromaticSource	AbsorbedPhotonDensity	vertex	Quantum Yield Models on page 544	$cm^{-3}s^{-1}$
AbsorbedPhotonDensityFromSpectrum	AbsorbedPhotonDensity	vertex	Quantum Yield Models on page 544	$cm^{-3}s^{-1}$
AbsorbedPhotonDensityIncoherent	AbsorbedPhotonDensity	vertex	Transfer Matrix Method on page 625	$cm^{-3}s^{-1}$
AccepMinusConcentration	AccepMinusConcentration	vertex	Doping Specification on page 11	cm^{-3}
AcceptorConcentration	AcceptorConcentration	vertex		cm^{-3}
AlphaChargeDensity	AlphaCharge	vertex	Alpha Particles on page 666	cm^{-3}
AlphaGeneration	AlphaGeneration	vertex	G^{Alpha}, Eq. 731, p. 667	$cm^{-3}s^{-1}$
AntimonyActiveConcentration	AntimonyActiveConcentration	vertex	Doping Specification on page 11	cm^{-3}
AntimonyConcentration	AntimonyConcentration	vertex	Sb, Doping Specification on page 11	cm^{-3}
AntimonyPlusConcentration	sbPlus	vertex	Sb$^+$, Chapter 13	cm^{-3}
ArsenicActiveConcentration	ArsenicActiveConcentration	vertex	Doping Specification on page 11	cm^{-3}
ArsenicConcentration	ArsenicConcentration	vertex	As, Doping Specification on page 11	cm^{-3}
ArsenicPlusConcentration	AsPlus	vertex	As$^+$, Chapter 13	cm^{-3}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
AugerRecombination	AugerRecombination	vertex	R^{A}, Eq. 425, p. 408	$\mathrm{cm}^{-3}\mathrm{s}^{-1}$
AutoOrientationSmoothing	AutoOrientationSmoothing	vertex	Auto-Orientation Framework on page 37	1
AvalancheGeneration	AvalancheGeneration	vertex	$G^{\parallel}$, Eq. 437, p. 413	$\mathrm{cm}^{-3}\mathrm{s}^{-1}$
AvalFlatElementMax	AvalFlatElementMax	element	Using Avalanche Generation on page 413	degree
AvalFlatElementMin	AvalFlatElementMin	element	Using Avalanche Generation on page 413	degree
Band2BandGeneration	Band2Band	vertex	$G_{\mathrm{net}}^{\mathrm{bb}}$, Band-to-Band Tunneling Models on page 431	$\mathrm{cm}^{-3}\mathrm{s}^{-1}$
BandGap	BandGap	vertex	E_{g}, Bandgap and Electron-Affinity Models on page 250	eV
BandgapNarrowing	BandGapNarrowing	vertex	E_{bgn}, Bandgap and Electron-Affinity Models on page 250	eV
BM_AngleVertex	BM_AngleVertex	vertex	Statistics About Non-Delaunay Elements on page 1022	degree
BM_EdgesPerVertex	BM_EdgesPerVertex	vertex		1
BM_ElementsPerVertex	BM_ElementsPerVertex	vertex		1
BM_ShortestEdge	BM_ShortestEdge	vertex		$\mu\mathrm{m}$
BM_AngleElements	BM_AngleElements	element		degree
BM_CoeffIntersectionNonDelaunayElements	BM_CoeffIntersectionNonDelaunayElements	element		1
BM_ElementsWithCommonObtuseFace	BM_ElementsWithCommonObtuseFace	element		1
BM_ElementsWithObtuseFaceOnBoundaryDevice	BM_ElementsWithObtuseFaceOnBoundaryDevice	element		1
BM_ElementVolume	BM_ElementVolume	element		$\mu\mathrm{m}^{3}$

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
`BM_IntersectionNonDelaunayElements`	`BM_IntersectionNonDelaunay Elements`	element	Statistics About Non-Delaunay Elements on page 1022	μm
`BM_VolumeIntersectionNon DelaunayElements`	`BM_VolumeIntersectionNon DelaunayElements`	element		μm^3
`BM_wCoeffIntersectionNon DelaunayElements`	`BM_wCoeffIntersectionNon DelaunayElements`	element		1
`BM_wElementsWithCommonObtuseFace`	`BM_wElementsWithCommonObtuse Face`	element		1
`BM_wElementsWithObtuseFaceOn BoundaryDevice`	`BM_wElementsWithObtuseFaceOn BoundaryDevice`	element		1
`BM_wIntersectionNonDelaunay Elements`	`BM_wIntersectionNonDelaunay Elements`	element		μm
`BM_wVolumeIntersectionNon DelaunayElements`	`BM_wVolumeIntersectionNon DelaunayElements`	element		μm^3
`BoronActiveConcentration`	`BoronActiveConcentration`	vertex	Doping Specification on page 11	cm^{-3}
`BoronConcentration`	`BoronConcentration`	vertex	B, Doping Specification on page 11	cm^{-3}
`BoronMinusConcentration`	`bMinus`	vertex	B^-, Chapter 13	cm^{-3}
`BuiltinPotential`	`BuiltinPotential`	vertex	ϕ_0, Eq. 98, p. 201	V
`CDL1Recombination`	`CDL1`	vertex	R_1, Coupled Defect Level (CDL) Recombination on page 405	$cm^{-3}s^{-1}$
`CDL2Recombination`	`CDL2`	vertex	R_2, Coupled Defect Level (CDL) Recombination on page 405	$cm^{-3}s^{-1}$
`CDLcRecombination`	`CDL3`	vertex	$R - R_1 - R_2$, Coupled Defect Level (CDL) Recombination on page 405	$cm^{-3}s^{-1}$

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
CDLRecombination	CDL	vertex	R , Coupled Defect Level (CDL) Recombination on page 405	$\text{cm}^{-3}\text{s}^{-1}$
cplxRefIndex, cplxExtCoeff, n_0, k_0, d_n_lambda, d_k_lambda, d_n_temp, d_n_carr, d_k_carr, d_n_gain	ComplexRefractiveIndex	vertex	Complex Refractive Index Model on page 578	1
ConductionBandEnergy	ConductionBandEnergy	element-vertex	E_C , Eq. 41, p. 176	eV
		vertex		
ConductionCurrentDensity	ConductionCurrent	vertex	$\lvert \vec{J_n} + \vec{J_p} \rvert$, Eq. 53, p. 181 or $\lvert \vec{J_\text{M}} \rvert$ in metals, Eq. 148, p. 239	Acm^{-2}
ConversePiezoelectricFieldXX, ConversePiezoelectricFieldXY, ConversePiezoelectricFieldXZ, ConversePiezoelectricFieldYY, ConversePiezoelectricFieldYZ, ConversePiezoelectricFieldZZ	ConversePiezoelectricField	vertex	Chapter 31	1
ConversePiezoelectricFieldXX	ConversePiezoelectricFieldXX	vertex	Components of converse piezoelectric field tensor	1
ConversePiezoelectricFieldXY	ConversePiezoelectricFieldXY			
ConversePiezoelectricFieldXZ	ConversePiezoelectricFieldXZ			
ConversePiezoelectricFieldYY	ConversePiezoelectricFieldYY			
ConversePiezoelectricFieldYZ	ConversePiezoelectricFieldYZ			
ConversePiezoelectricFieldZZ	ConversePiezoelectricFieldZZ			
CurECImACGreenFunction	CurECImACGreenFunction	vertex	Table 128 on page 710	1
CurECReACGreenFunction	CurECReACGreenFunction	vertex	Table 128 on page 710	1
CurETImACGreenFunction	CurETImACGreenFunction	vertex	Table 128 on page 710	V^{-1}
CurETReACGreenFunction	CurETReACGreenFunction	vertex	Table 128 on page 710	V^{-1}

Table 178　Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
CurGeoGreenFunction	CurGeoGreenFunction	vertex	Table 128 on page 710	Acm^{-3}
CurHCImACGreenFunction	CurHCImACGreenFunction	vertex	Table 128 on page 710	1
CurHCReACGreenFunction	CurHCReACGreenFunction	vertex	Table 128 on page 710	1
CurHTImACGreenFunction	CurHTImACGreenFunction	vertex	Table 128 on page 710	V^{-1}
CurHTReACGreenFunction	CurHTReACGreenFunction	vertex	Table 128 on page 710	V^{-1}
CurLTImACGreenFunction	CurLTImACGreenFunction	vertex	Table 128 on page 710	V^{-1}
CurLTReACGreenFunction	CurLTReACGreenFunction	vertex	Table 128 on page 710	V^{-1}
CurPotImACGreenFunction	CurPotImACGreenFunction	vertex	Table 128 on page 710	s^{-1}
CurPotReACGreenFunction	CurPotReACGreenFunction	vertex	Table 128 on page 710	s^{-1}
CurrentPotential	CurrentPotential	vertex	W, Current Potential on page 185	Acm^{-1}
DelVorWeight	DelVorWeight	vertex	Weighted Voronoï Diagram on page 1020	$\mathrm{\mu m}^{2}$
DeepLevels	DeepLevels	vertex	Energetic and Spatial Distribution of Traps on page 450	cm^{-3}
DielectricConstant	DielectricConstant	element	ε, Eq. 37, p. 173	1
DielectricConstant	DielectricConstant	vertex	ε, Eq. 37, p. 173	1
DielectricConstantAniso	DielectricConstantAniso	element	$\varepsilon_{\mathrm{aniso}}$, Anisotropic Electrical Permittivity on page 793	1

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
DielectricConstantAniso	DielectricConstantAniso	vertex	ε_{aniso}, Anisotropic Electrical Permittivity on page 793	1
DisplacementCurrentDensity	DisplacementCurrent	vertex	$\left|\vec{J}_D\right|$	Acm^{-2}
DonorConcentration	DonorConcentration	vertex	Doping Specification on page 11	cm^{-3}
DonorPlusConcentration	DonorPlusConcentration	vertex		cm^{-3}
DopingConcentration	Doping	vertex		cm^{-3}
DopingWells	DopingWells	vertex	Indices of doping wells, Initial Guess for Electrostatic Potential and Quasi-Fermi Potentials in Doping Wells on page 178	1
eAlphaAvalanche	eAlphaAvalanche	vertex	α_n, Eq. 437, p. 413	cm^{-1}
eAmorphousRecombination	eGapStatesRecombination	vertex	Chapter 17	$cm^{-3}s^{-1}$
eAmorphousTrappedCharge	eTrappedCharge	vertex	Chapter 17	cm^{-3}
eAugerRecombination	eAugerRecombination	vertex	R_n^A, Eq. 425, p. 408	$cm^{-3}s^{-1}$
eAvalancheGeneration	eAvalanche	vertex	G_n, Eq. 437, p. 413	$cm^{-3}s^{-1}$
eBand2BandGeneration	eBand2BandGeneration	vertex	Dynamic Nonlocal Path Band-to-Band Tunneling Model on page 436	$cm^{-3}s^{-1}$
eCDL1Lifetime	eCDL1lifetime	vertex	τ_{n1}, Coupled Defect Level (CDL) Recombination on page 405	s

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
eCDL2Lifetime	eCDL2lifetime	vertex	τ_{n2}, Coupled Defect Level (CDL) Recombination on page 405	s
eCurrentDensity	eCurrent	vertex	$\lvert \vec{J}_n \rvert$, Eq. 53, p. 181	Acm^{-2}
eDeformationPotential	eDeformationPotential	vertex	Using Deformation Potential Model on page 829	eV
eDensity	eDensity	vertex	n, Eq. 53, p. 181	cm^{-3}
eDifferentialGain	eDifferentialGain	vertex	Stimulated and Spontaneous Emission Coefficients on page 962	cm^2
eDiffusivityMobility	eDiffusivityMobility	vertex	$\mu_{n,\,diff}$ Non-Einstein Diffusivity on page 376	$cm^2V^{-1}s^{-1}$
eDirectTunnelCurrent	eSchenkTunnel	vertex	Direct Tunneling on page 718	Acm^{-2}
eDriftVelocity	eDriftVelocity	vertex	Electron drift velocity	$cm\ s^{-1}$
eeDiffusionLNS	eeDiffusionLNS	vertex	Table 128 on page 710	$C^2s^{-1}cm^{-1}$
eEffectiveField	eEffectiveField	vertex	E_n^{eff}, Eq. 469, p. 427	Vcm^{-1}
eEffectiveStateDensity	eEffectiveStateDensity	vertex	N_C, Effective Masses and Effective Density-of-States on page 261	cm^{-3}
eEffectiveStress	eEffectiveStress	vertex	Effective Stress on page 873	MPa
eeFlickerGRLNS	eeFlickerGRLNS	vertex	Table 128 on page 710	$C^2s^{-1}cm^{-1}$
eeMonopolarGRLNS	eeMonopolarGRLNS	vertex	Table 128 on page 710	$C^2s^{-1}cm^{-1}$

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
eEnormal	eEnormal	vertex	$F_\perp$, Eq. 327, p. 355 or $F_{n,\perp}$, Eq. 328, p. 355	Vcm^{-1}
eEparallel	eEparallel	vertex	F_n , Eq. 350, p. 370	Vcm^{-1}
eEquilibriumDensity	eEquilibriumDensity	vertex	n , Eq. 53, p. 181 at zero applied voltages (zero currents)	cm^{-3}
EffectiveBandGap	EffectiveBandGap	vertex	$E_g - E_{\text{bgn}}$, Bandgap and Electron-Affinity Models on page 250	eV
EffectiveIntrinsicDensity	EffectiveIntrinsicDensity	vertex	$n_{\text{i, eff}}$, Eq. 158, p. 249	cm^{-3}
eGradQuasiFermi	eGradQuasiFermi	vertex	$\lvert \nabla \Phi_n \rvert$, Eq. 352, p. 370	Vcm^{-1}
eHeatFlux	eHeatFlux	vertex	$\lvert \vec{S}_n \rvert$, Eq. 76, p. 196	Wcm^{-2}
eInterfaceTrappedCharge	eInterfaceTrappedCharge	vertex	Chapter 17	cm^{-2}
eIonIntegral	eIonIntegral	vertex	Approximate Breakdown Analysis on page 428	1
eJouleHeat	eJouleHeat	vertex	Table 28 on page 195	Wcm^{-3}
ElectricField	ElectricField	element	F	Vcm^{-1}
		vertex		
ElectronAffinity	ElectronAffinity	vertex	χ , Bandgap and Electron-Affinity Models on page 250	eV
ElectrostaticPotential	Potential	vertex	ϕ , Eq. 37, p. 173	V
eLifetime	eLifeTime	vertex	τ_n , Eq. 381, p. 392	s

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
eMLDAQuantumPotential	eMLDAQuantumPotential	vertex	MLDA Model on page 300	eV
eMobility	eMobility	element	μ_n, Chapter 15	$\mathrm{cm^2V^{-1}s^{-1}}$
eMobility	eMobility	vertex	μ_n, Chapter 15	$\mathrm{cm^2V^{-1}s^{-1}}$
eMobilityAniso	eMobilityAniso	element	μ_n^{aniso}, Anisotropic Mobility on page 786	$\mathrm{cm^2V^{-1}s^{-1}}$
eMobilityAniso	eMobilityAniso	vertex	μ_n^{aniso}, Anisotropic Mobility on page 786	$\mathrm{cm^2V^{-1}s^{-1}}$
eMobilityAnisoFactor	eMobilityAnisoFactor	vertex	r_e, Eq. 874, p. 786	1
eMobilityStressFactorXX	eMobilityStressFactorXX	vertex	Using Piezoresistance Mobility Model on page 861	1
eMobilityStressFactorXY	eMobilityStressFactorXY	vertex		1
eMobilityStressFactorXZ	eMobilityStressFactorXZ	vertex		1
eMobilityStressFactorYY	eMobilityStressFactorYY	vertex		1
eMobilityStressFactorYZ	eMobilityStressFactorYZ	vertex		1
eMobilityStressFactorZZ	eMobilityStressFactorZZ	vertex		1
eMVQMBandgapShift	eMVQMBandgapShiftl	vertex	MLDA Model on page 300	eV
eNLLTunnelingGeneration	eBarrierTunneling	vertex	Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722	$\mathrm{cm^{-3}s^{-1}}$
eNLLTunnelingPeltierHeat	eNLLTunnelingPeltierHeat	vertex	Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722	$\mathrm{Wcm^{-3}}$
eQuantumPotential	eQuantumPotential	vertex	Λ_n, Eq. 220, p. 283	eV

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
eQuasiFermiEnergy	eQuasiFermiEnergy	vertex	$E_{F,n}$ Quasi-Fermi Energy on page 201	eV
eQuasiFermiPotential	eQuasiFermi	vertex	Φ_n , Quasi-Fermi Potential With Boltzmann Statistics on page 175	V
EquilibriumPotential	EquilibriumPotential	vertex	ϕ , Eq. 37, p. 173 at zero applied voltages (zero currents)	V
eRelativeEffectiveMass	eRelativeEffectiveMass	vertex	m_n , Effective Masses and Effective Density-of-States on page 261	1
eSaturationVelocity	eSaturationVelocity	vertex	$v_{sat,n}$, Velocity Saturation Models on page 369	cm s^{-1}
eSaturationVelocityAniso	eSaturationVelocityAniso	vertex	$v_{sat,n}^{aniso}$, Anisotropic Mobility on page 786	cm s^{-1}
eSchenkBGN	eSchenkBGN	vertex	$-\Lambda_n$, Eq. 220, p. 283	eV
eSHEAvalancheGeneration	eSHEAvalancheGeneration	vertex	$G_{n,SHE}^{ii}$, Spherical Harmonics Expansion Method on page 746	cm^{-3}s^{-1}
eSHECurrentDensity	eSHECurrentDensity	vertex	$\vec{J}_{n,SHE}$, Spherical Harmonics Expansion Method on page 746	Acm^{-2}
eSHEDensity	eSHEDensity	vertex	n_{SHE} , Spherical Harmonics Expansion Method on page 746	cm^{-3}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
eSHEEnergy	eSHEEnergy	vertex	$T_{n,\,\mathrm{SHE}}$, Spherical Harmonics Expansion Method on page 746	K
eSHEVelocity	eSHEVelocity	vertex	$\left|\vec{v}_{n,\,\mathrm{SHE}}\right|$, Spherical Harmonics Expansion Method on page 746	cm s^{-1}
eSRHRecombination	eSRHRecombination	vertex	Dynamic Nonlocal Path Trap-Assisted Tunneling on page 400	cm^{-3}s^{-1}
eTemperature	eTemperature	vertex	T_n , Hydrodynamic Model for Temperatures on page 195	K
eTemperatureRelaxationTime	eTemperatureRelaxationTime	vertex	$\tau_{\mathrm{e}n}$, Eq. 84, p. 197	s
eTensorMobilityFactorXX	eTensorMobilityFactorXX	vertex	Chapter 31	1
eTensorMobilityFactorYY	eTensorMobilityFactorYY	vertex	Chapter 31	1
eTensorMobilityFactorZZ	eTensorMobilityFactorZZ	vertex	Chapter 31	1
eTensorMobilityXX	eTensorMobilityXX	vertex	Chapter 31	cm^2/(Vs)
eTensorMobilityYY	eTensorMobilityYY	vertex	Chapter 31	cm^2/(Vs)
eTensorMobilityZZ	eTensorMobilityZZ	vertex	Chapter 31	cm^2/(Vs)
eThermoElectricPower	eThermoelectricPower	vertex	P_n , Eq. 1078, p. 914	V K^{-1}
eVelocity	eVelocity	vertex	$v_n = \left|\vec{J}_n/nq\right|$	cm s^{-1}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
f1BandOccupancy001	f1BandOccupancy001	vertex	Using Intel Mobility Model on page 858	1
f1BandOccupancy010	f1BandOccupancy010	vertex		1
f1BandOccupancy100	f1BandOccupancy100	vertex		1
f2BandOccupancy001	f2BandOccupancy001	vertex		1
f2BandOccupancy010	f2BandOccupancy010	vertex		1
f2BandOccupancy100	f2BandOccupancy100	vertex		1
FowlerNordheim	FowlerNordheim	vertex	j_{FN} , Eq. 760, p. 717	Acm^{-2}
Grad2PoECACGreenFunction	Grad2PoECACGreenFunction	vertex	Table 128 on page 710	$\mathrm{V}^2\mathrm{s}^2\mathrm{C}^{-2}\mathrm{cm}^{-2}$
Grad2PoHCACGreenFunction	Grad2PoHCACGreenFunction	vertex	Table 128 on page 710	$\mathrm{V}^2\mathrm{s}^2\mathrm{C}^{-2}\mathrm{cm}^{-2}$
hAlphaAvalanche	hAlphaAvalanche	vertex	α_p , Eq. 437, p. 413	cm^{-1}
hAmorphousRecombination	hGapStatesRecombination	vertex	Chapter 17	$\mathrm{cm}^{-3}\mathrm{s}^{-1}$
hAmorphousTrappedCharge	hTrappedCharge	vertex	Chapter 17	cm^{-3}
hAugerRecombination	hAugerRecombination	vertex	R_p^{A} , Eq. 425, p. 408	$\mathrm{cm}^{-3}\mathrm{s}^{-1}$
hAvalancheGeneration	hAvalanche	vertex	G_p , Eq. 437, p. 413	$\mathrm{cm}^{-3}\mathrm{s}^{-1}$
hBand2BandGeneration	hBand2BandGeneration	vertex	Dynamic Nonlocal Path Band-to-Band Tunneling Model on page 436	$\mathrm{cm}^{-3}\mathrm{s}^{-1}$
hCDL1Lifetime	hCDL1lifetime	vertex	τ_{p1} , Coupled Defect Level (CDL) Recombination on page 405	s
hCDL2Lifetime	hCDL2lifetime	vertex	τ_{p2} , Coupled Defect Level (CDL) Recombination on page 405	s
hCurrentDensity	hCurrent	vertex	$\left|\vec{J_p}\right|$, Eq. 53, p. 181	Acm^{-2}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
hDeformationPotential	hDeformationPotential	vertex	Using Deformation Potential Model on page 829	eV
hDensity	hDensity	vertex	p , Eq. 53, p. 181	cm^{-3}
hDifferentialGain	hDifferentialGain	vertex	Stimulated and Spontaneous Emission Coefficients on page 962	cm^2
hDiffusivityMobility	hDiffusivityMobility	vertex	$\mu_{p,\,diff}$ Non-Einstein Diffusivity on page 376	$cm^2 V^{-1} s^{-1}$
hDirectTunnelCurrent	hSchenkTunnel	vertex	Direct Tunneling on page 718	Acm^{-2}
hDriftVelocity	hDriftVelocity	vertex	Hole drift velocity	$cm\ s^{-1}$
HeavyIonChargeDensity	HeavyIonChargeDensity	vertex	Heavy Ions on page 668	cm^{-3}
HeavyIonGeneration	HeavyIonGeneration	vertex	$G^{HeavyIon}$, Eq. 736, p. 669	$cm^{-3} s^{-1}$
hEffectiveField	hEffectiveField	vertex	E_p^{eff} , Eq. 470, p. 427	Vcm^{-1}
hEffectiveStateDensity	hEffectiveStateDensity	vertex	N_V , Effective Masses and Effective Density-of-States on page 261	cm^{-3}
hEffectiveStress	hEffectiveStress	vertex	Effective Stress on page 873	MPa
heiTemperature	HEItemperature	vertex	T_{hei} , hot-electron temperature, computed as postprocessing approach (`Carrier TempPost`), Chapter 25	K

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
hEnormal	hEnormal	vertex	$F_\perp$, Eq. 327, p. 355 or $F_{p,\perp}$, Eq. 328, p. 355	Vcm^{-1}
hEparallel	hEparallel	vertex	F_p , Eq. 350, p. 370	Vcm^{-1}
hEquilibriumDensity	hEquilibriumDensity	vertex	p , Eq. 53, p. 181 at zero applied voltages (zero currents)	cm^{-3}
hGradQuasiFermi	hGradQuasiFermi	vertex	$\lvert \nabla \Phi_p \rvert$, Eq. 352, p. 370	Vcm^{-1}
hhDiffusionLNS	hhDiffusionLNS	vertex	Table 128 on page 710	$\text{C}^2\text{s}^{-1}\text{cm}^{-1}$
hHeatFlux	hHeatFlux	vertex	$\lvert \vec{S_p} \rvert$, Eq. 77, p. 196	Wcm^{-2}
hhFlickerGRLNS	hhFlickerGRLNS	vertex	Table 128 on page 710	$\text{C}^2\text{s}^{-1}\text{cm}^{-1}$
hhMonopolarGRLNS	hhMonopolarGRLNS	vertex	Table 128 on page 710	$\text{C}^2\text{s}^{-1}\text{cm}^{-1}$
hInterfaceTrappedCharge	hInterfaceTrappedCharge	vertex	Chapter 17	cm^{-2}
hIonIntegral	hIonIntegral	vertex	Approximate Breakdown Analysis on page 428	1
hJouleHeat	hJouleHeat	vertex	Table 28 on page 195	Wcm^{-3}
hLifetime	hLifeTime	vertex	τ_p , Eq. 381, p. 392	s
hMLDAQuantumPotential	hMLDAQuantumPotential	vertex	MLDA Model on page 300	eV
hMobility	hMobility	element	μ_p , Chapter 15	$\text{cm}^2\text{V}^{-1}\text{s}^{-1}$
hMobility	hMobility	vertex	μ_p , Chapter 15	$\text{cm}^2\text{V}^{-1}\text{s}^{-1}$
hMobilityAniso	hMobilityAniso	element	μ_p^{aniso} , Anisotropic Mobility on page 786	$\text{cm}^2\text{V}^{-1}\text{s}^{-1}$

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
hMobilityAniso	hMobilityAniso	vertex	μ_p^{aniso}, Anisotropic Mobility on page 786	$cm^2V^{-1}s^{-1}$
hMobilityAnisoFactor	hMobilityAnisoFactor	vertex	r_h, Eq. 874, p. 786	1
hMobilityStressFactorXX	hMobilityStressFactorXX	vertex	Using Piezoresistance Mobility Model on page 861	1
hMobilityStressFactorXY	hMobilityStressFactorXY	vertex		1
hMobilityStressFactorXZ	hMobilityStressFactorXZ	vertex		1
hMobilityStressFactorYY	hMobilityStressFactorYY	vertex		1
hMobilityStressFactorYZ	hMobilityStressFactorYZ	vertex		1
hMobilityStressFactorZZ	hMobilityStressFactorZZ	vertex		1
hMVQMBandgapShift	hMVQMBandgapShift	vertex	MLDA Model on page 300	eV
hNLLTunnelingGeneration	hBarrierTunneling	vertex	Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722	$cm^{-3}s^{-1}$
hNLLTunnelingPeltierHeat	hNLLTunnelingPeltierHeat	vertex	Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722	Wcm^{-3}
HotElectronInj	HotElectronInjection	rivertex	Hot-electron current density j_{he} at interface, Eq. 794, p. 742, Eq. 800, p. 744	Acm^{-2}
		vertex		
HotHoleInj	HotHoleInjection	rivertex	Hot-hole current density j_{hh} at interface, Eq. 794, p. 742, Eq. 800, p. 744	Acm^{-2}
		vertex		
hQuantumPotential	hQuantumPotential	vertex	Λ_p, Eq. 220, p. 283	eV

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
hQuasiFermiEnergy	hQuasiFermiEnergy	vertex	$E_{F,p}$ Quasi-Fermi Energy on page 201	eV
hQuasiFermiPotential	hQuasiFermi	vertex	Φ_p, Quasi-Fermi Potential With Boltzmann Statistics on page 175	V
hRelativeEffectiveMass	hRelativeEffectiveMass	vertex	m_p, Effective Masses and Effective Density-of-States on page 261	1
hSaturationVelocity	hSaturationVelocity	vertex	$v_{\text{sat},p}$, Velocity Saturation Models on page 369	cm s^{-1}
hSaturationVelocityAniso	hSaturationVelocityAniso	vertex	$v_{\text{sat},p}^{\text{aniso}}$, Anisotropic Mobility on page 786	cm s^{-1}
hSchenkBGN	hSchenkBGN	vertex	$-\Lambda_p$, Eq. 220, p. 283	eV
hSHEAvalancheGeneration	hSHEAvalancheGeneration	vertex	$G_{p,\text{SHE}}^{\text{ii}}$, Spherical Harmonics Expansion Method on page 746	cm^{-3}s^{-1}
hSHECurrentDensity	hSHECurrentDensity	vertex	$\vec{J}_{p,\text{SHE}}$, Spherical Harmonics Expansion Method on page 746	Acm^{-2}
hSHEDensity	hSHEDensity	vertex	p_{SHE}, Spherical Harmonics Expansion Method on page 746	cm^{-3}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
hSHEEnergy	hSHEEnergy	vertex	$T_{p,\text{SHE}}$, Spherical Harmonics Expansion Method on page 746	K
hSHEVelocity	hSHEVelocity	vertex	$\left|\vec{v}_{p,\text{SHE}}\right|$, Spherical Harmonics Expansion Method on page 746	cm s^{-1}
hSRHRecombination	hSRHRecombination	vertex	Dynamic Nonlocal Path Trap-Assisted Tunneling on page 400	cm^{-3}s^{-1}
hTemperature	hTemperature	vertex	T_p, Hydrodynamic Model for Temperatures on page 195	K
hTemperatureRelaxationTime	hTemperatureRelaxationTime	vertex	τ_{ep}, Eq. 85, p. 197	s
hTensorMobilityFactorXX	hTensorMobilityFactorXX	vertex	Chapter 31	1
hTensorMobilityFactorYY	hTensorMobilityFactorYY	vertex	Chapter 31	1
hTensorMobilityFactorZZ	hTensorMobilityFactorZZ	vertex	Chapter 31	1
hTensorMobilityXX	hTensorMobilityXX	vertex	Chapter 31	cm^2/(Vs)
hTensorMobilityYY	hTensorMobilityYY	vertex	Chapter 31	cm^2/(Vs)
hTensorMobilityZZ	hTensorMobilityZZ	vertex	Chapter 31	cm^2/(Vs)
hThermoElectricPower	hThermoelectricPower	vertex	P_p, Eq. 1079, p. 914	V K^{-1}
hVelocity	hVelocity	vertex	$v_p = \left|\vec{J}_p/pq\right|$	cm s^{-1}
HydrogenAtom	HydrogenAtom	vertex	MSC–Hydrogen Transport Degradation Model on page 500	cm^{-3}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
HydrogenIon	HydrogenIon	vertex	MSC–Hydrogen Transport Degradation Model on page 500	cm^{-3}
HydrogenMolecule	HydrogenMolecule	vertex	MSC–Hydrogen Transport Degradation Model on page 500	cm^{-3}
ImeDensityResponse	ImeDensityResponse	vertex	$Im(\tilde{n})$ AC Response on page 1025	$cm^{-3}V^{-1}$
ImeeDiffusionLNVXVSD	ImeeDiffusionLNVXVSD	vertex	Table 128 on page 710	V^2scm^{-3}
ImeeFlickerGRLNVXVSD	ImeeFlickerGRLNVXVSD	vertex	Table 128 on page 710	V^2scm^{-3}
ImeeLNVXVSD	ImeeLNVXVSD	vertex	Table 128 on page 710	V^2scm^{-3}
ImeeMonopolarGRLNVXVSD	ImeeMonopolarGRLNVXVSD	vertex	Table 128 on page 710	V^2scm^{-3}
ImElectrostaticPotentialResponse	ImElectrostaticPotential Response	vertex	$Im(\tilde{\phi})$ AC Response on page 1025	1
ImeTemperatureResponse	ImeTemperatureResponse	vertex	$Im(\tilde{T}_n)$ AC Response on page 1025	KV^{-1}
ImhDensityResponse	ImhDensityResponse	vertex	$Im(\tilde{p})$ AC Response on page 1025	$cm^{-3}V^{-1}$
ImhhDiffusionLNVXVSD	ImhhDiffusionLNVXVSD	vertex	Table 128 on page 710	V^2scm^{-3}
ImhhFlickerGRLNVXVSD	ImhhFlickerGRLNVXVSD	vertex	Table 128 on page 710	V^2scm^{-3}
ImhhLNVXVSD	ImhhLNVXVSD	vertex	Table 128 on page 710	V^2scm^{-3}
ImhhMonopolarGRLNVXVSD	ImhhMonopolarGRLNVXVSD	vertex	Table 128 on page 710	V^2scm^{-3}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
ImhTemperatureResponse	ImhTemperatureResponse	vertex	$\mathrm{Im}(\tilde{T}_p)$ AC Response on page 1025	KV^{-1}
ImLatticeTemperatureResponse	ImLatticeTemperatureResponse	vertex	$\mathrm{Im}(\tilde{T})$ AC Response on page 1025	KV^{-1}
ImLNISD	ImLNISD	vertex	Table 128 on page 710	$\mathrm{A}^2\mathrm{scm}^{-3}$
ImLNVXVSD	ImLNVXVSD	vertex	Table 128 on page 710	$\mathrm{V}^2\mathrm{scm}^{-3}$
ImTrapLNISD	ImTrapLNISD	vertex	Table 128 on page 710	$\mathrm{A}^2\mathrm{scm}^{-3}$
ImTrapLNVSD	ImTrapLNVSD	vertex	Table 128 on page 710	$\mathrm{V}^2\mathrm{scm}^{-3}$
IndiumActiveConcentration	IndiumActiveConcentration	vertex	Doping Specification on page 11	cm^{-3}
IndiumConcentration	IndiumConcentration	vertex	In, Doping Specification on page 11	cm^{-3}
IndiumMinusConcentration	inMinus	vertex	In^-, Chapter 13	cm^{-3}
InsulatorElectricField	InsulatorElectricField	vertex	Electric field F on insulator.	Vcm^{-1}
InterfaceNBTICharge	InterfaceNBTICharge	vertex	Two-Stage NBTI Degradation Model on page 509	cm^{-2}
InterfaceNBTIState1	InterfaceNBTIState1	vertex	Two-Stage NBTI Degradation Model on page 509	cm^{-2}
InterfaceNBTIState2	InterfaceNBTIState2	vertex	Two-Stage NBTI Degradation Model on page 509	cm^{-2}
InterfaceNBTIState3	InterfaceNBTIState3	vertex	Two-Stage NBTI Degradation Model on page 509	cm^{-2}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
InterfaceNBTIState4	InterfaceNBTIState4	vertex	Two-Stage NBTI Degradation Model on page 509	cm^{-2}
InterfaceOrientation	InterfaceOrientation	vertex	Auto-Orientation Framework on page 37	1
IntrinsicDensity	IntrinsicDensity	vertex	n_i, Eq. 157, p. 249	cm^{-3}
JouleHeat	JouleHeat	vertex	Table 28 on page 195	Wcm^{-3}
LatticeHeatCapacity	LatticeHeatCapacity	vertex	c_L, Heat Capacity on page 899	$JK^{-1}cm^{-3}$
LatticeTemperature	LatticeTemperature, Temperature	vertex	T, Chapter 9, p. 189	K
LayerThickness	LayerThickness	vertex	LayerThickness Command on page 310	µm
LayerThicknessField	LayerThicknessField	vertex	LayerThickness Command on page 310	µm
lHeatFlux	lHeatFlux	vertex	$\left|\vec{S}_L\right|$, Eq. 78, p. 196	Wcm^{-2}
MeanIonIntegral	MeanIonIntegral	vertex	Approximate Breakdown Analysis on page 428	1
MetalConductivity	MetalConductivity	vertex	σ, Transport in Metals on page 239	$Acm^{-1}V^{-1}$
MetalWorkfunction	MetalWorkfunction	vertex	Metal Workfunction on page 242	eV

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
MobilityAcceptorConcentration	MobilityAcceptorConcentration	vertex	Mobility Doping File on page 384 or Add2TotalDoping (ChargedTraps), Doping Specification on page 11	cm^{-3}
MobilityDonorConcentration	MobilityDonorConcentration	vertex	Mobility Doping File on page 384 or Add2TotalDoping (ChargedTraps), Doping Specification on page 11	cm^{-3}
Mod_eGradQuasiFermi_ElectricField	Mod_eGradQuasiFermi_ ElectricField	vertex	$\left\|\nabla\tilde{\Phi}_n\right\|$, Interpolation of Driving Forces to Zero Field on page 373	Vcm^{-1}
Mod_eQuasiFermi_ElectricField_ Potential	Mod_eQuasiFermi_ElectricField _Potential	vertex	$\tilde{\Phi}_n$, Interpolation of Driving Forces to Zero Field on page 373	V
Mod_hGradQuasiFermi_ElectricField	Mod_hGradQuasiFermi_ ElectricField	vertex	$\left\|\nabla\tilde{\Phi}_p\right\|$, Interpolation of Driving Forces to Zero Field on page 373	Vcm^{-1}
Mod_hQuasiFermi_ElectricField_ Potential	Mod_hQuasiFermi_ElectricField _Potential	vertex	$\tilde{\Phi}_p$, Interpolation of Driving Forces to Zero Field on page 373	V
NDopantActiveConcentration	NDopantActiveConcentration	vertex	Doping Specification on page 11	cm^{-3}
NDopantConcentration	NdopantConcentration	vertex	NDopant, Doping Specification on page 11	cm^{-3}
NDopantPlusConcentration	NdopantPlus	vertex	NDopant$^+$, Chapter 13	cm^{-3}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
NearestInterfaceOrientation	NearestInterfaceOrientation	vertex	Auto-Orientation Framework on page 37	1
NegInterfaceCharge	NegInterfaceCharge	vertex	Mobility Degradation Components due to Coulomb Scattering on page 347	cm^{-2}
NitrogenActiveConcentration	NitrogenActiveConcentration	vertex	Doping Specification on page 11	cm^{-3}
NitrogenConcentration	NitrogenConcentration	vertex	N, Doping Specification on page 11	cm^{-3}
NitrogenPlusConcentration	NitrogenPlus	vertex	N^+, Chapter 13	cm^{-3}
OneOverDegradationTime	OneOverDegradationTime	vertex	Chapter 19	s^{-1}
OpticalAbsorption	OpticalAbsorptionHeat	vertex	Optical Absorption Heat on page 545	Wcm^{-3}
OpticalAbsorption(Bandgap)	OpticalAbsorptionHeat	vertex	Optical Absorption Heat on page 545	Wcm^{-3}
OpticalAbsorption(Vacuum)	OpticalAbsorptionHeat	vertex	Optical Absorption Heat on page 545	Wcm^{-3}
OpticalField	OpticalField	vertex	Plot optical intensity as well as real and imaginary parts of optical field.	W/m^{-3} V/m
OpticalGeneration	OpticalGeneration	vertex	G_0^{opt}, Eq. 707, p. 627	$cm^{-3}s^{-1}$
OpticalGenerationFromConstant	OpticalGeneration	vertex	Specifying the Type of Optical Generation Computation on page 534	$cm^{-3}s^{-1}$

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
OpticalGenerationFromFile	OpticalGeneration	vertex	Specifying the Type of Optical Generation Computation on page 534	$cm^{-3}s^{-1}$
OpticalGenerationFromMonochromatic Source	OpticalGeneration	vertex	Specifying the Type of Optical Generation Computation on page 534	$cm^{-3}s^{-1}$
OpticalGenerationFromSpectrum	OpticalGeneration	vertex	Specifying the Type of Optical Generation Computation on page 534	$cm^{-3}s^{-1}$
OpticalIntensity	OpticalIntensity	vertex	Solving the Optical Problem on page 553	Wcm^{-2}
OpticalIntensityCoherent	OpticalIntensity	vertex	Transfer Matrix Method on page 625	Wcm^{-2}
OpticalIntensityIncoherent	OpticalIntensity	vertex	Transfer Matrix Method on page 625	Wcm^{-2}
ParallelToInterfaceInBoundaryLayer Active	ParallelToInterfaceInBoundary LayerActive	element	Field Correction Close to Interfaces on page 375	1
PDopantActiveConcentration	PDopantActiveConcentration	vertex	Doping Specification on page 11	cm^{-3}
PDopantConcentration	pDopantConcentration	vertex	PDopant, Doping Specification on page 11	cm^{-3}
PDopantMinusConcentration	pDopantMinus	vertex	PDopant$^-$, Chapter 13	cm^{-3}
PE_Charge	PE_Charge	vertex	q_{PE}, Piezoelectric Datasets on page 888	cm^{-3}
PeltierHeat	PeltierHeat	vertex	Table 28 on page 195	Wcm^{-3}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
PhosphorusActiveConcentration	PhosphorusActiveConcentration	vertex	Doping Specification on page 11	cm^{-3}
PhosphorusConcentration	PhosphorusConcentration	vertex	P, Doping Specification on page 11	cm^{-3}
PhosphorusPlusConcentration	phPlus	vertex	P$^+$, Chapter 13	cm^{-3}
PiezoCharge	PiezoCharge	vertex	q_{PE}, Piezoelectric Datasets on page 888	cm^{-3}
PMIeNonLocalRecombination	PMIeNonLocalRecombination	vertex	R_n^{PMI}, Nonlocal Generation–Recombination Model on page 1097	$cm^{-3}s^{-1}$
PMIHeat	PMIHeat	vertex	Heat Generation Rate on page 1264	Wcm^{-3}
PMIhNonLocalRecombination	PMIhNonLocalRecombination	vertex	R_p^{PMI}, Nonlocal Generation–Recombination Model on page 1097	$cm^{-3}s^{-1}$
PMIRecombination	PMIRecombination	vertex	R^{PMI}, Generation–Recombination Model on page 1094	$cm^{-3}s^{-1}$
PMIUserField0	PMIUserField0	vertex	Command File of Sentaurus Device on page 1065	1
PMIUserField1	PMIUserField1	vertex		1
…	…	vertex		1
PMIUserField299	PMIUserField299	vertex		1
PoECImACGreenFunction	PoECImACGreenFunction	vertex	Table 128 on page 710	VsC^{-1}
PoECReACGreenFunction	PoECReACGreenFunction	vertex	Table 128 on page 710	VsC^{-1}
PoETImACGreenFunction	PoETImACGreenFunction	vertex	Table 128 on page 710	A^{-1}
PoETReACGreenFunction	PoETReACGreenFunction	vertex	Table 128 on page 710	A^{-1}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
PoGeoGreenFunction	PoGeoGreenFunction	vertex	Table 128 on page 710	Vcm^{-3}
PoHCImACGreenFunction	PoHCImACGreenFunction	vertex	Table 128 on page 710	VsC^{-1}
PoHCReACGreenFunction	PoHCReACGreenFunction	vertex	Table 128 on page 710	VsC^{-1}
PoHTImACGreenFunction	PoHTImACGreenFunction	vertex	Table 128 on page 710	A^{-1}
PoHTReACGreenFunction	PoHTReACGreenFunction	vertex	Table 128 on page 710	A^{-1}
PoLTImACGreenFunction	PoLTImACGreenFunction	vertex	Table 128 on page 710	A^{-1}
PoLTReACGreenFunction	PoLTReACGreenFunction	vertex	Table 128 on page 710	A^{-1}
PoPotImACGreenFunction	PoPotImACGreenFunction	vertex	Table 128 on page 710	VC^{-1}
PoPotReACGreenFunction	PoPotReACGreenFunction	vertex	Table 128 on page 710	VC^{-1}
Polarization	Polarization	vertex	$\left\|\vec{P}\right\|$, Chapter 29	Ccm^{-2}
PosInterfaceCharge	PosInterfaceCharge	vertex	Mobility Degradation Components due to Coulomb Scattering on page 347	cm^{-2}
QCEffectiveBandGap	QCEffectiveBandGap	vertex	$E_g - E_{bgn}$ $- q(\Lambda_n + \Lambda_n)$	eV
QCEffectiveIntrinsicDensity	QCEffectiveIntrinsicDensity	vertex	$n_{i, eff}$ with corrections due to Fermi statistics and quantization effects	cm^{-3}
QuantumYield	QuantumYield	vertex	Quantum Yield Models on page 544	1
QuasiFermiPotential	QuasiFermiPotential	vertex	Φ , Eq. 136, p. 225	V

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
QW_chEigenEnergy	QW_chEigenEnergy	vertex	Eigenenergies of the crystal-field split-hole bound states, Localized Quantum-Well Model on page 978	eV
QW_chNumberOfBoundStates	QW_chNumberOfBoundStates	vertex	Actual number of QW bound states for crystal-field split-holes, Localized Quantum-Well Model on page 978	1
QW_chRelativeEffectiveMass	QW_chRelativeEffectiveMass	vertex	Relative effective mass of crystal-field split-holes, Localized Quantum-Well Model on page 978	1
QW_chStrainBandShift	QW_chStrainBandShift	vertex	Shift in crystal-field split-hole band due to strain effects, Localized Quantum-Well Model on page 978	eV
QW_eEigenEnergy	QW_eEigenEnergy	vertex	Eigenenergies of the electron bound states, Localized Quantum-Well Model on page 978	eV
QW_ElectricFieldProjection	QW_ElectricFieldProjection	vertex	Electric field in the QW, Localized Quantum-Well Model on page 978	Vcm^{-1}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
`QW_eNumberOfBoundStates`	`QW_eNumberOfBoundStates`	vertex	Actual number of QW bound states for electrons, Localized Quantum-Well Model on page 978	1
`QW_eRelativeEffectiveMass`	`QW_eRelativeEffectiveMass`	vertex	Relative effective mass of electrons, Localized Quantum-Well Model on page 978	1
`QW_eStrainBandShift`	`QW_eStrainBandShift`	vertex	Shift in conduction band due to strain effects, Localized Quantum-Well Model on page 978	eV
`QW_hhEigenEnergy`	`QW_hhEigenEnergy`	vertex	Eigenenergies of the heavy-hole bound states, Localized Quantum-Well Model on page 978	eV
`QW_hhNumberOfBoundStates`	`QW_hhNumberOfBoundStates`	vertex	Actual number of QW bound states for heavy holes, Localized Quantum-Well Model on page 978	1
`QW_hhRelativeEffectiveMass`	`QW_hhRelativeEffectiveMass`	vertex	Relative effective mass of heavy holes, Localized Quantum-Well Model on page 978	1

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
QW_hhStrainBandShift	QW_hhStrainBandShift	vertex	Shift in heavy-hole band due to strain effects, Localized Quantum-Well Model on page 978	eV
QW_lhEigenEnergy	QW_lhEigenEnergy	vertex	Eigenenergies for the light-hole bound states, Localized Quantum-Well Model on page 978	eV
QW_lhNumberOfBoundStates	QW_lhNumberOfBoundStates	vertex	Actual number of QW bound states for light holes, Localized Quantum-Well Model on page 978	1
QW_lhRelativeEffectiveMass	QW_lhRelativeEffectiveMass	vertex	Relative effective mass of light holes, Localized Quantum-Well Model on page 978	1
QW_lhStrainBandShift	QW_lhStrainBandShift	vertex	Shift in light-hole band due to strain effects, Localized Quantum-Well Model on page 978	eV
QW_OverlapIntegral	QW_OverlapIntegral	vertex	Overlap integrals between electron and hole wavefunctions, Localized Quantum-Well Model on page 978	1

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
QW_QuantizationDirection	QW_QuantizationDirection	vertex	Quantization direction of the QW, Localized Quantum-Well Model on page 978	1
QW_Width	QW_Width	vertex	Extracted width of the QW, Localized Quantum-Well Model on page 978	μm
QWeDensity	QWeDensity	vertex	n, Eq. 1163, p. 974	cm^{-3}
QWeQuasiFermi	QWeQuasiFermi	vertex	Φ_n, Quasi-Fermi Potential With Boltzmann Statistics on page 175	V
QWhDensity	QWhDensity	vertex	p, Eq. 1164, p. 974	cm^{-3}
QWhQuasiFermi	QWhQuasiFermi	vertex	Φ_p, Quasi-Fermi Potential With Boltzmann Statistics on page 175	V
RadiationGeneration	RadiationGeneration	vertex	G_r, Eq. 720, p. 645	cm^{-3}s^{-1}
RadiativeRecombination	RadiativeRecombination	vertex	R, Eq. 424, p. 408	cm^{-3}s^{-1}
RandomizedDoping	RandomizedDoping	vertex	Statistical Impedance Field Method	cm^{-3}
RayTrees	RayTrees		Using the Raytracer on page 596	
RecombinationHeat	RecombinationHeat	vertex	Table 28 on page 195	Wcm^{-3}
ReeDensityResponse	ReeDensityResponse	vertex	$\mathrm{Re}(\tilde{n})$ AC Response on page 1025	cm^{-3}V^{-1}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
ReeeDiffusionLNVXVSD	ReeeDiffusionLNVXVSD	vertex	Table 128 on page 710	$\mathrm{V}^2\mathrm{scm}^{-3}$
ReeeFlickerGRLNVXVSD	ReeeFlickerGRLNVXVSD	vertex	Table 128 on page 710	$\mathrm{V}^2\mathrm{scm}^{-3}$
ReeeLNVXVSD	ReeeLNVXVSD	vertex	Table 128 on page 710	$\mathrm{V}^2\mathrm{scm}^{-3}$
ReeeMonopolarGRLNVXVSD	ReeeMonopolarGRLNVXVSD	vertex	Table 128 on page 710	$\mathrm{V}^2\mathrm{scm}^{-3}$
ReElectrostaticPotentialResponse	ReElectrostaticPotential Response	vertex	$\mathrm{Re}(\tilde{\phi})$ AC Response on page 1025	1
ReeTemperatureResponse	ReeTemperatureResponse	vertex	$\mathrm{Re}(\tilde{T}_n)$ AC Response on page 1025	KV^{-1}
RefractiveIndex	RefractiveIndex	element	n , Complex Refractive Index Model on page 578	1
RefractiveIndex	RefractiveIndex	vertex	n , Complex Refractive Index Model on page 578	1
RehDensityResponse	RehDensityResponse	vertex	$\mathrm{Re}(\tilde{p})$ AC Response on page 1025	$\mathrm{cm}^{-3}\mathrm{V}^{-1}$
RehhDiffusionLNVXVSD	RehhDiffusionLNVXVSD	vertex	Table 128 on page 710	$\mathrm{V}^2\mathrm{scm}^{-3}$
RehhFlickerGRLNVXVSD	RehhFlickerGRLNVXVSD	vertex	Table 128 on page 710	$\mathrm{V}^2\mathrm{scm}^{-3}$
RehhLNVXVSD	RehhLNVXVSD	vertex	Table 128 on page 710	$\mathrm{V}^2\mathrm{scm}^{-3}$
RehhMonopolarGRLNVXVSD	RehhMonopolarGRLNVXVSD	vertex	Table 128 on page 710	$\mathrm{V}^2\mathrm{scm}^{-3}$
RehTemperatureResponse	RehTemperatureResponse	vertex	$\mathrm{Re}(\tilde{T}_p)$ AC Response on page 1025	KV^{-1}
ReLatticeTemperatureResponse	ReLatticeTemperatureResponse	vertex	$\mathrm{Re}(\tilde{T})$ AC Response on page 1025	KV^{-1}

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
ReLNISD	ReLNISD	vertex	Table 128 on page 710	$\text{A}^2\text{scm}^{-3}$
ReLNVXVSD	ReLNVXVSD	vertex	Table 128 on page 710	$\text{V}^2\text{scm}^{-3}$
ReTrapLNISD	ReTrapLNISD	vertex	Table 128 on page 710	$\text{A}^2\text{scm}^{-3}$
ReTrapLNVSD	ReTrapLNVSD	vertex	Table 128 on page 710	$\text{V}^2\text{scm}^{-3}$
SemiconductorElectricField	SemiconductorElectricField	vertex	Electric field F on semiconductor.	Vcm^{-1}
SpaceCharge	SpaceCharge	vertex	Eq. 37, p. 173	cm^{-3}
SpontaneousRecombination	SpontaneousRecombination	vertex	Spontaneous Recombination Rate on page 965	$\text{cm}^{-3}\text{s}^{-1}$
SRHRecombination	SRHRecombination	vertex	$R_{\text{net}}^{\text{SRH}}$, Shockley–Read–Hall Recombination on page 391	$\text{cm}^{-3}\text{s}^{-1}$
StimulatedRecombination	StimulatedRecombination	vertex	Stimulated Recombination Rate on page 964	$\text{cm}^{-3}\text{s}^{-1}$
StressXX, StressXY, StressXZ, StressYY, StressYZ, StressZZ	Stress	vertex	Stress tensor, Chapter 31	Pa
StressXX	StressXX	vertex	Components of stress tensor, Chapter 31	Pa
StressXY	StressXY			
StressXZ	StressXZ			
StressYY	StressYY			
StressYZ	StressYZ			
StressZZ	StressZZ			
SurfaceRecombination	SurfaceRecombination	rivertex	Surface SRH Recombination on page 404	$\text{cm}^{-2}\text{s}^{-1}$
		vertex		
ThermalConductivity	ThermalConductivity	vertex	κ , Eq. 1042, p. 901	$\text{Wcm}^{-1}\text{K}^{-1}$

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
ThermalConductivityAniso	ThermalConductivityAniso	vertex	κ_{aniso}, Anisotropic Thermal Conductivity on page 794	$Wcm^{-1}K^{-1}$
ThermalizationYield(Bandgap)	ThermalizationYield	vertex	Optical Absorption Heat on page 545	1
ThermalizationYield(Vacuum)	ThermalizationYield	vertex	Optical Absorption Heat on page 545	1
ThomsonHeat	ThomsonHeat	vertex	Table 28 on page 195	Wcm^{-3}
TotalConcentration	TotalConcentration	vertex	Doping Specification on page 11	cm^{-3}
TotalCurrentDensity	Current	vertex	$\|\vec{J}_n + \vec{J}_p + \vec{J}_D\|$	Acm^{-2}
TotalHeat	TotalHeat	vertex	Sum of all heat generation terms, Chapter 9, Temperature in Metals on page 244	Wcm^{-3}
TotalInterfaceTrapConcentration	TotalInterfaceTrap Concentration	vertex	Chapter 17	cm^{-2}
TotalRecombination	TotalRecombination	vertex	Sum of all generation–recombination terms, Chapter 16	$cm^{-3}s^{-1}$
TotalTrapConcentration	TotalTrapConcentration	vertex	Chapter 17	cm^{-3}
tSRHRecombination	tSRHRecombination	vertex	Dynamic Nonlocal Path Trap-Assisted Tunneling on page 400	$cm^{-3}s^{-1}$
ValenceBandEnergy	ValenceBandEnergy	element-vertex	E_V, Eq. 42, p. 176	eV
		vertex		
VertexIndex	VertexIndex	vertex	Vertex numbers	1

Table 178   Scalar data (Continued)

Data name	Plot name	Location	Description	Unit
xMoleFraction	xMoleFraction	vertex	Abrupt and Graded Heterojunctions on page 10	1
yMoleFraction	yMoleFraction	vertex		1

Vector Data

Table 179   Vector data

Data name	Plot name	Location	Description	Unit
ConductionCurrentDensity	ConductionCurrent	vertex	$\vec{J}_n + \vec{J}_p$, Eq. 53, p. 181 or J_M in metals, Eq. 148, p. 239	Acm^{-2}
ContactSurfaceNormal	ContactSurfaceNormal	vertex	Contact surface normal	1
DisplacementCurrentDensity	DisplacementCurrent	vertex	$\vec{J}_D$	Acm^{-2}
eCurrentDensity	eCurrent	vertex	$\vec{J}_n$, Eq. 53, p. 181	Acm^{-2}
eDriftVelocity	eDriftVelocity	vertex	Electron drift velocity.	$cm\ s^{-1}$
eGradQuasiFermi	eGradQuasiFermi	vertex	$-\nabla\Phi_n$, Eq. 39, p. 175	Vcm^{-1}
eHeatFlux	eHeatFlux	vertex	$\vec{S}_n$, Eq. 76, p. 196	Wcm^{-2}
ElectricField	ElectricField	element	$\vec{F}$	Vcm^{-1}
		vertex		
EquilibriumElectricField	EquilibriumElectricField	vertex	$\vec{F}_{eq}$, Eq. 111, p. 209	Vcm^{-1}
eSHECurrentDensity	eSHECurrentDensity	vertex	$\vec{J}_{n,\ SHE}$, Spherical Harmonics Expansion Method on page 746	Acm^{-2}
eSHEVelocity	eSHEVelocity	vertex	$\vec{v}_{n,\ SHE}$, Spherical Harmonics Expansion Method on page 746	$cm\ s^{-1}$
eVelocity	eVelocity	vertex	$v_n = -\vec{J}_n/qn$	$cm\ s^{-1}$
GradPoECImACGreenFunction	GradPoECImACGreenFunction	vertex	Table 128 on page 710	$VsC^{-1}cm^{-1}$
GradPoECReACGreenFunction	GradPoECReACGreenFunction	vertex	Table 128 on page 710	$VsC^{-1}cm^{-1}$
GradPoETImACGreenFunction	GradPoETImACGreenFunction	vertex	Table 128 on page 710	$A^{-1}cm^{-1}$

Table 179   Vector data (Continued)

Data name	Plot name	Location	Description	Unit
GradPoETReACGreenFunction	GradPoETReACGreen Function	vertex	Table 128 on page 710	$\mathrm{A}^{-1}\mathrm{cm}^{-1}$
GradPoHCImACGreenFunction	GradPoHCImACGreen Function	vertex	Table 128 on page 710	$\mathrm{VsC}^{-1}\mathrm{cm}^{-1}$
GradPoHCReACGreenFunction	GradPoHCReACGreen Function	vertex	Table 128 on page 710	$\mathrm{VsC}^{-1}\mathrm{cm}^{-1}$
GradPoHTImACGreenFunction	GradPoHTImACGreen Function	vertex	Table 128 on page 710	$\mathrm{A}^{-1}\mathrm{cm}^{-1}$
GradPoHTReACGreenFunction	GradPoHTReACGreen Function	vertex	Table 128 on page 710	$\mathrm{A}^{-1}\mathrm{cm}^{-1}$
hCurrentDensity	hCurrent	vertex	$\vec{J_p}$, Eq. 53, p. 181	Acm^{-2}
hDriftVelocity	hDriftVelocity	vertex	Hole drift velocity	$\mathrm{cm\ s}^{-1}$
hGradQuasiFermi	hGradQuasiFermi	vertex	$-\nabla\Phi_p$, Eq. 352, p. 370	Vcm^{-1}
hHeatFlux	hHeatFlux	vertex	$\vec{S_p}$, Eq. 77, p. 196	Wcm^{-2}
hSHECurrentDensity	hSHECurrentDensity	vertex	$\vec{J}_{p,\mathrm{SHE}}$, Spherical Harmonics Expansion Method on page 746	Acm^{-2}
hSHEVelocity	hSHEVelocity	vertex	$\vec{v}_{p,\mathrm{SHE}}$, Spherical Harmonics Expansion Method on page 746	$\mathrm{cm\ s}^{-1}$
hVelocity	hVelocity	vertex	$\vec{v}_p = \vec{J_p}/qp$	$\mathrm{cm\ s}^{-1}$
ImConductionCurrentResponse	ImConductionCurrent Response	vertex	$\mathrm{Im}\left(\vec{\tilde{J}}_n + \vec{\tilde{J}}_p\right)$ AC Current Density Responses on page 1026	$\mathrm{Acm}^{-2}\mathrm{V}^{-1}$
ImDisplacementCurrentResponse	ImDisplacementCurrent Response	vertex	$\mathrm{Im}\left(\vec{\tilde{J}}_{\mathrm{D}}\right)$ AC Current Density Responses on page 1026	$\mathrm{Acm}^{-2}\mathrm{V}^{-1}$
ImeCurrentResponse	ImeCurrentResponse	vertex	$\mathrm{Im}\left(\vec{\tilde{J}}_n\right)$ AC Current Density Responses on page 1026	$\mathrm{Acm}^{-2}\mathrm{V}^{-1}$

Table 179   Vector data (Continued)

Data name	Plot name	Location	Description	Unit
ImeEnFluxResponse	ImeEnFluxResponse	vertex	$\mathrm{Im}\left(\vec{\tilde{S}}_n\right)$ AC Current Density Responses on page 1026	$\mathrm{Wcm}^{-2}\mathrm{V}^{-1}$
ImhCurrentResponse	ImhCurrentResponse	vertex	$\mathrm{Im}\left(\vec{\tilde{J}}_p\right)$ AC Current Density Responses on page 1026	$\mathrm{Acm}^{-2}\mathrm{V}^{-1}$
ImhEnFluxResponse	ImhEnFluxResponse	vertex	$\mathrm{Im}\left(\vec{\tilde{S}}_p\right)$ AC Current Density Responses on page 1026	$\mathrm{Wcm}^{-2}\mathrm{V}^{-1}$
ImlEnFluxResponse	ImlEnFluxResponse	vertex	$\mathrm{Im}\left(\vec{\tilde{S}}_\mathrm{L}\right)$ AC Current Density Responses on page 1026	$\mathrm{Wcm}^{-2}\mathrm{V}^{-1}$
ImTotalCurrentResponse	ImTotalCurrentResponse	vertex	$\mathrm{Im}\left(\vec{\tilde{J}}_n + \vec{\tilde{J}}_p + \vec{\tilde{J}}_\mathrm{D}\right)$ AC Current Density Responses on page 1026	$\mathrm{Acm}^{-2}\mathrm{V}^{-1}$
InsulatorElectricField	InsulatorElectricField	vertex	Electric field $\vec{F}$ on insulator.	Vcm^{-1}
lHeatFlux	lHeatFlux	vertex	$\vec{S}_\mathrm{L}$, Eq. 78, p. 196	Wcm^{-2}
Mod_eGradQuasiFermi_ ElectricField	Mod_eGradQuasiFermi_ ElectricField	vertex	$\nabla\tilde{\Phi}_n$, Interpolation of Driving Forces to Zero Field on page 373	Vcm^{-1}
Mod_hGradQuasiFermi_ ElectricField	Mod_hGradQuasiFermi_ ElectricField	vertex	$\nabla\tilde{\Phi}_p$, Interpolation of Driving Forces to Zero Field on page 373	Vcm^{-1}
NonLocalBackDirection	NonLocal	vertex	Visualizing Nonlocal Meshes on page 148	µm
NonLocalDirection	NonLocal	vertex		µm
OpticalField	OpticalField	vertex	Plot optical intensity as well as real and imaginary parts of optical field.	$\mathrm{W}/\mathrm{m}^{-3}$ V/m
PE_Polarization	PE_Polarization	vertex	P_PE, Piezoelectric Datasets on page 888	Ccm^{-2}
Polarization	Polarization	element	$\vec{P}$, Chapter 29	Ccm^{-2}
Polarization	Polarization	vertex	$\vec{P}$, Chapter 29	Ccm^{-2}

Table 179   Vector data (Continued)

Data name	Plot name	Location	Description	Unit
ReConductionCurrentResponse	ReConductionCurrent Response	vertex	$\mathrm{Re}\left(\vec{\tilde{J}}_n + \vec{\tilde{J}}_p\right)$ AC Current Density Responses on page 1026	$\mathrm{Acm^{-2}V^{-1}}$
ReDisplacementCurrentResponse	ReDisplacementCurrent Response	vertex	$\mathrm{Re}\left(\vec{\tilde{J}}_\mathrm{D}\right)$ AC Current Density Responses on page 1026	$\mathrm{Acm^{-2}V^{-1}}$
ReeCurrentResponse	ReeCurrentResponse	vertex	$\mathrm{Re}\left(\vec{\tilde{J}}_n\right)$ AC Current Density Responses on page 1026	$\mathrm{Acm^{-2}V^{-1}}$
ReeEnFluxResponse	ReeEnFluxResponse	vertex	$\mathrm{Re}\left(\vec{\tilde{S}}_n\right)$ AC Current Density Responses on page 1026	$\mathrm{Wcm^{-2}V^{-1}}$
RehCurrentResponse	RehCurrentResponse	vertex	$\mathrm{Re}\left(\vec{\tilde{J}}_p\right)$ AC Current Density Responses on page 1026	$\mathrm{Acm^{-2}V^{-1}}$
RehEnFluxResponse	RehEnFluxResponse	vertex	$\mathrm{Re}\left(\vec{\tilde{S}}_n\right)$ AC Current Density Responses on page 1026	$\mathrm{Wcm^{-2}V^{-1}}$
RelEnFluxResponse	RelEnFluxResponse	vertex	$\mathrm{Re}\left(\vec{\tilde{S}}_\mathrm{L}\right)$ AC Current Density Responses on page 1026	$\mathrm{Wcm^{-2}V^{-1}}$
ReTotalCurrentResponse	ReTotalCurrentResponse	vertex	$\mathrm{Re}\left(\vec{\tilde{J}}_n + \vec{\tilde{J}}_p + \vec{\tilde{J}}_\mathrm{D}\right)$ AC Current Density Responses on page 1026	$\mathrm{Acm^{-2}V^{-1}}$
SemiconductorElectricField	SemiconductorElectric Field	vertex	Electric field $\vec{F}$ on semiconductor.	$\mathrm{Vcm^{-1}}$
TotalCurrentDensity	Current	vertex	$\vec{J}_n + \vec{J}_p + \vec{J}_\mathrm{D}$	$\mathrm{Acm^{-2}}$

Special Vector Data

Table 180   Special vector data

Data name	Plot name	Location	Description	Unit
eSHEDistribution	eSHEDistribution	vertex	Electron energy distribution, SHE Distribution Hot-Carrier Injection on page 744	1
hSHEDistribution	hSHEDistribution	vertex	Hole energy distribution, SHE Distribution Hot-Carrier Injection on page 744	1

Tensor Data

Table 181   Tensor data

Data name	Plot name	Location	Description	Unit
ElasticStrain	ElasticStrain	vertex	Strain tensor from TDR file (Sentaurus Process or Sentaurus Interconnect), Strain Tensor on page 824	1
Strain	Strain	vertex	Strain tensor $\bar{\varepsilon}$, Stress and Strain in Semiconductors on page 821	1
Stress	Stress	vertex	Stress tensor $\bar{\sigma}$, Stress and Strain in Semiconductors on page 821	Pa

APPENDIX G Command File Overview

This appendix presents an overview of the command file of Sentaurus Device.

presents the topmost levels of the command file. Use this table to obtain a top-down overview of the command file. The remaining sections are ordered with respect to topics. The headings of the tables, therein, mostly start with a keyword. Use these tables to find details about keywords.

Organization of Command File Overview

The tables in this appendix have two or three columns, and their rows are ordered alphabetically with respect to the first (and, as far as applicable, the middle) column. Placeholders (cross references, user-supplied values in angle brackets (`<>`)) precede explicit keywords, irrespective of alphabetic order.

The left column contains keywords that can appear in the command file. In the topmost rows of some tables, the left column references another table. This means that all keywords in the referenced table can appear in the referring table as well. Some keywords are followed by an opening parenthesis or an opening brace to indicate that the keyword expects a selection of options listed in the middle column of the current and the following rows.

The middle column contains options or values to the keyword in the left column, one per row. For a selection of options, the last row indicates the closing parenthesis or the closing brace. For some tables, the middle column would be empty and is omitted.

The right column contains the description of keywords, options, and values of the row. As far as applicable, the right column also provides the following additional information:

- The default value, which can be:

  - An explicit value. Those values are written in Courier font, as you would type them.

  - + or – to indicate the default (true or false, respectively) for keywords that support the – prefix.

  - *on* or *off* for keywords that set and reset flags, but do not support the – prefix.

  - An asterisk (*) to indicate the default among mutually exclusive alternatives.

  - An exclamation mark (!) if no default exists and you must specify a value.

- The unit assumed for the given quantity. In unit specifications, *d* denotes the dimension of the mesh. For dimensionless quantities, no unit is specified.

- The location for which keywords should be specified, given as characters in parentheses:

  - (g) stands for global parameters that must not appear in region-specific, interface-specific, or contact-specific sections.

  - (r) stands for region-specific (or material-specific) parameters that usually do not make sense when specified for interfaces or contacts.

  - (c) and (i) stand for contact-specific or interface-specific parameters.

Furthermore, the tables use the following conventions:

- An ellipsis (…) denotes that the preceding item can be repeated an arbitrary number of times.

- An asterisk (*) followed by an integer, both typeset in Times font, denotes that the preceding item must appear the given number of times.

- Optional components of specifications are enclosed in brackets, and the brackets are *not* part of the syntax.

- Angle brackets (`<>`) indicate user-supplied values. Table 182 summarizes the common types of specification. More specific notation is explained in the last column of the table where it is used.

Some tables use additional conventions as necessary. They are explained in the text that precedes the respective table.

Table 182 Notation for user-supplied values

Specification	Description
`<(x,y)> <[x,y]>` `<(x,y]> <[x,y)>`	Range of floating-point numbers from x to y. Parentheses are used when the limits are excluded from the range; brackets are used when they are included. To denote ranges unbound on one side, the corresponding limit is omitted.
`<carrier>`	A carrier type, `Electron` or `Hole`.
`<float>`	A floating-point number (integers are special cases thereof).
`<ident>`	An identifier. This is like a string, but is not enclosed in double quotation marks.
`<int>`	An integer.
`<n..m>`	A range of integers, from `n` to `m`, inclusively. Either `n` or `m` can be omitted, to denote ranges that are unbound on one side.
`<string>`	A sequence of characters (including digits and special characters) included in double quotation marks. Unlike most Sentaurus Device input, strings are case sensitive.

Table 182   Notation for user-supplied values (Continued)

Specification	Description
`<vector>`	A sequence of up to three floating-point numbers, enclosed in parentheses, and separated by spaces, for example: `(1.0 3 0)`.
`<System_Coord>`	`CrystalSystem` or `SimulationSystem`.

Top Levels of Command File

Table 183 lists the top levels in the command file of Sentaurus Device.

Table 183   Top levels of command file

Table 184		Specification for single devices.
`Device`	`<string>` {Table 184}	Device name and device specifications (mixed mode). Device Section on page 54
`OpticalDevice`	`<string>` {Table 184}	Optical device name and device specification (mixed mode and Composite Method on page 656). Device Section on page 54
`Solve{`	Table 186}	The problem to be solved.
`System{`	Table 204}	The circuit (mixed mode). System Section on page 55

Device

Table 184   Device{} or single-device specification Chapter 2, p. 9

`CurrentPlot{`	`<ident>`	Use current plot PMI. Current Plot File of Sentaurus Device on page 1239
	`PMIModel` (Table 318)	Use current plot PMI with parameters. Current Plot File of Sentaurus Device on page 1239
	Table 178 (Table 330)	Plot scalar data to current file. Tracking Additional Data in the Current File on page 110
	Table 179/`Vector`(Table 330) }	Plot vectorial data to current file. Tracking Additional Data in the Current File on page 110
`Electrode{`	Table 206}	Electrode specification. Specifying Electrical Boundary Conditions on page 67
`eSHEDistributionPlot{`	`<vector>`...}	Electron-energy distribution plot. Visualizing Spherical Harmonics Expansion Method on page 757

Table 184   Device{} or single-device specification Chapter 2, p. 9 (Continued)

`Extraction{`	`<ident> [=] <ident>...}`	Process parameters. Extraction File on page 126
`File{`	Table 185}	Input and output files.
`GainPlot{`	Table 331}	Parameters for gain plot (LED).
`GridAdaptation(`	Table 222)	Perform grid adaptation. Adaptive Device Instances on page 994
`hSHEDistributionPlot{`	`<vector>...}`	Hole-energy distribution plot. Visualizing Spherical Harmonics Expansion Method on page 757
`HydrogenBoundary{`	Table 207}	Degradation model. Boundary Conditions on page 502
`IFM{`	Table 210}	Variations, noise models. IFM Section on page 707
`Math`	`[(`Table 336`)]`	Math specification, potentially restricted to a location.
`{`	Table 211}	
`MonteCarlo{`	`<options>}`	See the *Sentaurus™ Device Monte Carlo User Guide*.
`NoisePlot{`	Table 333}	Noise output data. Noise Output Data on page 710
	`(<vector>...) {`Table 334`}`	Nonlocal plot. Visualizing Data Defined on Nonlocal Meshes on page 148
`Physics`	`[(`Table 336`)]`	Physical models, potentially restricted to a location.
`{`	Table 233}	
`Plot{`	Table 328}	Plot data. Device Plots on page 122
`RayTraceBC{`	Table 208}	Raytrace boundary conditions.
`TensorPlot(`	Table 335)	Tensor plot for beam propagation method. Visualizing Results on Native Tensor Grid on page 655
`{`	`ComplexRefractiveIndex`	
	`OpticalField`	
	`OpticalIntensity}`	
`Thermode{`	Table 209}	Thermode specification. Specifying Thermal Boundary Conditions on page 70
`TrappedCarDistrPlot{`	`<vector>`	Trapped carrier charge plot at position `<vector>`. Visualizing Traps on page 466
	Table 339`={<vector>...}}`	Trapped carrier charge plot restricted to location.

File

In the description of Table 185, it is indicated whether a file is input or output, as well as the extensions (in Courier font) that Sentaurus Device appends to the user-supplied name to obtain the full name. The tags enclosed in at-signs (@) denote the default Sentaurus Workbench variables for the particular file name. (These defaults can be changed in tooldb.tcl, see Sentaurus™ Workbench User Guide, Global Configuration Files on page 286). (g) denotes keywords that must be used in global File sections only, while (d) denotes keywords that must be used in device-specific File sections only.

Table 185   File{}

ACExtract	=<string>	(g) Small-signal and noise analysis (output, _ac_des.plt, @acplot@). Small-Signal AC Analysis on page 96
Bandstructure	=<string>	(d) Base name for plotting local band structure data in an LED simulation (output, _kpbandstruc_vertexX_des.plt, _kpeigenfunc_vertexX_des.plt).
CMIPath	=<string>	(g) Search path for compact circuit files (extension .ccf) and the corresponding shared object files (extension .so.arch). The files are parsed and added to the System section of the command file. If the environment variable STROOT_ARCH_OS_LIB is defined, the directory $STROOT_ARCH_OS_LIB/sdevice is automatically added to CMIPath. System Section on page 55
Current	=<string>	Device currents, voltages, charges, temperatures, and times (output, _des.plt, @plot@). Current File on page 107
DephasingRates	=<string>	Directory for saving dephasing rates using the second Born approximation.
DevFields	=<string>	(d) Space distribution for trapped carrier charge density. Must match grid file (input .tdr). Energetic and Spatial Distribution of Traps on page 450
DevicePath	=<string>	(g) Load all files with the extension .device in the directory path <string>. The directory path has the format dir1:dir2:dir3. The devices found can be used in the System section. They are not overwritten by a definition with the same name in the command file. System Section on page 55
EmissionTable	=<string>	Tabulated emission data (output).
eSHEDistribution	=<string>	Electron distribution versus kinetic energy (output, _des.plt). Visualizing Spherical Harmonics Expansion Method on page 757
Extraction	=<string>	(d) Extraction file (output, extraction_des.xtr). Extraction File on page 126
Gain	=<string>	(d) Modal stimulated and spontaneous emission spectra (output, _gain_des.plt).

Table 185   File{} (Continued)

Grid	=<string>	(d) Device geometry and mesh (input, .tdr, or @tdr@). Exception for grid adaptation: base name for output grid files. Specifying Grid Adaptations on page 993
hSHEDistribution	=<string>	Hole distribution versus kinetic energy (output, _des.plt). Visualizing Spherical Harmonics Expansion Method on page 757
IlluminationSpectrum	=<string>	Illumination spectrum. Illumination Spectrum on page 536
LifeTime	=<string>	(d) Lifetime profiles (input, .tdr). Lifetime Profiles From Files on page 393
Load	=<string>	Old simulation results (input, .sav). Save and Load on page 157
MesherInput	=<string>	Base name of boundary and command file to be used for calling Sentaurus Mesh. Specifying the Optical Solver on page 554
MobilityDoping	=<string>	(d) File from which donor and acceptor concentrations for mobility calculations are read. Mobility Doping File on page 384
NewtonPlot	=<string>	Convergence monitoring (output). NewtonPlot on page 154
NonLocalPlot	=<string>	Data defined on nonlocal line meshes (output). Visualizing Data Defined on Nonlocal Meshes on page 148
OpticalGenerationFile	=<string>	Load optical generation from a file. Optical AC Analysis on page 661
OpticalGenerationInput	=<string>	File from which optical generation rate is loaded. Loading and Saving Optical Generation From and to File on page 542
OpticalGenerationOutput	=<string>	File to which optical generation rate is written. Loading and Saving Optical Generation From and to File on page 542
OpticalGenerationOutput (collected)	=<string>	File to which optical generation rate is written. Consecutive plots are written into one file instead of several enumerated files. Loading and Saving Optical Generation From and to File on page 542
OpticalSolverInput	=<string>	Command file of optical solver. Specifying the Optical Solver on page 554
OpticsOutput	=<string>	(g) Runtime log for optical solvers (output, _des.log, @optlog@).
Output	=<string>	"output" (g) Runtime log (output, _des.log, @log@).
ParameterPath	=<string>	(d) List of subdirectories in the $STROOT/tcad/$STRELEASE/lib/ sdevice/MaterialDB directory that are added to the search path for parameter files. Physical Model Parameters on page 21
Parameters	=<string>	(d) Device parameters (input, .par, @parameter@). Physical Model Parameters on page 21
Piezo	=<string>	(d) Stress data for piezoelectric model (input). Chapter 31, p. 821
Plot	=<string>	Spatially distributed simulation results (output, _des.tdr, @tdrdat@). Device Plots on page 122

Table 185   File{} (Continued)

Plot(collected)	=<string>	Spatially distributed simulation results (output, _des.tdr, @tdrdat@). Consecutive plots are written into one file instead of several enumerated files. Device Plots on page 122
PMIPath	=<string>	(g) Search path to load shared object files (extension .so.arch) for PMI models. Command File of Sentaurus Device on page 1065
PMIUserFields	=<string>	(d) File containing any of the fields PMIUserField0 to PMIUserField299.
SpectralPlot	=<string>	Spatially distributed simulation results (output, _des.tdr, @spectralplot@) for each entry of the illumination spectrum as well as spectral curves (_des.plt) for the results of the optical solver. Consecutive plots are written into one file instead of several enumerated files, that is, SpectralPlot(collected) is the default. Illumination Spectrum on page 536
SpectralPlot (-collected)	=<string>	Spatially distributed simulation results (output, _des.tdr, @spectralplot@) for each entry of the illumination spectrum as well as spectral curves (_des.plt) for the results of the optical solver. Consecutive plots are written into several enumerated files. Illumination Spectrum on page 536
TensorPlot	=<string>	Base name for saving tensor plot files when using beam propagation method. Visualizing Results on Native Tensor Grid on page 655
Save	=<string>	Simulation results for retrieval with Load (output, _des.sav). Save and Load on page 157
SaveOptField	=<string>	Base name for saving optical field data in an LED simulation.
SPICEPath	=<string>	Search path for SPICE circuit files (extension .scf). The files are parsed and added to the System section of the command file. If the environment variable STROOT_LIB is defined, the directory $STROOT_LIB/ sdevice/spice is automatically added to SPICEPath. SPICE Circuit Models on page 63
TrappedCarPlotFile	=<string>	Trapped carrier charge density, trap occupancy probability, and trap density versus energy (output, _des.plt). Visualizing Traps on page 466

Solve

Table 186   Solve{}

Table 199		Solve selected standalone problem.
[<ident>.] Table 191		Solve selected equation [for instance <ident>].
ACCoupled(	Table 187)	Perform small-signal and noise analysis. Small-Signal AC Analysis on page 96
{	[<ident>.] Table 191...}	Equations to be solved consistently.
Continuation(	Table 188)	Continuation options.
{	Table 186}	Problem to be solved.
Coupled(	Table 189)	Solve coupled equations consistently by Newton iteration.
{	[<ident>.] Table 191...}	Equations to be solved.
CurrentPlot	as Load	Control current output. When to Write to the Current File on page 107
HBCoupled(	Table 193)	Perform harmonic balance analysis. Harmonic Balance on page 101
{	[<ident>.] Table 191...}	Equations to be solved.
Load(	Table 194)	Load and continue with solution stored by Save. Save and Load on page 157
	Circuit	Load circuit.
	[{<ident>...}]	Devices to be loaded.
NewCurrentPrefix	=<string>	Use prefix <string> for current file. NewCurrentPrefix Statement on page 110
Plot(	Table 194)	Plot current solution. When to Plot on page 123
	[{<ident>...}]	Devices to be plotted.
Plugin(	Table 196)	Solve equations consistently by Gummel iteration.
{	Table 199	Solve selected standalone problem.
	[<ident>.] Table 191...	Solve selected equation (for example, <ident>).
	Coupled(Table 189) { [<ident>.] Table 191...} ...}	Solve coupled equations.
Quasistationary(	Table 197)	Quasistationary simulation options.
{	Table 186}	Problem to be solved.

Table 186   Solve{} (Continued)

Save	as Load	Save current solution for retrieval with Load. Save and Load on page 157
Set(	Table 198)	Set status according to Table 198.
SpectralPlot(	Table 194)	Plot spectral simulation results of current solution. When to Plot on page 123 and Illumination Spectrum on page 536
	[{<ident>...}]	Devices to be plotted.
System	(<string>)	Execute UNIX command <string> (ignore return status). System Command on page 170
+System	(<string>)	Execute UNIX command <string>; use its return status to decide whether it was successful. System Command on page 170
Transient(	Table 201)	Transient simulation options.
{	Table 186}	Problem to be solved.
Unset	(<ident>...)	Unset nodes. Mixed-Mode Electrical Boundary Conditions on page 69
	(TrapFilling)	Use the standard trap equations. Explicit Trap Occupation on page 468

Table 187   ACCoupled() Small-Signal AC Analysis on page 96

Table 189		Coupled() parameters.
ACCompute(	Table 194)	Restrict AC or noise analysis to selected points in a Quasistationary command.
ACExtract	=<string>	Prefix for the name of the file to which the results of AC analysis are written (overrides the specification from the File section).
ACMethod	=Blocked	Use Blocked solver.
ACPlot	=<string>	Plot the responses of the solution variables to the AC signals. <string> is a prefix for the names of the files to which the responses are written.
ACSubMethod	(<ident>)=Table 224	Super (1D and 2D), ILS (3D) Inner solver for device <ident>.
CircuitNoise		Compute noise from circuit elements. Noise From SPICE Circuit Elements on page 690
Decade		Use logarithmic intervals between the frequencies.
EndFrequency	=<(0,)>	! Hz Upper frequency.
Exclude	(<ident>...)	Devices that will be removed from the circuit for AC analysis.
Extraction{	Table 20}	List of frequency-dependent extraction curves. Extraction File on page 126

Table 187   ACCoupled() Small-Signal AC Analysis on page 96 (Continued)

Linear		Use linear intervals between the frequencies.
Node	(<ident>...)	Nodes for which to perform AC analysis.
NoisePlot	=<string>	Prefix for a file name. Chapter 23, p. 675
NumberOfPoints	=<0..>	! Number of frequencies for which to perform the analysis.
ObservationNode	(<ident>...)	Nodes for which to perform noise analysis; subset of those in Node. Chapter 23, p. 675
Optical		Perform optical AC analysis. Optical AC Analysis on page 100
StartFrequency	=<(0,)>	! Hz Lower frequency.
VoltageGreenFunctions		– Compute voltage responses for frequency zero. Analysis at Frequency Zero on page 677

Table 188   Continuation() Continuation Command on page 83

AcceptNewtonParameter		Apply relaxed Newton parameters. Relaxed Newton Method on page 143
BreakCriteria{	Table 214}	Break criteria. Break Criteria: Conditionally Stopping the Simulation on page 71
Decrement	=<float>	1.5 Divisor for step size on failure to solve.
DecrementAngle	=<float>	5 deg Angle for which step starts decreasing.
Digits	=<float>	3 Number of digits for relative error.
Error	=<float>	0.05 Absolute error target.
Iadapt	=<float>	! Lower current limit for adaptive algorithm.
Increment	=<float>	2 Multiplier for step size on successful solve.
IncrementAngle	=<float>	2.5 deg Angle up to which step increases.
InitialVstep	=<float>	! Initial voltage step.
MaxCurrent	=<float>	! Upper current limit.
MaxIfactor	=<float>	! Maximum-allowed current relative to previous point as a multiplication factor.
MaxIstep	=<float>	! Maximum-allowed current step.
MaxLogIfactor		! Maximum-allowed current relative to previous point as a multiplication factor, in orders of magnitude.
MaxStep	=<float>	Maximum step for the internal arc length variable.
MaxVoltage	=<float>	! Upper voltage limit.

Table 188   Continuation() Continuation Command on page 83 (Continued)

MaxVstep	=<float>	! Maximum-allowed voltage step.
MinCurrent	=<float>	! Lower current limit.
MinStep	=<float>	1e-5 Minimum step for the internal arc length variable.
MinVoltage	=<float>	! Lower voltage limit.
MinVoltageStep	=<float>	1e-2 Minimum voltage step controlling arc length step increase.
Name	=<ident>	Electrode to bias in continuation. It must be specified.
Normalized		Compute angles in a local scaled I–V coordinate system.
Rfixed	=<float>	0.001 Fixed resistor value.

Table 189   Coupled() Coupled Command on page 136

CheckRhsAfterUpdate		Check whether the RHS can be reduced further after the update error has converged. If CheckRhsAfterUpdate is specified in the Math section, -CheckRhsAfterUpdate can be used to disable it for this Coupled command.
Digits	=<float>	Relative error target.
GridAdaptation		Perform grid adaptation. Adaptive Solve Statements on page 1003
(	CurrentPlot	– Plot data obtained on intermediate grids to current file.
	MaxCLoops=<int>	1e5 Maximum number of adaptation iterations.
	Plot)	– Plot device data on intermediate grids.
IncompleteNewton		Incomplete Newton. Incomplete Newton Algorithm on page 140
(	RhsFactor=<float>	Maximum change in RHS to allow old Jacobian to be reused.
	UpdateFactor=<float>)	Maximum change in update to allow old Jacobian to be reused.
Iterations	=<0..>	Maximum number of iterations of the Newton algorithm.
LineSearchDamping	=<(0,1]>	Minimal coefficient for line search damping. 1 disables damping. Damped Newton Iterations on page 139
Method	=Table 224	Linear solver.
	=Blocked	Block decomposition solver.
NotDamped	=<0..>	Number of Newton iterations before Bank–Rose damping is applied. Damped Newton Iterations on page 139
RhsAndUpdateConvergence		Require both RHS and update error convergence.

Table 189   Coupled() Coupled Command on page 136 (Continued)

RhsMin	=<float>	Upper bound for RHS norm convergence.
SubMethod	[(<ident>)]=Table 224	Super (1D and 2D), ILS (3D) Inner solver (for device <ident>).
UpdateIncrease	=<float>	Maximum-allowed increase of update error per Newton step.
UpdateMax	=<float>	Maximum-allowed update error in Newton algorithm.

Table 190   Cyclic() Large-Signal Cyclic Analysis on page 93

Accuracy	=<float>		Tolerance ε_{cyc} .
Extrapolate(	Average		+ Use averaged factor r_{av}^o for each object. Factor r is defined separately for each vertex.
	Factor=<float>		1 Coefficient f for r_{av}^o estimation.
	Forward		– Proceed as in a standard transient, without cyclic extrapolation.
	MaxVal=<float>		25 Value of r_{max} .
	MinVal=<float>		1 Value of r_{min} .
	Print		+ Print averaged factors r_{av}^o for each object.
	QFtraps)		– Apply extrapolation to 'trap quasi-Fermi level' Φ_T instead of trap occupation probabilities f_T .
Period	=<float>		s Period of the cycle.
RelFactor	=<float>		Relaxation factor Υ.
StartingPeriod	=<2..>		2 Period from which the extrapolation procedure starts.

In the description column of Table 191, the default for `ErrRef` (first number; see Table 211 on page 1403) and its unit, and the default for `Error` (second number, see Table 211) are given.

Table 191   Equations

Charge	1.602192e-19 C 1e-3 Floating gate charge, available for `TransientErrRef` and `TransientError` only. Floating Gates on page 1035
Circuit	0.0258 V 1e-3 Circuit equations.
CondInsulator	0.0258 V 1e-3 Conductive insulator equations.
Contact	0.0258 V 1e-3 Contact equations.
Electron	1e10 cm^{-3} 1e-5 Electron continuity equation. Chapter 8, p. 181
eQuantumPotential	0.0258 V 1e-3 Electron quantum-potential equation. Density Gradient Quantization Model on page 294

Table 191   Equations (Continued)

eSHEDistribution	1 V 1e-3 Electron SHE distribution equation. Using Spherical Harmonics Expansion Method on page 750
eTemperature	300 K 1e-4 Electron temperature equation. Hydrodynamic Model for Temperatures on page 195
Hole	1e10 cm^{-3} 1e-5 Hole continuity equation. Chapter 8, p. 181
hQuantumPotential	0.0258 V 1e-3 Hole quantum potential equation. Density Gradient Quantization Model on page 294
hSHEDistribution	1 V 1e-3 Hole SHE distribution equation. Using Spherical Harmonics Expansion Method on page 750
hTemperature	300 K 1e-4 Hole temperature equation. Hydrodynamic Model for Temperatures on page 195
HydrogenAtom	1e10 cm^{-3} 1e-3 Hydrogen atom transport equation. Hydrogen Transport on page 500
HydrogenIon	1e10 cm^{-3} 1e-3 Hydrogen ion transport equation. Hydrogen Transport on page 500
HydrogenMolecule	1e10 cm^{-3} 1e-3 Hydrogen molecule transport equation. Hydrogen Transport on page 500
LLG	Landau–Lifshitz–Gilbert equation. Chapter 30, p. 805
Mechanics	Mechanical stress equation. Mechanics Solver on page 890
Poisson	0.0258 V 1e-3 Poisson equation. Electrostatic Potential on page 173
SingletExciton	Singlet exciton equation. Singlet Exciton Equation on page 235
TCircuit	Thermal circuit equations.
TContact	Thermal contact equations.
Temperature	300 K 1e-3 Temperature equation. Chapter 9, p. 189
Traps	1e-5 1 1e-3 Explicit trap equation. Trap-to-Trap Tunneling on page 461

Table 192   Goal{} Quasistationary Ramps on page 74

Charge	=<float>	C Target charge for contact.
Contact	=<string1>.<string2>	Name of instance and contact to be ramped.
Current	=<float>	A µm^{d-3} Target current for contact.
Device	=<string>	Name of the device where the parameter will be ramped.
DopingWell	(<vector>)	Semiconductor well defined by point <vector> where quasi-Fermi potential will be ramped.

Table 192   Goal{} Quasistationary Ramps on page 74 (Continued)

DopingWells	(Material=<string>)	Semiconductor wells in material <string> where quasi-Fermi potential will be ramped.
	(Region=<string>)	Semiconductor wells in the region <string> where quasi-Fermi potential will be ramped.
	(Semiconductor)	All device semiconductor wells where Fermi potential will be ramped.
eQuasiFermi	=<float>	V Target electron quasi-Fermi potential for semiconductor wells. Ramping Quasi-Fermi Potentials in Doping Wells on page 76
hQuasiFermi	=<float>	V Target hole quasi-Fermi potential for semiconductor wells. Ramping Quasi-Fermi Potentials in Doping Wells on page 76
Material	=<string>	Name of material where the parameter will be ramped.
MaterialInterface	=<string>	Name of material interface where parameter will be ramped.
Model	=<string>	Name of model for which the parameter will be ramped.
ModelParameter	=<string>	Parameter path or name of parameter that is ramped when using Parameter Ramping on page 573.
Name	=<string>	Name of contact to be ramped.
	=Regexp(<string>)	Regular expression for matching contacts.
Node	=<string>	Name of node for which the voltage will be ramped.
Parameter	=<string>	Name of parameter that will be ramped.
	=<string1>.<string2>	Name of instance and parameter that will be ramped. This syntax only applies to circuit parameters, but not device parameters.
Power	=<float>	Target heat for contact.
Region	=<string>	Name of region where the parameter will be ramped.
RegionInterface	=<string>	Name of region interface where parameter will be ramped.
Temperature	=<float>	K Target temperature for contact.
Value	=<float>	Target value for parameter.
Voltage	=<float>	V Target voltage for node or contact.
WellContactName	=<string>	Name of contact defining the well where quasi-Fermi potential will be ramped.

Table 193   HBCoupled() Harmonic Balance on page 101

Table 189		Coupled() parameters.
CNormPrint		+ Print instance equation errors per Newton step (MDFT mode only).
Derivative		– Use complete Jacobian for HB Newton.
GMRES		Use GMRES linear solver; requires Method=ILS.
(	MaxIterations=<int>	200 Maximal number of iterations.
	Restart=<int>	20 Size of minimization subspace.
	Tolerance=<float>)	1e-4 Required residuum reduction.
Initialize	=DCMode	0-th harmonic from DC solution; others, zero.
	=HBMode	All harmonics from previous harmonic balance (HB) solution.
	=MixedMode	0-th harmonic from DC; others, from previous HB solution.
Method	=ILS	Required for GMRES.
	=Pardiso	Use PARDISO to solve linear system (SDFT mode only).
Name	=<string>	Name component of plot files. Default is Coupled_<number>, where <number> is the global index of all Coupled, ACCoupled, and HBCoupled solve entries.
RhsScale	(Table 191)=<float>	Scaling of RHS in Newton (MDFT mode only).
SolveSpectrum	=<string>	Referenced solve spectrum (MDFT mode only).
Tone		Multiple specification for multitone (MDFT mode only).
(	Frequency=<freqspec>	! Hz Base frequency. Performing Harmonic Balance Analysis on page 102
	NumberOfHarmonics=<int>)	! Number of harmonics H . Eq. 25, p. 101
UpdateScale	(Table 191)=<float>	Scaling of update in Newton (MDFT mode only).
ValueMin	(Table 191)=<float>	Lower bound for quantity in time domain (MDFT mode only).
ValueVariation	(Table 191)=<float>	Allowed variation of quantity in time domain (MDFT mode only).

Table 194   Load(), Plot(), Save(), SpectralPlot() in Solve{} When to Plot on page 123

Current	(Difference=<float>)	A Only for Continuation simulations. Write save or plot files when the difference between the actual and previous plotting current values on the continuation contact is greater than the specified Difference.
	(Intervals=<int>)	A Only for Continuation simulations. Divide the range specified with MinCurrent and MaxCurrent of Continuation into <int> intervals, and write save or plot files every time the current enters one of these intervals. When LogCurrent is specified in Continuation section, logarithmic ($\mathrm{asinh}(10^{100}$ current)) current range is used. Write save or plot file when the current enters a new logarithmic interval.
	(LogDifference=<(0,)>)	A Only for Continuation simulations. LogCurrent must be specified in Continuation section. Write save or plot files when the difference between the actual and previous logarithmic plotting current values is greater than the specified Difference.
Explicit		– Write datasets specified in Plot section only. Explicit is ignored by SpectralPlot.
FilePrefix	=<string>	Prefix of file name. File names consist of the prefix, the instance name, an optional local number (depending on Overwrite and noOverwrite), and an extension. The default file prefix is save<globalsaveindex> for Save and plot<globalplotindex> for Plot.
Iterations	=(<int>;…)	(0;1;...) Save or plot at certain Plugin iterations.
IterationStep	=<int>	Save or plot all <int> steps of plugins, quasistationaries, continuations, or transients.
Loadable		+ Write additional information required to load a simulation from a .tdr file. Loadable is not supported for SpectralPlot.
noOverwrite		off Give each new save or plot file a new name by numbering.
Number	=<int>	Number of the solution to be retrieved by Load.
Overwrite		on Rewrite the same file name at each loop.
Time=(	<float>	Time point for plot. When to Plot on page 123
	decade	Use logarithmic range subdivision. When to Plot on page 123
	intervals=<int>	Number of subdivisions. When to Plot on page 123
	range=(<float>*2);...)	Plotting range. When to Plot on page 123

Table 194   Load(), Plot(), Save(), SpectralPlot() in Solve{} When to Plot on page 123
(Continued)

Voltage	(Difference=<float>)	V Only for `Continuation` simulations. Write save or plot files when the difference between current and previous plotting voltages is greater than the specified `Difference`.
	(Intervals=<int>)	Only for `Continuation` simulations. Divide the range specified with `MinVoltage` and `MaxVoltage` of `Continuation` into `<int>` intervals, and write save or plot files every time the voltage enters one of these intervals.
When		Generate output whenever the target was crossed the between the previous and the current iteration i, $X_{i-1} < X_T \leq X_i$ or $X_{i-1} > X_T \geq X_i$. Available for `Plot`, `SpectralPlot`, `Save`, and `CurrentPlot` inside a `Quasistationary`, `Transient`, or `Continuation`.
(	Contact= [<string>.]<string>	[Instance and] contact name for target. The instance name defaults to " ", appropriate for single-device simulation.
	Current=<float>	A Target current X_T.
	Node=<string>	Node name for target.
	Voltage=<float>)	V Target voltage X_T.

Table 195   MSConfigs() in Set() in Solve{} Manipulating MSCs During Solve on page 486

Frozen		+ Freeze MSCs.
MSConfig		Set occupations for the specified MSC.
(	Device=<string>	Device instance name to where the MSC belongs.
	Name=<string>	Name of MSC.
	State(Name=<string> Value=<float>)...)	Set occupation of MSC state `<string>` to given value.

Table 196   Plugin() Plugin Command on page 145

BreakOnFailure		Stop when an inner `Coupled` fails.
Digits	=<float>	Relative precision target.
Iterations	=<int>	Maximum number of iterations. `0` is used to perform one loop without error testing.

Table 197   Quasistationary() Quasistationary Ramps on page 74

AcceptNewtonParameter		Apply relaxed Newton parameters. Relaxed Newton Method on page 143
(	ReferenceStep=<float>)	`1.e-9` Apply relaxed Newton parameters for step size < `ReferenceStep`.
BreakCriteria{	Table 214}	Break criteria. Break Criteria: Conditionally Stopping the Simulation on page 71
Decrement	=<float>	`2` Divisor for the step size when last step failed.
DoZero		+| – The equations are solved for $t = 0$.
Extraction{	Table 20}	List of voltage-dependent extraction curves. Extraction File on page 126
Extrapolate		Use extrapolation. Extrapolation on page 81
(	Order=<int>)	`1` Order of extrapolation.
Goal{	Table 192}	Goal for ramping.
GridAdaptation		Perform grid adaptation. Adaptive Solve Statements on page 1003
(	CurrentPlot	– Write currents obtained on intermediate grids.
	Iterations=(<int>;...)	Adapt grid at given iterations.
	IterationStep=<int>	`1` Adapt grid any <int> steps.
	MaxCLoops=<int>	`1e5` Maximum number of adaptation iterations.
	Plot	– Plot device data on intermediate grids.
	Time=(Range= (<float>*2);...))	Adapt grid when time falls into a given range.
Increment	=<float>	`2` Multiplier for the step size when last step was successful.
InitialStep	=<float>	`0.1` Initial step size.
MaxStep	=<float>	`1` Maximum step size.
MinStep	=<float>	`0.001` Minimum step size.
NewtonPlotStep	=<float>	Upper limit for step size for which to write Newton plot files. NewtonPlot on page 154
NonlocalPath	(Table 229)	Dynamic Nonlocal Path Band-to-Band Tunneling Model on page 436, Handling of Derivatives on page 442

Table 197   Quasistationary() Quasistationary Ramps on page 74 (Continued)

Plot{	Intervals=<int>	! Number of intervals in `Range`. Saving and Plotting During a Quasistationary on page 81
	Range=(<float>*2)}	! Range of t for which to generate plots.
PlotBandstructure	as Plot	Plot band structure data in an LED simulation.
PlotLEDRadiation	as Plot	Optical far field of LED.
PlotGain	as Plot	Plot stimulated and spontaneous emission data in LED simulation.
ReadExtrapolation		+ Try to use the extrapolation information from a previous Quasistationary if it is available and compatible. Extrapolation on page 81
SaveOptField	as Plot	Save optical field data in an LED simulation.
SpectralPlot	as Plot	Plot spectral simulation results. Illumination Spectrum on page 536
StoreExtrapolation		+ Store the extrapolation information internally at the end of the Quasistationary. Extrapolation on page 81

NOTE   Multiple entries from Table 198 must be specified in multiple `Set()` definitions, because `Set()` only takes a single option.

Table 198   Set() in Solve{}

<ident>	=<float>	Set node. Mixed-Mode Electrical Boundary Conditions on page 69
<ident>.<string>	=<float>	Set parameter <string> of compact circuit instance <ident>. Mixed-Mode Electrical Boundary Conditions on page 69
<ident>	mode Charge	Use charge boundary condition for contact <ident>. Changing Boundary Condition Type During Simulation on page 68
<ident>	mode Current	Use current boundary condition for contact <ident>. Changing Boundary Condition Type During Simulation on page 68
<ident>	mode Voltage	Use voltage boundary condition for contact <ident>. Changing Boundary Condition Type During Simulation on page 68
MSConfigs(	Table 195)	Set MSCs. Manipulating MSCs During Solve on page 486
(PreFactor	=<float> [Device=<string>] [MSConfig=<string>] [Transition=<string>])	Set MSC transition prefactors for emission, capture, or both using EPreFactor, CPreFactor, or PreFactor, respectively. Manipulating Transition Dynamics on page 487
eSHEDistributions(	Frozen)	Freeze or unfreeze (-Frozen) the electron distribution function. Using Spherical Harmonics Expansion Method on page 750
hSHEDistribution(	Frozen)	Freeze or unfreeze (-Frozen) the hole distribution function. Using Spherical Harmonics Expansion Method on page 750

Table 198   Set() in Solve{} (Continued)

HydrogenAtom	=<string>	Set the concentration of hydrogen atom. Hydrogen Transport on page 500
HydrogenIon	=<string>	Set the concentration of hydrogen ion. Hydrogen Transport on page 500
HydrogenMolecule	=<string>	Set the concentration of hydrogen molecule. Hydrogen Transport on page 500
TrapFilling	=Table 203	Set trap filling. Explicit Trap Occupation on page 468
Traps(	Table 203)	Set traps. Explicit Trap Occupation on page 468

Table 199   Standalone

Optics	Optical problem.
Wavelength	Update wavelength according to optical problem.

Table 200   Time conditions Time-Stepping on page 89, When to Write to the Current File on page 107, When to Plot on page 123

<float>	s A time point.
Range=(<float>*2)	Interval on time axis.
Range=(<float>*2) Intervals=<int> [Decade | Linear*]	Subdivided interval on time axis. Subdivision on logarithmic or linear scale.

Table 201   Transient() Transient Command on page 87

Table 232		Time step control.
AcceptNewtonParameter		Apply relaxed Newton parameters. Relaxed Newton Method on page 143
(	ReferenceStep=<float>)	1.e-9 s Apply relaxed Newton parameters for step size < ReferenceStep.
BreakCriteria{	Table 214}	Break criteria. Break Criteria: Conditionally Stopping the Simulation on page 71
Cyclic(	Table 190)	Cyclic analysis. Large-Signal Cyclic Analysis on page 93
Decrement	=<float>	2 Divisor for the step size when last step failed.
FinalTime	=<float>	s Final time.

Table 201   Transient() Transient Command on page 87 (Continued)

Increment	=<float>	2 Multiplier for the step size when last step was successful.
InitialStep	=<float>	0.1 s Initial step size.
InitialTime	=<float>	0 s Start time.
MaxStep	=<float>	1 s Maximum step size.
MinStep	=<float>	0.001 s Minimum step size.
NewtonPlotStep	=<float>	Upper limit for step size for which to write Newton plot files. NewtonPlot on page 154
NonlocalPath	(Table 229)	Dynamic Nonlocal Path Band-to-Band Tunneling Model on page 436, Handling of Derivatives on page 442
Plot{	Intervals=<int>	Number of intervals in Range.
	Range=(<float>*2)}	s Range of *t* for which to generate plots. Saving and Plotting During a Quasistationary on page 81
ReadExtrapolation		+ Try to use the extrapolation information from a previous Transient if it is available and compatible. Extrapolation on page 81
SpectralPlot	as Plot	Plot spectral simulation results. Illumination Spectrum on page 536
StoreExtrapolation		+ Store the extrapolation information internally at the end of the Transient. Extrapolation on page 81
TurningPoints(	(<float1> <float2>)...	Time point <float1> and associated advancing time-step limit <float2>.
	(Condition(Time(Table 200 [; Table 200]...)) Value=<float>)...)	Time point conditions and associated advancing time-step limit Value.

Table 202   TrapFilling= in Set() in Solve {} Explicit Trap Occupation on page 468

0	Set trap occupation to be in equilibrium with zero electron and hole concentration.
-Degradation	Return trap concentrations to initial values. Device Lifetime and Simulation on page 496
Empty	(deprecated) Set all traps to empty.
Frozen	Keep the current trap occupation unchanged until the next Set or UnSet.
Full	(deprecated) Set all traps to fully occupied.

Table 202   TrapFilling= in Set() in Solve {} Explicit Trap Occupation on page 468 (Continued)

n	(deprecated) Set trap occupation to be in equilibrium with a very high electron and zero hole concentration.
p	(deprecated) Set trap occupation to be in equilibrium with a very high hole and zero electron concentration.

Table 203   Traps() in Set() in Solve {} Explicit Trap Occupation on page 468

`[<string1>.]<string2>=<float>...`	Set occupation of trap `<string2>` of device `<string1>` to specified value.
`[<string1>.]value=<float>...`	Set occupation of traps of device `<string1>` to specified value.
`Frozen`	+ Freeze traps.

System

Table 204   System{} System Section on page 55

`<ident1>`	`<ident2>` `(<string>=<ident3>...)`	Create device instance `<ident2>` from device `<ident1>` and connect electrode `<string>` to node `<ident3>`.
`<ident1>`	`<ident2>(<ident3>...){` `<ident4>=<pvalue>...}`	Create instance `<ident2>` from parameter set `<ident1>`, connect terminals to nodes `<ident3>`, and override parameter `<ident4>` by `<pvalue>`, the type of which depends on the parameter.

`<ident1>`	`<ident2>(OpticalDevice`
	`= ["<optdev1" ...])`
	`{<ident3>=<pvalue>...}`
		Create instance `<ident2>` from parameter set `<ident1>`, connect instance to optical device instances `<optdev1>`, and override parameter `<ident4>` by `<pvalue>`, the type of which depends on the parameter.

`ACPlot(`	Table 205)	Define circuit quantities for AC analysis output. AC System Plot on page 61
`Electrical`	`(<ident>...)`	List of electrical nodes. System Section on page 55
`HBPlot`	`[<string>]`(Table 205)	Define circuit quantities for HB analysis output. Harmonic Balance on page 101
`Hint(`	`<ident>=<float>)`	Set node only for the first solve. Set, Unset, Initialize, and Hint on page 60
`Initialize(`	`<ident>=<float>)`	Set node until first transient. Set, Unset, Initialize, and Hint on page 60.
`Netlist`	`=<string>`	HSPICE netlist file. Netlist Files on page 45
`Plot`	`[<string>]` (Table 205)	Plot circuit quantities to file named `<string>`.

Table 204   System{} System Section on page 55 (Continued)

Set(	<ident>=<float>	Set node. Set, Unset, Initialize, and Hint on page 60
	<ident>.<string>= <float>)	Set parameter <string> of compact circuit instance <ident>.
Thermal	(<ident>...)	List of thermal nodes. System Section on page 55
Unset(	<ident>)	Unset node. Set, Unset, Initialize, and Hint on page 60

Table 205   Plot(), ACPlot(), and HBPlot() in System{} System Plot on page 61, AC System Plot on page 61, Harmonic Balance on page 101

<ident>		Print the voltage at node <ident>.
freq	()	Print the current AC analysis frequency.
h	(<ident1> <ident2>)	Print the heat that exits device <ident1> through node <ident2>.
i	(<ident1> <ident2>)	Print the current that exits device <ident1> through node <ident2>.
p	(<ident1> <ident2>)	Print attribute <ident2> of circuit element <ident1>.
t	(<ident>)	Print the temperature at node <ident>.
	(<ident1> <ident2>)	Print the temperature difference between two given nodes.
time	()	Print the current time in transient analysis, or quasistationary t parameter for frequency-domain analysis.
v	(<ident>)	Print the voltage at node <ident>.
	(<ident1> <ident2>)	Print the voltage difference between two given nodes.

Boundary Conditions

Table 206   Electrode{} Specifying Electrical Boundary Conditions on page 67

AreaFactor	=<float>	1 Multiplier for electrode current. Reading a Structure on page 9
Barrier	=<float>	V Barrier voltage.
Charge	=<float>	C Charge for floating electrode. Voltage must not be specified. Floating Contacts on page 223
	=(<float1> At <float2>[,] ...)	C, s Transient charge behavior. A list of pairs of charges <float1> at time <float2>, piecewise linearly interpolated.

Table 206   Electrode{} Specifying Electrical Boundary Conditions on page 67 (Continued)

Current	=<float>	$A\mu m^{d-3}$ Current boundary condition. `Voltage` is used as initial guess only.
	=(<float1> At <float2>[,] ...)	$A\mu m^{d-3}$, s Transient current behavior. A list of pairs of currents `<float1>` at time `<float2>`, piecewise linearly interpolated.
DistResist	=<float>	Ωcm^2 Distributed resistance. Resistive Contacts on page 213
	=SchottkyResist	Use Schottky contact resistance model. Resistive Contacts on page 213
eRecVelocity	=<[0,)>	$2.573e6\ cm s^{-1}$ Electron recombination velocity. Schottky Contacts on page 204
Extraction{	bulk	Specify electrode as bulk for extraction purposes. Extraction File on page 126
	drain	Specify electrode as drain for extraction purposes. Extraction File on page 126
	gate	Specify electrode as gate for extraction purposes. Extraction File on page 126
	source}	Specify electrode as source for extraction purposes. Extraction File on page 126
FGcap=(	value=<float>	$F\mu m^{d-3}$ Additional capacitance for floating electrode. Floating Metal Contacts on page 223
	name=<string>)	Coupling to electrode `<string>`. Floating Metal Contacts on page 223
hRecVelocity	=<[0,)>	$1.93e6\ cm s^{-1}$ Hole recombination velocity. Schottky Contacts on page 204
Material	=<string>	Electrode material. Contacts on Insulators on page 203
	=<string> (N=<(0,)>)	cm^{-3} Electrode material with n-doping. Contacts on Insulators on page 203
	=<string> (P=<(0,)>)	cm^{-3} Electrode material with p-doping. Contacts on Insulators on page 203
Name	=<string>	Name of electrode.
	=Regexp(<string>)	Regular expression for matching structure contacts.
Poisson	=Dirichlet	* Use Dirichlet-like boundary condition for Poisson equation.
	=Neumann	Use homogeneous Neumann boundary condition for Poisson equation at Ohmic contacts.
Resist	=<float>	$\Omega\mu m^{3-d}$ Contact resistance. Resistive Contacts on page 213
Schottky		off Contact is a Schottky contact. Schottky Contacts on page 204
SRDoping		Include the image force lowering of the potential energy barrier at Schottky contact. Resistive Contacts on page 213

Table 206 Electrode{} Specifying Electrical Boundary Conditions on page 67 (Continued)

Voltage	=<float>	V Contact voltage.
	=(<float1> At <float2>[,] ...)	V,s Transient voltage behavior. A list of pairs of voltages <float1> at time <float2>, piecewise linearly interpolated.
Workfunction	=<float>	eV Electrode workfunction. Contacts on Insulators on page 203

Table 207 HydrogenBoundary{} Boundary Conditions on page 502

HydrogenAtom	=<float>	cm^{-3} Boundary concentration.
	=reflective	Homogeneous Neumann boundary condition
HydrogenIon	=<float>	cm^{-3} Boundary concentration.
	=reflective	Homogeneous Neumann boundary condition.
HydrogenMolecule	=<float>	cm^{-3} Boundary concentration.
	=reflective	Homogeneous Neumann boundary condition.
Name	=<string>	Name of the hydrogen contact.

Table 208 RayTraceBC{} Boundary Condition for Raytracing on page 605

Fresnel		Fresnel boundary condition.
Name	=<string>	Name of the reflectivity contact or photon-recycling contact.
LayerStructure{	<float> <string> [; <float> <string>] ...}	Definition of multilayer structure used for TMM calculation. First column contains thickness of layer in μm . Second column contains material name of layer.
MapOptGenToRegions(	<string> <string> ...)	Specify list of regions to map the lumped TMM BC optical generation to.
PMIModel	=<ident> [(Table 341)]	Name of the PMI model associated with this BC contact.
QuantumEfficiency	=<float>	Define the quantum efficiency of the TMM BC optical generation.
ReferenceMaterial	=<string>	Definition of LayerStructure orientation. The topmost layer in the LayerStructure specification is connected to the region with material ReferenceMaterial.
ReferenceRegion	=<string>	Definition of LayerStructure orientation. The topmost layer in the LayerStructure specification is connected to the region with name ReferenceRegion.
Reflectivity	=<[0,1]>	0 Reflectivity.

Table 208   RayTraceBC{} Boundary Condition for Raytracing on page 605 (Continued)

{Side	="X" Periodic}	Define periodic BC at opposing x-surfaces. Periodic Boundary Condition on page 614
	="Y" Periodic}	Define periodic BC at opposing y-surfaces.
	="Z" Periodic}	Define periodic BC at opposing z-surfaces.
Transmittivity	=<[0,1]>	0 Transmittivity.

Table 209   Thermode{} Boundary Conditions for Lattice Temperature on page 226

AreaFactor	=<float>	1 Multiplier for heat fluxes. Reading a Structure on page 9
Name	=<string>	Name of thermode.
	=Regexp(<string>)	Regular expression for matching structure contacts.
Power	=<float>	$\mathrm{W\,cm}^{-2}$ Heat flux boundary condition.
SurfaceConductance	=<float>	$\mathrm{cm}^{-2}\mathrm{K}^{-1}\mathrm{W}$ Contact thermal conductance.
SurfaceResistance	=<float>	$\mathrm{cm}^{2}\mathrm{K}\mathrm{W}^{-1}$ Contact thermal resistivity.
Temperature	=<float>	K Contact temperature.

IFM

Table 210   IFM{} IFM Section on page 707

DeterministicVariation(	Table 285)	(g) Deterministic variations. Deterministic Doping Variations on page 703
Noise	[<string>] (Table 313)	(r) Noise sources. Noise Sources on page 680
RandomizedVariation	<string> (Table 319)	(g) Set sIFM models. Statistical Impedance Field Method on page 691

Math

Table 211   Math{}

Table 232		Transient time-step control.
AcceptNewtonParameter (	Table 212)	(g) Relaxed Newton method. Relaxed Newton Method on page 143
ACMethod	=Blocked	* Use block decomposition solver for ACCoupled.
ACSubMethod	=Table 224	Inner linear solver for Blocked method for ACCoupled.
AllowLayerThickness	=Everywhere	(g) Account for LayerThickness in all materials. LayerThickness Command on page 310
	=Insulator	(g) Account for LayerThickness in insulators only.
	=Metal	(g) Account for LayerThickness in metals only.
	=Semiconductor	* (g) Account for LayerThickness in semiconductors only.
AnisoSG		off (g) Use anisotropic Scharfetter–Gummel approximation for anisotropic models. Chapter 28, p. 779
AutoCNPMinStepFactor		2.0 (g) Multiplier of MinStep for the automatic activation of CNormPrint. Automatic Activation of CNormPrint and NewtonPlot on page 155
AutomaticCircuitContact		on Poisson covers the circuit. Additional Equations Available in Mixed Mode on page 141
AutoNPMinStepFactor		2.0 (g) Multiplier of MinStep for the automatic activation of NewtonPlot. Automatic Activation of CNormPrint and NewtonPlot on page 155
AutoOrientation	=(<int>...)	Miller indices for surface orientations supported by AutoOrientation. Changing Orientations Used With Auto-Orientation on page 38
AutoOrientationSmoothing Distance	=<float>	$0.0\ \mu m$ (r) Auto-orientation smoothing distance. Auto-Orientation Smoothing on page 38
AvalFlatElementExclusion	=<float>	0.0 degree (g) Exclude elements from contributing to avalanche generation. Using Avalanche Generation on page 413
AvalDerivatives		+ Compute analytic derivatives of avalanche generation. Derivatives on page 140

Table 211   Math{} (Continued)

`AvalPostProcessing`		off Impact ionization–generated carriers are not included self-consistently in the solution. Approximate Breakdown Analysis With Carriers on page 430
`AverageAniso`		+ (g) Use average-aniso approximation for anisotropic models. Chapter 28, p. 779
`AverageBoxMethod`		+ Use element-oriented element intersection box method algorithm. If disabled, use quadrilateral box method algorithm. Box Method Coefficients in 3D Case on page 1013
`BM_ExtendedPrecision`		+ Use "long double" precision to compute box method coefficients and control volumes. Extended Precision on page 1012
`BoxCoefficientsFromFile`	`[(GrdNumbering)]`	Try to read sections of the geometry file. Saving and Restoring Box Method Coefficients on page 1021
`BoxMeasureFromFile`	`[(GrdNumbering)]`	Try to read sections of the geometry file. Saving and Restoring Box Method Coefficients on page 1021
`BoxMethodFromFile`		+ Read Voronoï surface from this file if the grid file has a `VoronoiFaces` section. Box Method Coefficients in 3D Case on page 1013
`BreakAtIonIntegral`	`(<int> <float>)`	1 1 Terminate the quasistationary simulation when the `<int>` largest ionization integrals are greater than `<float>`. Approximate Breakdown Analysis on page 428
`BreakCriteria{`	Table 214`}`	Break criteria. Break Criteria: Conditionally Stopping the Simulation on page 71
`BroadeningIntegration(GaussianQuadrature(Order`	`=<int>))`	Use Gaussian quadrature to integrate the broadening spectrum of an LED simulation. Accelerating Gain Calculations and LED Simulations on page 930
`CDensityMin`		`3e-8` Acm^2 (r) Current limit for parallel electric-field computation. Electric Field Parallel to the Interface on page 371
`CheckRhsAfterUpdate`		– Check whether the RHS can be reduced further after the update error has converged. Convergence and Error Control on page 137
`CheckUndefinedModels`		+ (g) Check for undefined physical parameters. Undefined Physical Models on page 33
`CNormPrint`		(g) Convergence monitoring. CNormPrint on page 154
`ComputeDopingConcentration`		– (g) Recompute net doping based on individual doping species. Doping Specification on page 11

Table 211   Math{} (Continued)

ComputeGradQuasiFermiAt Contacts	=UseElectrostaticPotential	* Use the electrostatic potential to compute the `GradQuasiFermi` driving force within elements touching a contact. Eq. 353, p. 370
	=UseQuasiFermi	Use the quasi-Fermi potential to compute the `GradQuasiFermi` driving force within elements touching a contact. Eq. 352, p. 370
ComputeIonizationIntegrals		off Compute ionization integrals for paths that cross local field maxima in a semiconductor. Approximate Breakdown Analysis on page 428
	(WriteAll)	off Output information for all computed paths.
ConstRefPot	=<float>	eV Value for ϕ_{ref}. Quasi-Fermi Potential With Boltzmann Statistics on page 175
CoordinateSystem{	Table 1}	(g) Coordinate system of explicit coordinates in command file. Reading a Structure on page 9
cT_Range	=(<float*2)	10 80000 K (g) Lower and upper limit for carrier temperature. Numeric Parameters for Temperature Equations on page 199
CurrentPlot(	Digits=<float>	6 Number of digits in the names of quantities in the current plot file. CurrentPlot Options on page 114
	IntegrationUnit=<string>)	um Length unit for current plot integration. CurrentPlot Options on page 114
CurrentWeighting		off Compute contact currents using an optimal weighting scheme. Numeric Approaches for Contact Current Computation on page 185
Cylindrical	(<float>)	off Use the 2D mesh to simulate a 3D cylindrical device. The device is assumed to be rotationally symmetric around the vertical axis given by x = `<float>`μm. `<float>` must be less than or equal to the smallest horizontal device coordinate, and defaults to `0`. Reading a Structure on page 9
	(xAxis=<float>)	This is same as (`<float>`).
	(yAxis=<float>)	The device is assumed to be rotationally symmetric around the horizontal axis given by y = `<float>`μm. `<float>` must be less than or equal to the smallest vertical device coordinate.
DensityIntegral	(<int>)	30 (g) Defines a number of Gauss–Laguerre quadrature integration points. Using Multivalley Band Structure on page 270
DensLowLimit	=<float>	1e-100 cm^{-3} (g) Lower limit for carrier densities. Numeric Parameters for Continuity Equation on page 184

Table 211   Math{} (Continued)

Derivatives		+ Compute analytic derivatives of mobility and avalanche generation. Derivatives on page 140
Digits	=<float>	5 Approximate number of digits to which equations must be solved to be considered as converged. Convergence and Error Control on page 137
DirectCurrent		off Compute contact currents directly, using only contact nodes and their neighbors. Numeric Approaches for Contact Current Computation on page 185
DualGridInterpolation	(Method=Conservative)	Use conservative element-based interpolation for dual-grid simulations. Dual-Grid Setup for Raytracing on page 623, Single-Grid Versus Dual-Grid LED Simulation on page 922
	(Method=Simple)	Use bilinear vertex-based interpolation for dual-grid simulations. Dual-Grid Setup for Raytracing on page 623, Single-Grid Versus Dual-Grid LED Simulation on page 922
eB2BGenWithinSelectedRegions		+ (g) Restrict nonlocal path band-to-band electron generation to regions where model is active. Dynamic Nonlocal Path Band-to-Band Tunneling Model on page 436
eDrForceRefDens	=<[0,)>	0 cm^{-3} (r) Damping parameter for high-field mobility driving force, alias for RefDens_eGradQuasiFermi_Zero. Interpolation of Driving Forces to Zero Field on page 373
ElementEdgeCurrent		– (g) Use an alternative element-edge approximation of the current density compared to the default edge approximation.
ElementVolumeAvalanche		– (g) Use truncated element-vertex volumes for avalanche generation. Using Avalanche Generation on page 413
eMobilityAveraging	=Element	* (r) Use element averaged electron mobility. Mobility Averaging on page 384
	=ElementEdge	(r) Use element-edge averaged electron mobility. Mobility Averaging on page 384
EnormalInterface(	MaterialInterface= [<string>...]	Material interfaces for normal electric field computation. Normal to Interface on page 355
	RegionInterface= [<string>...])	Region interfaces for normal electric field computation. Normal to Interface on page 355

Table 211   Math{} (Continued)

EparallelToInterface(		Options for EparallelToInterface driving force. Electric Field Parallel to the Interface on page 371
	Direction=<vector>	! Direction of the current.
	Box=(<vector> <vector>))	Restrict Direction vector to vertices contained in box.
EquilibriumSolution(	Table 220)	(g) Parameters for equilibrium solution used with conductive insulators. Conductive Insulators on page 244
Error	(Table 191)=<float>	Value of ε_A . Convergence and Error Control on page 137
ErrRef	(Table 191)=<float>	Value of x_{ref} . Convergence and Error Control on page 137
ExitOnFailure		(g) off Terminate the simulation as soon as a Solve command fails.
ExitOnUnknownParameterRegion		+ (g) Exit when unknown region, region interface, or electrode appears in parameter file.
-ExitOnUnknownParameterRegion		off (g) Print warning message when unknown region, region interface, or electrode appears in parameter file.
ExtendedPrecision	[(Table 26)]	(g) off Use extended precision floating-point arithmetic. Extended Precision on page 168
Extrapolate(		off Use extrapolation to obtain an initial guess for the next solution based on the previous solutions. Extrapolation on page 81, Extrapolation on page 91
	Order=<int>)	1 Order of extrapolation in quasistationary command.
GeometricDistances		+ (g) Use enhanced distance and normal to interface computation for mobility and MLDA. Normal to Interface on page 355
HB	{Table 223}	Harmonic Balance on page 101; not device specific.
hDrForceRefDens	=<[0,)>	0 cm^{-3} (r) Damping parameter for high-field mobility driving force, alias for RefDens_hGradQuasiFermi_Zero. Interpolation of Driving Forces to Zero Field on page 373
hMobilityAveraging	=Element	(r) Use element averaged hole mobility. Mobility Averaging on page 384
	=ElementEdge	* (r) Use element-edge averaged hole mobility. Mobility Averaging on page 384

Table 211   Math{} (Continued)

IgnoreTdrUnits		off (g) Ignore TDR units when loading data from a .tdr file. Reading a Structure on page 9
ILSrc	=<string>	ILS options. Linear Solvers on page 145
ImplicitACSystem		- (g) Construct implicit AC system. AC Analysis in Single-Device Mode on page 99
IncompleteNewton		– (g) Incomplete Newton. Incomplete Newton Algorithm on page 140
(	RhsFactor=<float>	10 Maximum change in RHS to allow old Jacobian to be reused.
	UpdateFactor=<float>)	0.1 Maximum change in update to allow old Jacobian to be reused.
Interrupt	=BreakRequest	Write .tdr or .sav file and abort actual solve statement after signal INT occurs. Snapshots on page 124
	=PlotRequest	Write .tdr or .sav file and continue simulation after signal INT occurs. Snapshots on page 124
Iterations	=<0..>	50 Maximum number of Newton iterations. Convergence and Error Control on page 137
LineSearchDamping	=<(0,1]>	1 Smallest allowed damping coefficient for line search damping. Damped Newton Iterations on page 139
lT_Range	=(<float*2)	50 5000 K (g) Lower and upper limit for lattice temperature. Numeric Parameters for Temperature Equations on page 199
MeshDomain	<string> (Table 225...)	Define a named mesh domain. Mesh Domains on page 1002
MetalConductivity		+ Conductivity of metals. The thermal conductivity is simulated in any case. Transport in Metals on page 239
Method	=Table 224	Linear solver for Coupled.
	=Blocked	* Use block decomposition solver for Coupled. Linear Solvers on page 145
MixAverageBoxMethod		– Use mix average box method algorithm. Box Method Coefficients in 3D Case on page 1013
MLDAbox({	Table 226}...)	A box within which the interface is confined for the calculation of the MLDA distance function. Modified Local-Density Approximation on page 300

Table 211   Math{} (Continued)

MLDAMinDistanceToContact	=<float>	`75e-8` µm (g) Minimum distance to contact where MLDA model is switched off. MLDA Model on page 300
MVMLDAcontrols(	Table 227)	Multivalley MLDA controlling options. Using MLDA on page 304
NaturalBoxMethod		– Use edge-oriented element intersection BM algorithm. Box Method Coefficients in 3D Case on page 1013
NewtonPlot		(g) Convergence monitoring. NewtonPlot on page 154
(	Error	Write the error of all solution variables.
	MinError	Write file only if error decreases.
	NewtonPlotStep= <float>	Upper limit for step size for which to write files.
	Plot	Write everything specified in the `Plot` section. Device Plots on page 122
	Residual	Write the residuals (right-hand sides) of all equations.
	Update)	Write the updates of all solution variables from the previous step.
NoAutomaticCircuitContact		off (g) Poisson excludes the circuit. Additional Equations Available in Mixed Mode on page 141
NonLocal	(Table 228)	(cir) Nonlocal mesh. Nonlocal Meshes on page 146
	<string> (Table 228)	(g) Named nonlocal mesh.
NonLocalLengthLimit	=<float>	`1e-4` cm (g) Limit for nonlocal line length. Nonlocal Meshes on page 146
NonLocalPath	(Table 229)	Dynamic Nonlocal Path Band-to-Band Tunneling Model on page 436, Handling of Derivatives on page 442
NormalFieldCorrection	=<float>	(r) Normal field correction factor for mobility on interface points. Field Correction on Interface on page 356
NoSRHperPotential		off Omit potential derivatives of SRH recombination rate. Using Field Enhancement on page 396
NoSRHperT		off Omit temperature derivatives of SRH recombination rate. Using Field Enhancement on page 396

Table 211   Math{} (Continued)

NotDamped	=<0..>	1000 (g) Number of iterations in each Newton iteration before Bank–Rose damping is activated. Damped Newton Iterations on page 139
NumberOfAssemblyThreads	=<int>	1 (g) Number of threads for linear solver. Parallelization on page 166
NumberOfSolverThreads	=<int>	1 (g) Number of threads for assembly. Parallelization on page 166
NumberOfThreads	=<int>	1 (g) Number of threads for linear solver and assembly. Parallelization on page 166
Numerically	[(Table 191...)]	off (g) Use numeric derivatives. The optional list restricts the numeric computation to specific Jacobian blocks. Derivatives on page 140
ParallelLicense	(Table 25)	(g) Determine the behavior if insufficient parallel licenses are available.
ParallelToInterfaceInBoundary Layer		+ (r) Controls the computation of driving forces for mobility and avalanche models along interfaces. Field Correction Close to Interfaces on page 375
(	ExternalBoundary	+ Include the external boundary in the interface for which this feature applies.
	ExternalXPlane	+ Include external x-planes in the interface for which this feature implies.
	ExternalYPlane	+ Include external y-planes in the interface for which this feature implies.
	ExternalZPlane	+ Include external z-planes in the interface for which this feature implies.
	FullLayer	off Apply switch to all elements that touch an interface either by a face, an edge, or a vertex.
	Interface	+ Include semiconductor–insulator region interfaces in the interface for which this feature applies.
	PartialLayer)	on Apply switch only to elements that touch an interface by an edge (2D) or a face (in 3D).
ParameterInheritance	=Flatten	* Region parameters inherit materialwise parameter settings. Combining Parameter Specifications on page 30
	=None	Region parameter settings cause materialwise settings to be ignored.

Table 211   Math{} (Continued)

PeriodicBC		(g) Periodic boundary conditions (PBCs). Periodic Boundary Conditions on page 227
((	Table 191	Equation for which to apply PBCs. If omitted, apply to all equations (RPBC only).
	Coordinates=(<float>*2)	μm Coordinate of `Direction` axis where the PBCs will be applied. Sentaurus Device replaces coordinates outside the device with coordinates at the outer boundary (RPBC only).
	Direction=<0..2>	Direction of periodicity: `0` for x-axis, `1` for y-axis, and `2` for z-axis.
	Factor=<float>	`1e8` Tuning parameter α (RPBC only).
	MortarSide=<side>	`XMin` | `YMin` | `ZMin` Mortar side with `<side>` one of `XMin`, `XMax`, `YMin`, `YMax`, `ZMin`, or `ZMax` (MPBC only).
	Type=<type>)...)	RPBC Select PBC mode where `<type>` is one of `RPBC` or `MPBC`.
PlotExplicit		– (g) All `Plot` statements write datasets specified in `Plot` section only.
PlotLoadable		+ (g) All `Plot` statements write additional information required to load a simulation from a `.tdr` file.
PostProcess	(Transient=<ident> [(Table 341)])	(g) Use PMI `<ident>` to postprocess data. Postprocess for Transient Simulation on page 1244
PrintLinearSolver		(g) Print additional information regarding the linear solver being used. Linear Solvers on page 145
RandomizedVariation	<string> (Table 231)	(g) Use statistical impedance field method. Statistical Impedance Field Method on page 691
RecBoxIntegr	(<float> <int> <int>)	`(1e-2 10 1000)`Maximum relative deviation of covered volume, maximum number of levels, maximum number of total rectangles per box.
RecomputeQFP		Keep density variables constant, and recompute quasi-Fermi potentials when the electrostatic potential changes and carrier equations are not solved. Introduction to Carrier Transport Models on page 181
RefDens_eEparallel_ ElectricField	=<float>	0 cm^{-3} (r) Damping parameter for electron high-field mobility and avalanche driving forces. Interpolation of the Eparallel Driving Force on page 374 and Interpolation of Avalanche Driving Forces on page 426

Table 211   Math{} (Continued)

RefDens_eEparallel_ ElectricField_Aval	=<float>	0 cm^{-3} (r) Damping parameter for electron avalanche driving force. Interpolation of Avalanche Driving Forces on page 426
RefDens_eEparallel_ ElectricField_HFS	=<float>	0 cm^{-3} (r) Damping parameter for the electron high-field mobility driving force. Interpolation of the Eparallel Driving Force on page 374
RefDens_eGradQuasiFermi_ ElectricField	=<float>	0 cm^{-3} (r) Damping parameter for electron high-field mobility and avalanche driving forces. Interpolation of the GradQuasiFermi Driving Force on page 373
RefDens_eGradQuasiFermi_ ElectricField_HFS	=<float>	0 cm^{-3} (r) Damping parameter for electron high-field mobility driving force. Interpolation of the GradQuasiFermi Driving Force on page 373
RefDens_eGradQuasiFermi_ EparallelToInterface_HFS	=<float>	0 cm^{-3} (r) Damping parameter for electron high-field mobility driving force. Interpolation of the GradQuasiFermi Driving Force on page 373
RefDens_eGradQuasiFermi_Zero	=<float>	0 cm^{-3} (r) Damping parameter for electron high-field mobility driving force, alias for eDrForceRefDens. Interpolation of Driving Forces to Zero Field on page 373
RefDens_Eparallel_ ElectricField	=<float>	0 cm^{-3} (r) Damping parameter for electron and hole high-field mobility and avalanche driving forces. Interpolation of the Eparallel Driving Force on page 374 and Interpolation of Avalanche Driving Forces on page 426
RefDens_Eparallel_ ElectricField_Aval	=<float>	0 cm^{-3} (r) Damping parameter for electron and hole avalanche driving forces. Interpolation of Avalanche Driving Forces on page 426
RefDens_Eparallel_ ElectricField_HFS	=<float>	0 cm^{-3} (r) Damping parameter for the electron and hole high-field mobility driving forces. Interpolation of the Eparallel Driving Force on page 374
RefDens_GradQuasiFermi_ ElectricField	=<float>	0 cm^{-3} (r) Damping parameter for electron and hole high-field mobility and avalanche driving forces. Interpolation of the GradQuasiFermi Driving Force on page 373
RefDens_GradQuasiFermi_ ElectricField_HFS	=<float>	0 cm^{-3} (r) Damping parameter for electron and hole high-field mobility driving forces. Interpolation of the GradQuasiFermi Driving Force on page 373
RefDens_GradQuasiFermi_ EparallelToInterface_HFS	=<float>	0 cm^{-3} (r) Damping parameter for electron and hole high-field mobility driving forces. Interpolation of the GradQuasiFermi Driving Force on page 373

Table 211   Math{} (Continued)

RefDens_GradQuasiFermi_Zero	=<float>	0 cm^{-3} (r) Damping parameter for electron and hole high-field mobility driving forces, alias for DrForceRefDens. Interpolation of Driving Forces to Zero Field on page 373
RefDens_hEparallel_ElectricField	=<float>	0 cm^{-3} (r) Damping parameter for hole high-field mobility and avalanche driving forces. Interpolation of the Eparallel Driving Force on page 374 and Interpolation of Avalanche Driving Forces on page 426
RefDens_hEparallel_ElectricField_Aval	=<float>	0 cm^{-3} (r) Damping parameter for hole avalanche driving force. Interpolation of Avalanche Driving Forces on page 426
RefDens_hEparallel_ElectricField_HFS	=<float>	0 cm^{-3} (r) Damping parameter for the hole high-field mobility driving force. Interpolation of the Eparallel Driving Force on page 374
RefDens_hGradQuasiFermi_ElectricField	=<float>	0 cm^{-3} (r) Damping parameter for hole high-field mobility and avalanche driving forces. Interpolation of the GradQuasiFermi Driving Force on page 373
RefDens_hGradQuasiFermi_ElectricField_HFS	=<float>	0 cm^{-3} (r) Damping parameter for hole high-field mobility driving force. Interpolation of the GradQuasiFermi Driving Force on page 373
RefDens_hGradQuasiFermi_EparallelToInterface_HFS	=<float>	0 cm^{-3} (r) Damping parameter for hole high-field mobility driving force. Interpolation of the GradQuasiFermi Driving Force on page 373
RefDens_hGradQuasiFermi_Zero	=<float>	0 cm^{-3} (r) Damping parameter for hole high-field mobility driving force, alias for hDrForceRefDens. Interpolation of Driving Forces to Zero Field on page 373
RelErrControl		+ Use relative error control. Convergence and Error Control on page 137
RelTermMinDensity	=<(0,)>	1e3 cm^{-3} (g) Stabilization parameter for temperature relaxation term. Hydrodynamic Model Parameters on page 198
RelTermMinZeroDensity	=<(0,)>	2e8 cm^{-3} (g) Stabilization parameter for temperature relaxation term. Hydrodynamic Model Parameters on page 198
RhsAndUpdateConvergence		– Newton converged if both RHS and update are converged. Convergence and Error Control on page 137
RhsFactor	=<float>	1e10 Maximum increase of the L_2-norm of the RHS between Newton iterations. Convergence and Error Control on page 137

Table 211   Math{} (Continued)

RhsMax	=<float>	1e15 Maximum of L_2-norm of the RHS in each Newton iteration. Used only during transient simulations. Convergence and Error Control on page 137
RhsMin	=<float>	1e-5 Minimum of L_2-norm of the RHS in each Newton iteration. Convergence and Error Control on page 137
SHECutoff	=<[0,)>	5.0 (g) Maximum kinetic energy to be plotted in the SHE distribution model. Using Spherical Harmonics Expansion Method on page 750
SHEIterations	=<0..>	20 (g) Number of iterations in the SHE distribution model. Using Spherical Harmonics Expansion Method on page 750
SHEMethod	=Table 224	super (g) Linear solver for the SHE distribution model. Using Spherical Harmonics Expansion Method on page 750
SHERefinement	=<1..>	1 (g) Number of energy grid intervals inside the phonon energy spacing in the SHE distribution model. Using Spherical Harmonics Expansion Method on page 750
SHESOR		+ Use the successive over-relaxation method in the SHE distribution model. Using Spherical Harmonics Expansion Method on page 750
SHESORParameter	=<[1,2]>	1.1 (g) Successive over-relaxation parameter in the SHE distribution model. Using Spherical Harmonics Expansion Method on page 750
SHETopMargin	=<[0,)>	1.0 (g) Top energy margin in the SHE distribution model. Using Spherical Harmonics Expansion Method on page 750
SimStats		off (g) Write simulation statistics to current plot file. Simulation Statistics for Plotting and Output on page 156
	(WriteDOE	Write simulation statistics as DOE variables.
	DOE_prefix=<string>)	Use the specified prefix for DOE variables.
Smooth		off Keep mobility and recombination rates from the previous step to obtain better initial conditions for extreme nonlinear iterations.
Spice_gmin	=<float>	1e-12 S (g) SPICE minimum conductance. Mixed-Mode Math Section on page 64
Spice_Temperature	=<float>	300.15 K (g) Temperature of SPICE circuit. Mixed-Mode Math Section on page 64

Table 211   Math{} (Continued)

SponEmissionIntegration(GaussianQuadrature(Order	=<int>))	Use Gaussian quadrature to integrate the spontaneous emission spectrum of an LED simulation. Accelerating Gain Calculations and LED Simulations on page 930
StackSize	=<int>	1000000 byte (g) Stack size per thread. Parallelization on page 166
StressLimit	=<float>	1e100 Pa (g) Upper limit on stress values read from files or specified. Values exceeding the limit will be truncated to the limit. Stress Limits on page 825
StressMobilityDependence	=TensorFactor	Stress Tensor Applied to Low-Field Mobility on page 882
StressSG		off (g) Use anisotropic Scharfetter–Gummel approximation for piezo mobility models. Chapter 28, p. 779
SubMethod	=Table 224	(g) Inner linear solver for Blocked method. Linear Solvers on page 145
Surface	<string> (Table 338...)	(g) Define a surface. Mobility Degradation Components due to Coulomb Scattering on page 347, Random Geometric Fluctuations on page 684
TensorGridAniso		off (g) Use tensor-grid approximation for anisotropic piezo mobility. Tensor Grid Option on page 881
TensorGridAniso(	Piezo	off (g) Same as TensorGridAniso.
	Aniso)	off (g) Use tensor-grid approximation for anisotropic models. Chapter 28, p. 779
ThinLayer(	Mirror=(<mirror>*3))	(g) Mirror planes for simulation system axes. <mirror> is Min, Max, None, or Both. Geometric Parameters of LayerThickness Command on page 312
TransferredElectronEffect2_ eMinDerivativePerField	=<float>	-1e100 $\mathrm{cm^2V^{-1}s^{-1}}$ (r) Lower bound for velocity derivative $\partial v / \partial F_{\mathrm{hfs}}$ (electrons only). Transferred Electron Model 2 on page 365
TransferredElectronEffect2_ hMinDerivativePerField	=<float>	-1e100 $\mathrm{cm^2V^{-1}s^{-1}}$ (r) Lower bound for velocity derivative $\partial v / \partial F_{\mathrm{hfs}}$ (holes only). Transferred Electron Model 2 on page 365
TransferredElectronEffect2_ MinDerivativePerField	=<float>	-1e100 $\mathrm{cm^2V^{-1}s^{-1}}$ (r) Lower bound for velocity derivative $\partial v / \partial F_{\mathrm{hfs}}$ (electrons and holes). Transferred Electron Model 2 on page 365

Table 211   Math{} (Continued)

Transient	=BE	(g) Backward Euler method. Backward Euler Method on page 1032
	=TRBDF	* (g) TRBDF method. TRBDF Composite Method on page 1033
TrapDLN	=<int>	13 (g) Levels to approximate trap energy distribution. Energetic and Spatial Distribution of Traps on page 450
Traps(	Damping=<[0,)>	10 Damping for traps for the nonlinear Poisson equation. A value of 0 disables damping. Chapter 17, p. 449
	RegionWiseAssembly)	– Apply regionwise assembly for traps.
UpdateIncrease	=<float>	1.e100 (g) Maximum-allowed update error increase factor per Newton step.
UpdateMax	=<float>	1.e100 (g) Maximum-allowed update error in Newton algorithm.
UseSchurSolver		– (g) Replace Blocked by specialized MPBC solver. Specialized Linear Solver for MPBC on page 230
Volume	<string> (Table 337...)	(g) Define a volume. Random Band Edge Fluctuations on page 688
Wallclock		– (g) Report wallclock times rather than CPU times after each step in the simulation.
WeightedVoronoiBox		off (g) Compute-weighted coefficients and measure. Weighted Box Method Coefficients on page 1019

Table 212   AcceptNewtonParameter() Relaxed Newton Method on page 143

Digits	=<integer>	Number of relative error digits.
Error (	Electron=<float>	Absolute error parameter for electrons.
	eQuantumPotential=<float>	Absolute error parameter for electron quantum potential.
	eTemperature=<float>	Absolute error parameter for electron temperature.
	Hole=<float>	Absolute error parameter for holes.
	hQuantumPotential=<float>	Absolute error parameter for hole quantum potential.
	hTemperature=<float>	Absolute error parameter for hole temperature.
	Poisson=<float>	Absolute error parameter for potential.
	Temperature=<float>)	Absolute error parameter for lattice temperature.
ErrRef (	Electron=<float>	cm^{-3} Reference error parameter for electrons.
	eQuantumPotential=<float>	V Reference error parameter for electron quantum potential.
	eTemperature=<float>	K Reference error parameter for electron temperature.
	Hole=<float>	cm^{-3} Reference error parameter for holes.
	hQuantumPotential=<float>	V Reference error parameter for hole quantum potential.
	hTemperature=<float>)	K Reference error parameter for hole temperature.
InvokeAtDivergence		– Allow relaxed convergence to be considered for diverged solutions.
RelErrControl		Use relative error control.
RhsAndUpdateConvergence		Require both RHS and update error convergence.
RhsMin	=<float>	Minimum of RHS norm.
UpdateScale	=<float>	Additional factor for the update error.

Table 213 AxisAligned2d(),AxisAligned3d() in Meshing() Parameters Affecting Meshing Engine on page 998

GeometricAccuracy	=<float>	1.e-6 µm
MaxAngle	=<float>	165 deg
MaxAspectRatio	=<float>	1.e6
MaxBoundaryCutRatio	=<float>	0.01
MaxNeighborRatio	=<float>	4.
MinEdgeLength	=<float>	1.e-7 µm
Smoothing		off (in `AxisAligned2d`) on (in `AxisAligned3d`)

Table 214 BreakCriteria{} Break Criteria: Conditionally Stopping the Simulation on page 71

Current(	absval=<float>	$\mathrm{A}\,\mu\mathrm{m}^{d-3}$ Upper limit for absolute current value.
	contact=<string>	! Name of contact with break criterion.
	DevName=<ident>	Identifier of circuit device name (mixed mode only).
	maxval=<float>	$\mathrm{A}\,\mu\mathrm{m}^{d-3}$ Upper limit for current.
	minval=<float>	$\mathrm{A}\,\mu\mathrm{m}^{d-3}$ Lower limit for current.
	Node=<ident>)	Identifier of circuit node name (mixed mode only).
CurrentDensity(	DevName=<ident>	Identifier of device (mixed mode only).
	maxval=<float>)	$\mathrm{A}\mathrm{cm}^{-2}$ (r) Maximum current density.
DevicePower | OuterDevicePower(	absval=<float>	$\mathrm{W}\,\mu\mathrm{m}^{d-3}$ Upper limit for absolute power value.
	DevName=<ident>	Identifier of circuit device name (mixed mode only).
	maxval=<float>	$\mathrm{W}\,\mu\mathrm{m}^{d-3}$ Upper limit for power value.
	minval=<float>)	$\mathrm{W}\,\mu\mathrm{m}^{d-3}$ Lower limit for power value.
ElectricField(	DevName=<ident>	Identifier of circuit device name (mixed mode only).
	maxval=<float>)	$\mathrm{V}\mathrm{cm}^{-1}$ (r) Maximum electric field.
InnerDevicePower	as DevicePower	$\mathrm{W}\,\mu\mathrm{m}^{d-3}$ Break criteria based on inner device power.
LatticeTemperature(	DevName=<ident>	Identifier of circuit device name (mixed mode only).
	maxval=<float>)	K (r) Maximum lattice temperature.
Voltage	as Current	V Voltage break criteria.

Table 215   Criterion() Parameters Common to All Refinement Criteria on page 999

Criterion <string>		Parameter for AGM criterion with name <string>.
(	MaxElementSize=(<float>*d)	µm Maximal element size in axis directions.
	MeshDomain=<string>	Name of definition domain.
	MinElementSize=(<float>*d)	µm Minimal element size in axis directions.
	RefinementScale=<float>	8. Refinement scale per coupled adaptation iteration.
	Type=	– Select type of criterion.
	Element	Element-specific parameters in Table 216.
	| Integral0	Integral0-specific parameters in Table 217.
	| Residual	Residual-specific parameters in Table 218.

Table 216   Criterion() of Type Element Criterion Type: Element on page 1000

Criterion <string>	(Type=Element	Criterion of type Element.
	Table 215	Common criterion parameters.
	AbsError=<float>	Absolute error target.
	DataName="Table 178")	Dataset for criterion (must be defined on vertices).
	Logarithmic	– Use logarithmic formula.
	RelError=<float>)	Relative error target.

Table 217   Criterion() of Type Integral0 Criterion Type: Integral0 on page 1001

Criterion <string>	(Type=Integral0	Criterion of type Integral0.
	Table 215	Common criterion parameters.
	DataName="Table 178")	Dataset for criterion (must be defined on vertices).
	IsotropicRefinement	Choose isotropic refinement.
	QuantityPower=<float>	1. Power exponent of quantity.
	ReferenceElementSize= (<float>*d)	Extension of reference volume.
	ReferenceQuantityRange= (<float1> <float2>)	Range for reference value.

Table 218   Criterion() of Type Residual Criterion Type: Residual on page 1002

Criterion <string>	(Type=Residual	Criterion of type `Residual`.
	Table 215	Common criterion parameters.
	AbsError=<float>	Absolute error target.
	RelError=<float>)	Relative error target.

Table 219   Delaunizer2d()/Delaunizer3d() in Meshing() Parameters Affecting Meshing
Engine on page 998

CoplanarityAngle	=<float>	179. deg
CoplanarityDistance	=<float>	1.e-5 µm
DelaunayTolerance	=<float>	1.e-4
EdgeProximity	=<float>	0.05
FaceProximity	=<float>	0.05
MaxAngle	=<float>	180. deg (only for two dimensions)
MaxConnectivity	=<float>	1.e30
MaxNeighborRatio	=<float>	1.e30
MaxSolidAngle	=<float>	360. deg (only for three dimensions)
MinAngle	=<float>	0. deg
MinEdgeLength	=<float>	1.e-8 µm
SliverAngle	=<float>	175. deg
SliverDistance	=<float>	0.01

Table 220   EquilibriumSolution() Equilibrium Solution on page 175

Digits	=<float>	Relative error target.
Iterations	=<0..>	50 Maximum number of Newton iterations. Convergence and Error Control on page 137
LineSearchDamping	=<(0,1]>	1 Smallest allowed damping coefficient for line search damping. Damped Newton Iterations on page 139
NotDamped	=<0..>	1000 (g) Number of iterations in each Newton iteration before Bank–Rose damping is activated. Damped Newton Iterations on page 139
RelErrControl		+ Use relative error control. Convergence and Error Control on page 137

Table 221   FromElementGrid() in Meshing() Initialization From Element Grid File on page 995

ElementSize(	Resolution=<vector>)	0. µm Stop refinement at given size.
Gaussian(	Alpha=<float>)	3. Tuning parameter.
Method	=ElementSize | Gaussian | Laplacian	ElementSize Select method.

Table 222   GridAdaptation() in Device{} Adaptive Device Instances on page 994

AvaHomotopy(	Extrapolate	+ Use extrapolation during avalanche homotopy.
	Iterations=<int>	5 Number of Newton iterations in avalanche homotopy.
	LinearParametrization	+ Use linear parameterization of avalanche generation.
	Off)	– Disable avalanche homotopy.
Criterion <string>	(Table 215)	Specify a criterion with name <string>.
ElementLimit (		Control adaptation based on element numbers.
	Fraction=<float>	Fraction of number of marked leaf elements.
	Ignore=<float>	Absolute limit of leaf elements.
	Maximum=<float>	Ignore adaptation for number of leaf elements larger than <float>.
	Minimum=<float>)	Perform adaptation for number of leaf elements smaller than <float>.
MaxCLoops	=<int>	1e5 Maximal number of iterations per adaptive coupled system.

Table 222   GridAdaptation() in Device{} Adaptive Device Instances on page 994 (Continued)

Meshing(	AxisAligned2d(Table 213)	Parameters for quadtree approach in two dimensions.
	AxisAligned3d(Table 213)	Parameters for octree approach in three dimensions.
	Delaunizer2d(Table 219)	Parameters for delaunizer in two dimensions.
	Delaunizer3d(Table 219)	Parameters for delaunizer in three dimensions.
	FromElementGrid (Table 221)	Parameters for initialization method FromElementGrid.
	InitializationMethod= FromBoundaryAndCommand | FromElementGrid	FromBoundaryAndCommand Select the initialization method.
	UseMeshCommandFileRefinement)	+ Use refinement specifications in mesh command file for initial grid.
Poisson		+ Perform EPC smoothing step.
Smooth		+ Perform NBJI smoothing step.
Weights(	Avalanche=<float>	1 Avalanche weight in AGM dissipation rate.
	eCurrent=<float>	1 Electron current weight in AGM dissipation rate.
	hCurrent=<float>	1 Hole current weight in AGM dissipation rate.
	Recombination=<float>)	1 Recombination weight in AGM dissipation rate.

Table 223   HB{} Harmonic Balance on page 101

MDFT		– Use MDFT mode.
RhsScale	(Table 191)=<float>	Scaling of RHS in Newton (MDFT mode only).
SolveSpectrum(	Name=<string>)	Solve spectrum with (mandatory) name.
{	(<int>*n)...}	List of spectrum multi-indices. n is the number of tones. Solve Spectrum on page 103
UpdateScale	(Table 191)=<float>	Scaling of update in Newton (MDFT mode only).
ValueMin	(Table 191)=<float>	Lower bound for quantity in time domain (MDFT mode only).
ValueVariation	(Table 191)=<float>	Allowed variation of quantity in time domain (MDFT mode only).

Table 224   Linear solvers (Solvers User Guide)

ILS		Parallel, iterative linear solver. Customizable, high accuracy, and parallel performance for all problems.
(	`MultipleRHS`	– Solve linear systems with multiple right-hand sides (only for AC analysis).
	`Set=<int>)`	Use ILS options from set `<int>`.
ParDiSo		Parallel, supernodal direct solver. High accuracy and parallel performance for small and medium problems.
(	`IterativeRefinement`	– Perform up to two iterative refinement steps to improve the accuracy of the solution.
	`MultipleRHS`	– Solve linear systems with multiple right-hand sides (only for AC analysis).
	`NonsymmetricPermutation`	+ Compute an initial nonsymmetric matrix permutation and scaling, which places large matrix entries on the diagonal.
	`RecomputeNonsymmetricPermutation )`	– Compute a nonsymmetric matrix permutation and scaling before each factorization.
Super		Supernodal direct solver. Best accuracy for small problems, not parallelized.

Table 225   MeshDomain() in Math {} Mesh Domains on page 1002

Box	`( (<float1>*d) (<float2>*d) )`	Domain covered by box given by minimum `<float1>` and maximum `<float2>` values in axis directions.
MeshDomain	`=<string>`	Domain covered by referenced mesh domain.
Region	`=<string>`	Domain covered by referenced region.
Type	`= Cap | Cup`	`Cup` Build intersection (`Cap`) or union (`Cup`).

Table 226   MLDAbox({}...) Modified Local-Density Approximation on page 300

MaxX	`=<float>`	µm Upper x-coordinate of the box.
MaxY	`=<float>`	µm Upper y-coordinate of the box.
MaxZ	`=<float>`	µm Upper z-coordinate of the box.
MinX	`=<float>`	µm Lower x-coordinate of the box.
MinY	`=<float>`	µm Lower y-coordinate of the box.
MinZ	`=<float>`	µm Lower z-coordinate of the box.

Table 227   MVMLDAcontrols() Using MLDA on page 304

AveDistanceFactor	=<float>	`0.05` Factor that controls computation of an averaged distance from a vertex to the interface for the multivalley MLDA model.
Load	=<string>	Name of file from which to load energy-dependent data.
LoadWithInterpolation	=<string>	Name of file from which to load energy-dependent data, possibly obtained for different mesh.
MaxDoping4Majority	=<float>	`1e22` cm^{-3} Maximum doping concentration where the multivalley MLDA model is applied to majority carriers.
MaxIntDistance	=<float>	`1e-6` cm Distance from the interface up to which the multivalley MLDA model is applied.
Save	=<string>	Name of file where to save energy-dependent data.

Table 228   Nonlocal() Nonlocal Meshes on page 146

Table 338		(g) Interface that is part of the reference surface.
Barrier	(Table 337...)	– (g) Regions that form the tunneling barrier.
Digits	=<float>	2 (cgi) Accuracy for nonlocal tunneling currents. Nonlocal Tunneling Parameters on page 726
Direction	=<vector>	`(0 0 0)` (cgi) If nonzero, suppress the construction of nonlocal mesh lines with a direction more than `MaxAngle` degrees different from `<vector>`.
Discretization	=<float>	`1e100` cm (cgi) Maximum distance between nonlocal mesh points on a nonlocal line.
Electrode	=<string>	(g) Electrode that is part of the reference surface.
Endpoint		(r) Allow nonlocal lines that end in the region. Default is `Endpoint` for semiconductors; otherwise, `-Endpoint`.
	(Table 337...)	(g) Regions where nonlocal lines can or cannot end.
EnergyResolution	=<(0,)>	`0.005` eV (cgi) Minimum energy resolution for integrals in computation of nonlocal tunneling current. Nonlocal Tunneling Parameters on page 726
Length	=<float>	cm (cgi) Distance from the interface or contact up to which nonlocal mesh lines are constructed.
MaxAngle	=<float>	`180` deg (cgi) Suppress construction of nonlocal mesh lines that enclose an angle of more than `<float>` degrees with the vector specified by `Direction`.
Outside		+ (cgi) Allow nonlocal mesh lines to leave the device.

Table 228   Nonlocal() (Continued)

Permeable		+ (r) Allow extension of nonlocal lines (as specified by the `Permeation` parameter) into or across the region.
	(Table 337...)	+ (g) Regions into or across which nonlocal lines can or cannot be extended.
Permeation	=<float>	`0 cm` (cgi) Length by which nonlocal mesh lines are extended across the interface or contact.
Refined		+ (r) Autorefine nonlocal lines inside the region.
	(Table 337...)	+ (g) Regions in which nonlocal lines are or are not autorefined.
Transparent		+ (r) Allow nonlocal lines crossing the region.
	(Table 337...)	+ (g) Regions that nonlocal lines can or cannot cross.

Table 229   NonlocalPath() in Math{}, Quasistationary(), and Transient()

Derivative	=<int>	`0`: Without derivative computation (default) `1`: With derivative computation Handling of Derivatives on page 442
Direction	=<vector>	Frozen tunneling direction.
MaxStep	<float>	(`1.0`) Higher boundary for step-size control.
MinStep	<float>	(`1.0e-6`) Lower boundary for step-size control.
N	=<int>	(`3`) Number of Newton iterations where Jacobian entries are collected.
Postprocessing		– Switch on and off postprocessing mode.
Strategy	=<int>	Strategy for filling of system Jacobian: `1`: Collect all `2`: Collect last `N` (default) `3`: Collect last `N` with step size control

Table 230   RandomField() Spatial Correlations and Random Fields on page 693

AverageGrainSize	=<vector>	µm Average grain size along main axes.
CorrelationFunction	=Exponential	Use exponential correlations.
	=Gaussian	Use Gaussian correlations.
	=Grain	* Use grain-based correlations.
Lambda	=<vector>	µm Correlation length for main axes
MaxInternalPoints	=<int>	2147483647 Maximum-allowed number of points for Fourier transform.
Resolution	=<vector>	(0.25 0.25 0.25) Spatial resolution of exponential and Gaussian randomization.

Table 231   RandomizedVariation() in Math{} Statistical Impedance Field Method on page 691

ExtrudeTo3D		– For correlated variations, internally extrude 2D structures to three dimensions.
NumberOfSamples	=<0..>	! Number of samples.
RandomField(	Table 230)	(g) Declare random field. Spatial Correlations and Random Fields on page 693
Randomize	=<int>	0 Seed for random number generator.

Table 232   Transient time-step control Numeric Control of Transient Analysis on page 88

CheckTransientError		off Error control of transient integration method.
NoCheckTransientError		on No error control of transient integration method.
TransientDigits	=<float>	3 Relative accuracy for time-step control.
TransientError	(Table 191)=<float>	Absolute error for time-step control.
TransientErrRef	(Table 191)=<float>	Error reference for time-step control.
TrStepRejectionFactor	=<float>	Factor f_{rej} . Controlling Transient Simulations on page 1034

Physics

Table 233　Physics{} Part II on page 171

Active(	Type=QuantumWell)	Activate the localized QW model or the nonlocal QW model to use in conjunction with QWLocal or Schroedinger, respectively.
Affinity	(<ident> [(Table 341)])	(r) Use PMI model <ident> for electron affinity. Electron Affinity on page 1151
AlphaParticle(	Table 276)	(g) Generation by alpha particles. Alpha Particles on page 666
AnalyticTEP		(g) Analytic expression for thermoelectric power. Thermoelectric Power (TEP) on page 913
Aniso(	Table 279)	Anisotropic properties. Chapter 28, p. 779
AreaFactor	=<float>	1 (g) Multiplier for current and heat flux densities at electrodes and thermodes. Reading a Structure on page 9
BarrierLowering		off (c) Use barrier lowering for Schottky contact. Barrier Lowering at Schottky Contacts on page 208
Charge((	Table 282)...)	Oxide and insulator interface charges. Insulator Fixed Charges on page 471
ComplexRefractiveIndex(	Table 283)	off (g) Use complex refractive index model. Complex Refractive Index Model on page 578
CondInsulator		(r) Turn an insulator into a conductive insulator. Conductive Insulators on page 244
DefaultParametersFromFile		Initialize default parameters from parameter files instead of using built-in values. Default Parameters on page 35
DeterministicVariation(	Table 285)	(g) Deterministic variations. Deterministic Variations on page 703
Dipole(		(i) Use dipole interface model. Dipole Layer on page 174
	Reference=<string>)	! Reference side <string> (either region or material name).
Discontinuity		Create discontinuous interface(s). Discontinuous Interfaces on page 231
DistResist	=<float>	$\Omega\mathrm{cm}^2$ (i) Distributed resistance at metal–semiconductor interface. Transport in Metals on page 239
	=SchottkyResist	Emulate a Schottky interface. Transport in Metals on page 239

Table 233 Physics{} Part II on page 171 (Continued)

eBarrierTunneling	`<string>` [(Table 238)]	off (g) Nonlocal tunneling from and to conduction band. Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722
EffectiveIntrinsicDensity	(Table 290)	(r) Band gap and bandgap narrowing. Band Gap and Electron Affinity on page 249
EffectiveMass	(GaussianDOS)	(r) Use simplified Gaussian density-of-states model for organic semiconductors. Gaussian Density-of-States for Organic Semiconductors on page 264
	(`<ident>` [(Table 341)])	(r) Use PMI model `<ident>` for effective mass. Effective Mass on page 1154
eMLDA	[()]	– (r) MLDA model for electrons. Modified Local-Density Approximation on page 300
(	LambdaTemp)	+ (r) Use temperature-dependent λ for both electrons and holes.
eMobility(	Table 272)	(r) Electron mobility model. Chapter 15, p. 317
eMultiValley		off (r) Multivalley statistics. Multivalley Band Structure on page 267, Multivalley Band Structure on page 835
eMultiValley(	DensityIntegral	off (r) Numeric density computation. Using Multivalley Band Structure on page 270
	kpDOS	off (r) Two-band $k \cdot p$ models for electron Δ_2 valleys. Using Multivalley Band Structure on page 270
	mcDOS	off (r) Monte Carlo DOS. Using Multivalley Band Structure on page 270, Using MLDA on page 304
	MLDA	off (r) Multivalley MLDA quantization model. Modified Local-Density Approximation on page 300, Using Multivalley Band Structure on page 837, Inversion Layer on page 844
	MLDA(-Nonparabolicity)	off (r) Exclude band nonparabolicity in MLDA model. Using MLDA on page 304
	Nonparabolicity	off (r) Band nonparabolicity. Nonparabolic Band Structure on page 268
	parfile	on (r) With kpDOS, it adds the parameter file valleys. Using Multivalley Band Structure on page 270
	RelativeToDOSMass	off (r) Multivalley effective DOS. Using Multivalley Band Structure on page 270
	ThinLayer)	off (r) Geometric quantization model. Using Multivalley Band Structure on page 270, Using MLDA on page 304

Table 233   Physics{} Part II on page 171 (Continued)

EnergyRelaxationTimes	(<ident> [(Table 341)])	Use PMI model <ident> to compute energy relaxation times. Energy Relaxation Times on page 1158
	(constant)	Use constant energy relaxation times.
	(formula)	Use the value of formula in the parameter file.
	(irrational)	Use the ratio of two irrational polynomials. Energy-Dependent Energy Relaxation Time on page 769
eNMP(	Table 292)	(i) Extended nonradiative multiphonon (eNMP) model. Extended Nonradiative Multiphonon Model on page 513
eQCvanDort		off (r) van Dort model for electrons. van Dort Quantization Model on page 284
eQuantumPotential	[(Table 294)]	– (r) Activate electron density gradient quantum correction. Density Gradient Quantization Model on page 294
eQuasiFermi	=<float>	V (r) Initial quasi-Fermi potential specification for electrons. Regionwise Specification of Initial Quasi-Fermi Potentials on page 179
eRecVelocity	=<[0,)>	$2.573e6 \ cms^{-1}$ (i) Electron recombination velocity. Electric Boundary Conditions for Metals on page 240
eSHEDistribution		off (r) Specify the region where the electron SHE distribution is calculated. Using Spherical Harmonics Expansion Method on page 750
	(Table 295)	
eThermionic		(i) Thermionic emission model for electrons. Conductive Insulators on page 244, Thermionic Emission Current on page 763
	(HCI)	(i) Inject hot electrons locally. Destination of Injected Current on page 738
	(Organic_Gaussian)	(i) Thermionic-like Gaussian emission model at organic heterointerfaces for electrons. Gaussian Transport Across Organic Heterointerfaces on page 766
ExternalSchroedinger	<string> (Table 296)	(g) Connection to external 2D Schrödinger solver. External 2D Schrödinger Solver on page 292
Fermi		off (g) Fermi statistics. Fermi Statistics on page 176
	(-WithJoyceDixon)	(g) Fermi statistics with old Wuensche approximation for Fermi integrals. Fermi Statistics on page 176
FloatCoef	=<float>	0 (g) Interpolation coefficient for initial guess in floating wells. Initial Guess for Electrostatic Potential and Quasi-Fermi Potentials in Doping Wells on page 178
GateCurrent(	Table 297)	(i) Gate currents (hot-carrier injection, some of the tunneling models).

Table 233   Physics{} Part II on page 171 (Continued)

GaussianDOS_full		(r) Use Gaussian density-of-states model for organic semiconductors. Gaussian Density-of-States for Organic Semiconductors on page 264
hBarrierTunneling	`<string>` [(Table 238)]	off (g) Nonlocal tunneling from and to valence band. Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722
HeatCapacity(	Table 302)	(r) Heat capacity.
HeatPreFactor	`=<float>`	1. (r) Scaling factor for lattice heat generation. Scaling of Lattice Heat Generation on page 200
HeatSource(	`<ident>)`	Name of the PMI model.
HeavyIon(	Table 277)	off (g) Generation by heavy ions. Heavy Ions on page 668
HeteroInterface		(i) Double points at interfaces. Abrupt and Graded Heterojunctions on page 10
hMLDA(	`[()]`	– (r) MLDA model for holes. Modified Local-Density Approximation on page 300
	`LambdaTemp)`	+ (r) Use temperature-dependent λ for both electrons and holes.
hMobility(	Table 272)	(r) Hole mobility model. Chapter 15, p. 317
hMultiValley		off (r) Multivalley statistics. Multivalley Band Structure on page 267, Multivalley Band Structure on page 835

Table 233   Physics{} Part II on page 171 (Continued)

hMultiValley(	DensityIntegral	off (r) Numeric density computation. Using Multivalley Band Structure on page 270
	kpDOS	off (r) Six-band $k \cdot p$ model for hole bands. Multivalley Band Structure on page 267
	mcDOS	off (r) Monte carlo DOS. Using Multivalley Band Structure on page 270, Using MLDA on page 304
	MLDA	off (r) Multivalley MLDA quantization model. Modified Local-Density Approximation on page 300, Using Multivalley Band Structure on page 837
	MLDA(-Nonparabolicity)	off (r) Exclude band nonparabolicity in MLDA. Using MLDA on page 304
	Nonparabolicity	off (r) Band nonparabolicity. Nonparabolic Band Structure on page 268
	parfile	on (r) With kpDOS, it adds the parameter file valleys. Using Multivalley Band Structure on page 270
	RelativeToDOSMass	off (r) Multivalley effective DOS. Using Multivalley Band Structure on page 270
	ThinLayer)	off (r) Geometric quantization model. Using Multivalley Band Structure on page 270, Using MLDA on page 304
hQCvanDort		off (r) van Dort model for holes. van Dort Quantization Model on page 284
hQuantumPotential	[(Table 294)]	– (r) Activate hole density gradient quantum correction. Density Gradient Quantization Model on page 294
hQuasiFermi	=<float>	V (r) Initial quasi-Fermi potential specification for holes. Regionwise Specification of Initial Quasi-Fermi Potentials on page 179
hRecVelocity	=<[0,)>	$1.93e6$ cms^{-1} (i) Hole recombination velocity. Electric Boundary Conditions for Metals on page 240
hSHEDistribution		off (r) Specify the region where the hole SHE distribution is calculated. Using Spherical Harmonics Expansion Method on page 750
	(Table 295)	
hThermionic		(i) Thermionic emission model for holes. Conductive Insulators on page 244, Thermionic Emission Current on page 763
	(HCI)	(i) Inject hot holes locally. Destination of Injected Current on page 738
	(Organic_Gaussian)	(i) Thermionic-like Gaussian emission model at organic heterointerfaces for holes. Gaussian Transport Across Organic Heterointerfaces on page 766

Table 233   Physics{} Part II on page 171 (Continued)

Hydrodynamic	[()]	(g) Hydrodynamic model for electrons and holes. Hydrodynamic Model for Current Densities on page 184, Hydrodynamic Model for Temperatures on page 195
	(eTemperature)	(g) Hydrodynamic model for electrons only. Hydrodynamic Model for Current Densities on page 184, Hydrodynamic Model for Temperatures on page 195
	(hTemperature)	(g) Hydrodynamic model for holes only. Hydrodynamic Model for Current Densities on page 184, Hydrodynamic Model for Temperatures on page 195
HydrogenDiffusion		off (ri) Hydrogen transport model without reaction or hydrogen type specification. Using MSC–Hydrogen Transport Degradation Model on page 507
	(Table 304)	off (ri) Hydrogen transport model with reaction or hydrogen type specification. Using MSC–Hydrogen Transport Degradation Model on page 507
IncompleteIonization(	Table 306)	Incomplete ionization. Chapter 13, p. 277
LatticeTemperatureLimit	=<float>	K Maximum lattice temperature. Break Criteria: Conditionally Stopping the Simulation on page 71
LayerThickness		off Thickness extraction command. LayerThickness Command on page 310
(	ChordWeight=<float>	0 Weight of chord length. Thickness Extraction on page 313
	MaxFitWeight=<float>	0 Thickness Extraction on page 313
	MinAngle=(<float>*2)	0 0 Angle constraints. Thickness Extraction on page 313
	Thickness=<float>)	µm Explicit thickness value.
LED(	Table 268)	Activate LED framework.
MagneticField	=<vector>	T (g) Magnetic field. Chapter 32, p. 897
Mechanics(	Table 307)	(g) Mechanical stress solver. Mechanics Solver on page 890
MetalResistivity(	<ident> [(Table 341)])	PMI for metal resistivity. Metal Resistivity on page 1260
MetalWorkfunction(	Table 308)	(r) Metal workfunction. Metal Workfunction on page 242
Mobility(	Table 272)	(r) Mobility model. Chapter 15, p. 317
MoleFraction(	Table 310)	Mole fractions. Mole-Fraction Specification on page 17
MSConfigs(	MSConfig (Table 311...)...)	(r) Multistate configurations. Specifying Multistate Configurations on page 475

Table 233   Physics{} Part II on page 171 (Continued)

MSPeltierHeat		(i) Peltier heat at metal–semiconductor interfaces or semiconductor contacts. Heating at Contacts, Metal–Semiconductor and Conductive Insulator–Semiconductor Interfaces on page 916
MultiValley		off (r) Multivalley statistics. Multivalley Band Structure on page 267, Multivalley Band Structure on page 835
MultiValley(	DensityIntegral	off (r) Numeric density computation. Using Multivalley Band Structure on page 270
	kpDOS	off (r) $k \cdot p$ model for electrons and holes. Using Multivalley Band Structure on page 270
	MLDA	off (r) Multivalley MLDA quantization model. Modified Local-Density Approximation on page 300, Using Multivalley Band Structure on page 837, Inversion Layer on page 844
	MLDA(-Nonparabolicity)	off (r) Exclude band nonparabolicity in MLDA. Using MLDA on page 304
	Nonparabolicity	off (r) Band nonparabolicity. Nonparabolic Band Structure on page 268
	parfile	on (r) With kpDOS, it adds the parameter file valleys. Using Multivalley Band Structure on page 270
	RelativeToDOSMass)	off (r) Multivalley effective DOS. Using Multivalley Band Structure on page 270
NBTI(	Table 312)	(i) NBTI degradation model. Two-Stage NBTI Degradation Model on page 509
Noise	[<string>] (Table 313)	(r) Noise sources. Noise Sources on page 680
OpticalAbsorptionHeat(	ScalingFactor=<float>	1 Optical Absorption Heat on page 928
	Table 259)	Optical Absorption Heat on page 928
Optics(	Table 315)	Specifying the Type of Optical Generation Computation on page 534
Piezo(	Table 317)	(r) Stress and strain models. Using Stress and Strain on page 823
Piezoelectric_Polarization	(<ident> [(Table 341)])	Use PMI model <ident> to compute piezoelectric polarization. Piezoelectric Polarization on page 1219
	(strain)	Use strain model to compute piezoelectric polarization. Strain Model on page 883
	(stress)	Use stress model to compute piezoelectric polarization. Stress Model on page 885

Table 233 Physics{} Part II on page 171 (Continued)

Polarization		off (r) Use ferroelectric model. Chapter 29, p. 797
	`(Memory=<2..>)`	`10` Maximum nesting of minor loops. Using Ferroelectrics on page 797
PostTemperature		(g) Use simplified self-heating model. Uniform Self-Heating on page 190
		* Compute dissipated power as integral of Joule heat over entire device.
	`(IV_diss)`	(g) Compute dissipated power as $\sum IV$ over all electrodes.
	`(IV_diss(<string>...))`	(g) Compute dissipated power as $\sum IV$ over user-selected electrodes.
QWLocal(	Table 250)	Localized QW model parameters. Localized Quantum-Well Model on page 978
Radiation(	Table 278)	Radiation model. Chapter 22, p. 665
RandomizedVariation	`<string>` (Table 319)	(g) Set sIFM models. Statistical Impedance Field Method on page 691
RayTraceBC(	Table 252)	Physics material or region interface–based definition of boundary conditions. Boundary Condition for Raytracing on page 605
RecGenHeat		(g) Generation–recombination processes act as heat sources. Hydrodynamic Model for Temperatures on page 195
(	`OptGenOffset=<float>`	`0.5` Divide contribution of optical generation rate into energy gain/loss terms H_n and H_p. Hydrodynamic Model for Temperatures on page 195
	`OptGenWavelength=<float>)`	µm Wavelength if optical generation is loaded from file. Hydrodynamic Model for Temperatures on page 195
Recombination(	Table 234)	Generation–recombination model. Chapter 16, p. 391
Schottky		off (i) Use Schottky boundary conditions. Electric Boundary Conditions for Metals on page 240
Schroedinger	(Table 320)	(i) Schrödinger solver. 1D Schrödinger Solver on page 285
	`<string>` (Table 320)	(g) Schrödinger solver on named nonlocal mesh.

Table 233   Physics{} Part II on page 171 (Continued)

SingletExciton		off (ri) Activate region or interface for singlet exciton equation.
(	FluxBC	off (i) Impose a zero flux boundary condition on specified interface. Using the Singlet Exciton Equation on page 237
	BarrierType (Table 281)	(i) Set the barrier type at organic heterointerface. Using the Singlet Exciton Equation on page 237
	Recombination (Table 254))	off (r) Switch on generation and recombination terms in singlet exciton equation. Using the Singlet Exciton Equation on page 237
TATNonlocalPathNC	=<float>	cm^{-3} (i) Room temperature effective density-of-states N_C for electron trap-assisted tunneling from Schottky contacts or Schottky metal–semiconductor interfaces. Using Dynamic Nonlocal Path TAT Model on page 402
Temperature	=<float>	300 K (g) Device (lattice) temperature.
TEPower	(<string>)	(gr) Use PMI to compute thermoelectric power. Using Thermoelectric Power on page 915
	(Analytic)	(gr) Use analytic thermoelectric power. Using Thermoelectric Power on page 915
ThermalConductivity(	Table 323)	(r) Thermal conductivity.
Thermionic		(i) Thermionic emission model for electrons and holes. Conductive Insulators on page 244, Thermionic Emission Current on page 763
	(HCI)	(i) Inject hot carriers locally. Destination of Injected Current on page 738
	(Organic_Gaussian)	(i) Thermionic-like Gaussian emission model at organic heterointerfaces. Gaussian Transport Across Organic Heterointerfaces on page 766
Thermodynamic		off (g) Thermodynamic transport model. Thermodynamic Model for Current Densities on page 183, Thermodynamic Model for Lattice Temperature on page 193
Traps((	Table 325)...)	Traps. Chapter 17, p. 449

Generation and Recombination

Table 234   Recombination() Chapter 16, p. 391

`<ident>`	`[(Table 341)]`	Use PMI model `<ident>`. Generation–Recombination Model on page 1094
`Auger`		off (r) Auger recombination. Auger Recombination on page 408
	`(WithGeneration)`	off (r) Auger recombination and generation.
`Avalanche(`	Table 235)	off (r) Impact ionization. Avalanche Generation on page 413
`Band2Band(`	Table 236)	off (r) Band-to-Band Tunneling Models on page 431
`CDL(`	Table 258)	off (r) Coupled defect level recombination. Coupled Defect Level (CDL) Recombination on page 405
`ConstantCarrierGeneration`	`(value=<float>)`	off (r) Constant carrier generation. Constant Carrier Generation on page 412
`eAvalanche(`	Table 235)	off (r) Electron impact ionization. Avalanche Generation on page 413
`hAvalanche(`	Table 235)	off (r) Hole impact ionization. Avalanche Generation on page 413
`intrinsicRichter`		off (r) Extended recombination model for silicon, covering Auger and radiative recombination. Intrinsic Recombination Model for Silicon on page 409
`Radiative`		– (r) Radiative recombination. Radiative Recombination on page 407
`SRH(`	Table 258)	off (r) Shockley–Read–Hall recombination. Shockley–Read–Hall Recombination on page 391
`SurfaceSRH`		off (i) Interface Shockley–Read–Hall recombination. Surface SRH Recombination on page 404
`TrapAssistedAuger`		off (r) Trap-assisted Auger recombination. Trap-Assisted Auger Recombination on page 403

Table 235   Avalanche() Avalanche Generation on page 413

`<ident> [(Table 341)]`	Use PMI model `<ident>`. Avalanche Generation Model on page 1100
`BandgapDependence`	– Include a dependency on the energy bandgap in the avalanche generation models. Using Avalanche Generation on page 413
`CarrierTempDrive`	Use temperature driving force (default for hydrodynamic simulation). Avalanche Generation With Hydrodynamic Transport on page 427
`ElectricField`	Use plain electric field driving force. Approximate Breakdown Analysis on page 428
`Eparallel`	Use current-parallel electric field driving force. Driving Force on page 426
`GradQuasiFermi`	* Use gradient quasi-Fermi potential driving force. For hydrodynamic simulation, default is `CarrierTempDrive`. Driving Force on page 426
`Hatakeyama`	Use Hatakeyama model. Hatakeyama Avalanche Model on page 423
`Lackner`	Use Lackner model. Lackner Model on page 418
`Okuto`	Use Okuto–Crowell model. Okuto–Crowell Model on page 417
`UniBo`	Use University of Bologna model. University of Bologna Impact Ionization Model on page 419
`UniBo2`	Use new University of Bologna impact ionization model. New University of Bologna Impact Ionization Model on page 421
`vanOverstraeten`	* Use van Overstraeten model. van Overstraeten – de Man Model on page 416

Table 236   Band2Band() Band-to-Band Tunneling Models on page 431

`DensityCorrection`	`=Local`	Use density correction. Schenk Density Correction on page 434
	`=None`	* Use plain densities. Schenk Density Correction on page 434
`FranzDispersion`		– Use Franz dispersion in the direct nonlocal path model. Using Nonlocal Path Band-to-Band Model on page 440
`InterfaceReflection`		+ Consider interface reflection in the nonlocal path model. Using Band-to-Band Tunneling on page 431

Table 236   Band2Band() Band-to-Band Tunneling Models on page 431 (Continued)

Model	=E1	Use simple model with $P = 1$. Simple Band-to-Band Models on page 434
	=E1_5	Use simple model with $P = 1.5$. Simple Band-to-Band Models on page 434
	=E2	Use simple model with $P = 2$. Simple Band-to-Band Models on page 434
	=Hurkx	Use Hurkx model. Hurkx Band-to-Band Model on page 435
	=NonlocalPath	Use nonlocal path model. Dynamic Nonlocal Path Band-to-Band Tunneling Model on page 436
	=Schenk	Use Schenk model. Schenk Model on page 433
ParameterSetName	=(<string>...)	Named parameter sets to be used. Using Band-to-Band Tunneling on page 431

Table 237   BPM() Beam Propagation Method on page 647

Bidirectional(	Error=<float>	! Relative error used as a break criterion for iterative algorithm in bidirectional beam propagation method.
	Iterations=<int>)	! Maximum number of iterations used as a break criterion for iterative algorithm in bidirectional beam propagation method.
Boundary(	GridNodes=<float>*2	! Number of PML boundary grid nodes to be inserted at left and right sides.
	Order=<1..2>	! Order of spatial variation of complex stretching parameter.
	Side=<string>	! "X", "Y", or "Z".
	StretchingParameterImag= (<float>*2)	! Minimum and maximum values of imaginary part of stretching parameter.
	StretchingParameterReal= (<float>*2)	! Minimum and maximum values of real part of stretching parameter.
	Type="PML"	! Use PML boundary conditions.
	VacuumGridNodes= (<float>*2))	! Number of vacuum grid nodes to be inserted at left and right sides.

Table 237   BPM() Beam Propagation Method on page 647 (Continued)

Excitation(	CenterGauss=<vector>	μm Gaussian center. Size of vector is $d-1$.
	SigmaGauss=<vector>	μm Gaussian half width. Size of vector is $d-1$.
	TruncationPositionX= (<float>*2)	Left and right truncation positions of plane wave for x-axis.
	TruncationPositionY= (<float>*2)	Left and right truncation positions of plane wave for y-axis.
	TruncationSlope=<vector>	Plane-wave truncation slope. Size of vector is $d-1$.
	Type="Gaussian"	Use Gaussian excitation.
	Type="PlaneWave")	Use truncated plane wave excitation.
GridNodes	=<vector>	! Number of grid nodes in each spatial dimension.
ReferenceRefractiveIndex	=<float>	! Value for reference refractive index. General on page 649
	=average	Use average refractive index in propagation plane as reference refractive index.
	=fieldweighted	Use field-weighted refractive index in propagation plane as reference refractive index.
	=maximum	Use maximum refractive index in propagation plane as reference refractive index.
ReferenceRefractiveIndexDelta	=<float>	`ReferenceRefractiveIndexDelta` is added to `ReferenceRefractiveIndex` in the calculation. To be used for fine-tuning the numerics. General on page 649

Table 238   eBarrierTunneling() and hBarrierTunneling() Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722

Band2Band	=None	* No band-to-band tunneling.
	=Full	Include band-to-band tunneling with consistent parallel momentum integral with the direct nonlocal path band-to-band tunneling model.
	=Simple	Include band-to-band tunneling with simple parallel momentum integral.
	=UpsideDown	Include band-to-band tunneling with nonphysical parallel momentum integral.
BandGap		– Allow tunneling into the band gap at the interface for which tunneling is specified. Use this option for backward compatibility only.
BarrierLowering		– Apply a position-dependent barrier lowering for tunneling barrier.

Table 238   eBarrierTunneling() and hBarrierTunneling() Nonlocal Tunneling at Interfaces, Contacts, and Junctions on page 722 (Continued)

Multivalley		– Use multivalley band structure. Band-to-Band Contributions to Nonlocal Tunneling Current on page 734
PeltierHeat		– Include Peltier heating terms for tunneling carriers. Eq. 788, p. 735
Schroedinger		– Schrödinger equation–based model instead of WKB for tunneling probabilities. This option does not work with the `TwoBand` or `Band2Band` option. Schrödinger Equation–Based Tunneling Probability on page 731
Transmission		– Use additional interface transmission coefficients. Eq. 778, p. 730
TwoBand		– Use two-band dispersion relation. Eq. 777, p. 730

Table 239   ElectricField() in SRH() and CDL() SRH Field Enhancement on page 396

DensityCorrection	=Local	(r) Use density correction. Schenk TAT Density Correction on page 398
	=None	* (r) Use local densities.
Lifetime	=Constant	* (r) No field-enhanced lifetime.
	=Hurkx	(r) Use Hurkx model for lifetime enhancement. Hurkx TAT Model on page 399
	=Schenk	(r) Use Schenk model for lifetime enhancement. Schenk Trap-Assisted Tunneling (TAT) Model on page 397

Table 240   Farfield(...) in Physics{Optics(OpticalSolver(RayTracing(...)))} Far Field and Sensors for Raytracing on page 620

Origin	=Auto	Automatically compute origin as the center of the device. `Auto` is the default.
	=<vector>	User-specified origin as a vector in micrometers.
Discretization	=<int>	Default is `360` for two dimensions, and `36` for three dimensions.
ObservationRadius	=<float>	Radius in micrometers. Default is `1e6` μm , that is, 1 m.
Sensor(	Table 256)	Specify a sensor detector.
SensorSweep(	Table 257)	Specify sensor sweep.

Table 241   FDTD() Specifying the Optical Solver on page 554

GenerateMesh		Control of tensor mesh generation using Sentaurus Mesh.
(	ForEachWavelength	Generate tensor mesh whenever the wavelength changes compared with the previous FDTD solution.
	Once	Generate tensor mesh once at the beginning of the simulation.
	Wavelength=(<float>*<0..m>))	Specify list of strictly monotonically increasing wavelengths between which the tensor mesh is generated only once.

Table 242   FromFile() Loading Solution of Optical Problem From File on page 640 and
Controlling Interpolation When Loading Optical Generation Profiles on page 659

DatasetName	=AbsorbedPhotonDensity | OpticalGeneration	AbsorbedPhotonDensity Name of dataset to be loaded from file.
GridInterpolation	=Conservative | Simple	Interpolation algorithm to be used if source and destination grid are different.
IdentifyingParameter	=(<string>...)	! Name of identifying parameters or parameter paths.
ImportDomain(	Table 243)	Specify source and destination regions as well as domain truncation for interpolation.
ProfileIndex	=<int>	0 ID of loaded profiles after sorting with respect to leading IdentifyingParameter.
ShiftVector	=<vector>	(0,0,0) Displacement of source grid.
SpectralInterpolation	=Linear | Off | PiecewiseConstant	Off Type of interpolation between loaded profiles.
WeightedAPDintegrationlayers	=<int>	Default is the number of regions with a limit of 20. However, you can choose a higher number. Accurate Absorbed Photon Density for 1D Optical Solvers on page 575
WeightedAPDIntegrationSet Boundaries	=(<float>...)	Specifies the boundaries of layers measured from the illumination window in propagation direction.

Table 243   ImportDomain() Controlling Interpolation When Loading Optical Generation
Profiles on page 659

DestinationBoxCorner1	=<vector>	(-Inf, -Inf, -Inf) Lower-left corner of box in destination grid used to restrict interpolation domain.
DestinationBoxCorner2	=<vector>	(Inf, Inf, Inf) Upper-right corner of box in destination grid used to restrict interpolation domain.
DestinationRegions	=(<string>...)	Regions in destination grid selected for interpolation.
SourceBoxCorner1	=<vector>	(-Inf, -Inf, -Inf) Lower-left corner of box in source grid used to restrict interpolation domain.
SourceBoxCorner2	=<vector>	(Inf, Inf, Inf) Upper-right corner of box in source grid used to restrict interpolation domain.
SourceRegions	=(<string>...)	Regions in source grid selected for interpolation.

Table 244   Medium() Transfer Matrix Method on page 625

ExtinctionCoefficient	=<float>	1
Location	=top	! Position of medium with respect to extracted layer structure.
	=bottom	Position of medium with respect to extracted layer structure.
Material	=<string>	Name of material.
RefractiveIndex	=<float>	1

Table 245   NonlocalPath() in SRH() Dynamic Nonlocal Path Trap-Assisted Tunneling on
page 400

Fermi		– Use Fermi statistics.
Lifetime	=Hurkx	* Use Hurkx model for lifetime enhancement.
	=Schenk	Use Schenk model for lifetime enhancement.
TwoBand		– Use Two-band dispersion for the transmission coefficient.

Table 246   OptBeam(()...) Using Optical Beam Absorption Method on page 646

LayerStackExtraction(	ComplexRefractiveIndexThreshold=<float>	0 Choose threshold value for layer creation when using ElementWise extraction mode.
	Mode=RegionWise | ElementWise	RegionWise Specify whether layer stack is created on a per-element or per-region basis.
	Position=(<float>*3)	Specify starting point of extraction line.
	WindowName=<string>	Reference to illumination window in Excitation section.
	WindowPosition=<ident>)	Center Specify starting point of extraction line in terms of a cardinal direction (North, South, East, West, NorthEast, SouthEast, NorthWest, SouthWest).

Table 247   OpticalGeneration{} Specifying the Type of Optical Generation Computation on page 534 and Controlling Interpolation When Loading Optical Generation Profiles on page 659

AutomaticUpdate		+ Controls whether optical generation is recomputed if quantities on which it depends are not up-to-date.
ComputeFromMonochromaticSource		Optical Generation From Monochromatic Source on page 536
(	Scaling=<float>	1
	TimeDependence (Table 261))	

Table 247   OpticalGeneration{} Specifying the Type of Optical Generation Computation on
page 534 and Controlling Interpolation When Loading Optical Generation Profiles
on page 659 (Continued)

ComputeFromSpectrum		Illumination Spectrum on page 536
(	KeepSpectralData	Keep spectral data (for example, for plotting or to avoid recomputation of optics) when computing the optical generation resulting from an illumination spectrum.
	RefreshEveryTime	Force recomputation of respective optical generation contribution at every occasion.
	Scaling=<float>	1
	Select (Table 255)	Active parameters of multidimensional spectrum file.
	TimeDependence (Table 261))	
QuantumYield	=<float>	1 Quantum Yield Models on page 544
QuantumYield(	EffectiveAbsorption	Quantum Yield Models on page 544
	Factor=<float>	1 Quantum Yield Models on page 544
	StepFunction (Table 260)	Quantum Yield Models on page 544
	Unity)	Quantum Yield Models on page 544
ReadFromFile		Loading and Saving Optical Generation From and to File on page 542
(	DatasetName= AbsorbedPhotonDensity | OpticalGeneration	
	TimeDependence (Table 261)	
	Scaling=<float>	1
	RefreshEveryTime	Force recomputation of respective optical generation contribution at every occasion.
	GridInterpolation= Simple | Conservative	Interpolation algorithm to be used if source and destination grid are different.
	ShiftVector=<vector>	(0,0,0) Displacement of source grid.
	ImportDomain (Table 243))	Specify source and destination regions as well as domain truncation for interpolation.
Scaling	=<float>	1

Table 247   OpticalGeneration{} Specifying the Type of Optical Generation Computation on page 534 and Controlling Interpolation When Loading Optical Generation Profiles on page 659 (Continued)

SetConstant		Constant Optical Generation on page 543
(	RefreshEveryTime	Force recomputation of respective optical generation contribution at every occasion.
	TimeDependence(Table 261)	
	Value=<float>)	$s^{-1} cm^{-3}$ Value for optical generation rate.
TimeDependence(	Table 261)	Specification of type of time dependency.

Table 248   OpticalTurningPoints() Optical Turning Points on page 552

Dt	=<float>	Limiting time step for range $[t_0 t_3]$ for time-dependence FromFile only. The default value is given by the smallest time interval specified in the OptGenTransientScaling file defined in the File section. For all other types of time dependence, use Dt to set DtRise, DtPlateau, and DtFall to the same value instead of setting each keyword separately. If any of these keywords is set, it overwrites the value of Dt.
DtFall	=<float>	0 s Limiting time step for range $[t_2 t_3]$. Does not apply to time-dependence FromFile.
DtFallEnd	=<float>	$(t_1 - t_0)/10$ s Limiting time step at t_3.
DtFallStart	=<float>	$(t_1 - t_0)/10$ s Limiting time step at t_2. Does not apply to time-dependence FromFile.
DtPlateau	=<float>	0 s Limiting time step for range $[t_1 t_2]$. Does not apply to time-dependence FromFile.
DtRise	=<float>	0 s Limiting time step for range $[t_0 t_1]$. Does not apply to time-dependence FromFile.
DtRiseEnd	=<float>	$(t_1 - t_0)/10$ s Limiting time step at t_1. Does not apply to time-dependence FromFile.
DtRiseStart	=<float>	$(t_1 - t_0)/10$ s Limiting time step at t_0.
MinAmplitude	=<float>	0.01 Signal amplitude used to define time points t_0 and t_3 for analytic signals with asymptotic tails.

Table 249   Physics(...){ RayTraceBC(TMM(...)) }

LayerStructure{	`<float> <string>;`
	`<float> <string>;`
	`...`
	`<float> <string>}`
		Definition of multilayer structure used for TMM calculation. First column contains thickness of layer in μm . Second column contains material name of layer.

MapOptGenToRegions(	`<string> <string>` `...)`	Set list of regions to which the lumped optical generation of the TMM BC is mapped.
QuantumEfficiency	`=<float>`	Specify the quantum efficiency of the TMM BC optical generation.
ReferenceMaterial	`=<string>`	Definition of `LayerStructure` orientation. The topmost layer in the `LayerStructure` specification is connected to the region with material `ReferenceMaterial`.
ReferenceRegion	`=<string>`	Definition of `LayerStructure` orientation. The topmost layer in the `LayerStructure` specification is connected to the region with name `ReferenceRegion`.

Table 250   QWLocal() Localized Quantum-Well Model on page 978

eDensityCorrection		– Activate electron quantization model in the quantum well. Quantum-Well Quantization Model on page 309
ElectricFieldDep		+ Switch on electric field dependency for the localized QW model.
hDensityCorrection		– Activate hole quantization model in the quantum well. Quantum-Well Quantization Model on page 309
MaxElectricField	`=<float>`	`1e6` V/cm Cutoff value for electric field.
NumberOfCrystalFieldSplit HoleSubbands	`=<int>`	Set the maximum number of crystal-field split-hole subbands.
NumberOfElectronSubbands	`=<int>`	Set the maximum number of electron subbands.
NumberOfHeavyHoleSubbands	`=<int>`	Set the maximum number of heavy-hole subbands.
NumberOfLightHoleSubbands	`=<int>`	Set the maximum number of light-hole subbands.
NumberOfValenceBands	`=<int>`	`2` Set the number of valence bands.
Polarization	`= TE │ TM │ Mixed`	`TE` Set the polarization used for the computation of the optical transition matrix element. Optical Transition Matrix Element for Wurtzite Crystals on page 971

Table 250   QWLocal() Localized Quantum-Well Model on page 978 (Continued)

PolarizationFactor	=<[0,1]>	1 Set the polarization factor used for the computation of the optical transition matrix element in mixed polarization simulations. Optical Transition Matrix Element for Wurtzite Crystals on page 971
WidthExtraction(	Table 264)	Set QW width extraction parameters.

Table 251   RayDistribution() Distribution Window of Rays on page 602

Dx	=<float>	Specify discretized x-size for Mode=Equidistant.
Dy	=<float>	Specify discretized y-size for Mode=Equidistant.
Mode	=AutoPopulate	Automatically populate rays within the excitation shape.
	=Equidistant	Equidistant distribution of rays within the excitation shape.
	=MonteCarlo	Monte Carlo distribution of rays within the excitation shape.
NumberOfRays	=<int>	Set number of rays for Mode=MonteCarlo or Mode=AutoPopulate.
Scaling	=<float>	Multiply the rays in this window by a scaling factor.
WindowName	=<string>	Specify name of the ray distribution window. No name sets the RayDistribution section as global.

Table 252   RayTraceBC() in Physics material or region interface–based definition of boundary condition

Fresnel		Fresnel boundary condition.
PMIModel	=<ident> [(Table 341)]	Name of the PMI model associated with this BC contact.
Reflectivity	=<[0,1]>	0 Reflectivity.
TMM(	Table 249)	Specification of TMM multilayer structure.
Transmittivity	=<[0,1]>	0 Transmittivity.

Table 253   RayTracing(()...) in Physics{Optics(OpticalSolver(...))}, unified raytracing interface
Raytracing on page 556

`CompactMemoryOption`		Activate the compact memory model of raytracing.
`DepthLimit`	`=<int>`	Stop tracing a ray after passing through more than `<int>` material boundaries.
`ExternalMaterialCRIFile`	`=<string>`	Include a CRI file to define the external media. External Material in Raytracer on page 615
`Farfield(`	Table 240`)`	Activate the far field and sensor feature. Far Field and Sensors for Raytracing on page 620
`MinIntensity`	`=<float>`	Stop tracing a ray when its intensity becomes less than `<float>` times the original intensity. `RelativeMinIntensity` is an equivalent keyword.
`MonteCarlo`		Activate Monte Carlo raytracing.
`NonSemiconductorAbsorption`		Include optical generation calculation in nonsemiconductor region or material.
`OmitReflectedRays`		Discard all reflected rays from raytracing process.
`OmitWeakerRays`		Discard the weaker ray at a material interface. This is chosen by comparing the reflectivity and transmittivity.
`PlotInterfaceFlux`		Activate plotting of interface fluxes on all BCs. Plotting Interface Flux on page 618
`PolarizationVector`	`=Random`	Default. Automatically choose a random polarization vector that is perpendicular to the starting ray direction.
	`=<vector>`	Set a fixed polarization vector for the starting ray.
`Print`		Create the raytree in the output `.tdr` file.
`Print(Skip(`	`<int>))`	Create a reduced raytree by omitting every user-defined subtree count.
`RayDistribution(`	Table 251`)`	Create a ray distribution to be used in conjunction with the excitation illumination window.
`RedistributeStoppedRays`		Distribute the total power accumulated at terminated rays back into the raytree.
`RetraceCRIchange`	`=<float>`	Fractional change of the complex refractive index to force retracing of rays.
`UserWindow(`	Table 263`)`	Input a set of starting rays from a file that is specified by the user. User-Defined Window of Rays on page 600

Table 253   RayTracing(()...) in Physics{Optics(OpticalSolver(...))}, unified raytracing interface
Raytracing on page 556 (Continued)

VirtualRegions{	<string> <string> ...}	Specify virtual regions whereby the raytracer will ignore their existence.
WeightedOpticalGeneration		Switch on weighted method to distribute optical generation from element to vertices. Weighted Interpolation for Raytrace Optical Generation on page 617

Table 254   Recombination() in SingletExciton()

Bimolecular		off (r) Switch on bimolecular recombination in continuity and singlet exciton equations. Singlet Exciton Equation on page 235, Bimolecular Recombination on page 444
Dissociation		off (i) Switch on interface exciton dissociation in continuity and singlet exciton equations. Singlet Exciton Equation on page 235, Exciton Dissociation Model on page 445
eQuenching		off (r) Switch on quenching of singlet exciton due to free electrons. Singlet Exciton Equation on page 235
hQuenching		off (r) Switch on quenching of singlet exciton due to free holes. Singlet Exciton Equation on page 235
radiative		off (r) Switch on directly radiative decay of singlet exciton associated with light emission.
trappedradiative		off (r) Switch on trap-assisted radiative decay of singlet exciton associated with light emission.

Table 255   Select() Enhanced Spectrum Control on page 538

AllowDuplicates		off (g) Control whether duplicate entries of the spectrum are ignored.
Condition	=<string>	"true" Define a Boolean Tcl expression to select a subset of a multidimensional spectrum.
Parameter	=(<string>...)	Active parameters of multidimensional spectrum file.
Var	=<float>	0 Auxiliary parameter that is used to provide more flexibility when specifying a selection condition for the multidimensional spectrum.

Table 256   Sensor(...) in unified raytracing far field Far Field and Sensors for Raytracing on
page 620

Angular(	Phi=(<float>*2)	Define the range of ϕ for the angular sensor.
	Theta=(<float>*2))	Define the range of θ for the angular sensor.
Line(	Corner1=<vector>	Define first point of line sensor.
	Corner2=<vector>	Define second point of line sensor.
	UseNormalFlux)	Compute the projected-to-normal flux.
Name	=<string>	Name of the sensor.
Rectangle(	AxisAligned	Take `Corner1` and `Corner2` as opposing corners of the rectangle sensor.
	Corner1=<vector>	Define first corner of rectangle sensor.
	Corner2=<vector>	Define second corner of rectangle sensor.
	Corner3=<vector>	Define third corner of rectangle sensor.
	UseNormalFlux)	Compute the projected-to-normal flux.

Table 257   SensorSweep in unified raytracing far field Far Field and Sensors for Raytracing
on page 620

Name	=<string>	Specify name of sensor sweep.
Ndivisions	=<int>	Set number of subdivisions for the collection ring.
Phi	=(<float>*2)	Specify range of ϕ for the sensor ring.
Theta	=(<float>*2)	Specify range of θ for the sensor ring.
VaryPhi		Set the sensor sweep as a latitude ring.
VaryTheta		Set the sensor sweep as a longitudinal ring.

Table 258   SRH() and CDL() Shockley–Read–Hall Recombination on page 391, Coupled
Defect Level (CDL) Recombination on page 405

<ident>	[(Table 341)]	Use PMI model <ident> to compute lifetimes. Lifetimes on page 1162
DopingDependence		Doping dependence. SRH Doping Dependence on page 393
ElectricField(	Table 239)	(r) Field enhancement. SRH Field Enhancement on page 396
ExpTempDependence		Exponential temperature dependence. SRH Temperature Dependence on page 394

Table 258   SRH() and CDL() Shockley–Read–Hall Recombination on page 391, Coupled
Defect Level (CDL) Recombination on page 405 (Continued)

NonlocalPath(	Table 245)	(r) Nonlocal trap-assisted tunneling enhancement. Dynamic Nonlocal Path Trap-Assisted Tunneling on page 400
TempDependence		Temperature dependence. SRH Temperature Dependence on page 394

Table 259   StepFunction() Optical Absorption Heat on page 928

Bandgap		Use $E_g - E_{bgn}$ as the cutoff energy for interband absorption.
EffectiveBandgap		Use $(E_g - E_{bgn} + 2 \cdot (3/2)kT)$ as the cutoff energy for interband absorption.
Energy	=<float>	eV Use specified value as the cutoff energy for interband absorption.
Wavelength	=<float>	µm Use specified value as the cutoff energy for interband absorption.

Table 260   StepFunction() Quantum Yield Models on page 544

Bandgap		Use E_g as the cutoff energy for interband absorption.
EffectiveBandgap		Use $E_g - E_{bgn}$ as the cutoff energy for interband absorption.
Energy	=<float>	eV Use specified value as the cutoff energy for interband absorption.
Wavelength	=<float>	µm Use specified value as the cutoff energy for interband absorption.

Table 261   TimeDependence() Specifying Time Dependency for Transient Simulations on
page 547

FromFile		off Reads the time dependency as a table from file.
OpticalTurningPoints(	Table 248)	+ (g) Specification of optical turning points. Optical Turning Points on page 552.
Scaling	=<float>	1 Scaling factor for optical generation.
WavePeriods	=<int>	Number of periods of the periodic signal.
WaveTime	=(<float>*2)	s Time interval (t_{min}, t_{max}) when the optical generation rate is constant.
WaveTPeriod	=<float>	s Period of periodic signal.
WaveTPeriodOffset	=<float>	s Offset of periodic signal (only applies to linear and Gaussian time dependency).

Table 261   TimeDependence() Specifying Time Dependency for Transient Simulations on page 547 (Continued)

WaveTSigma	=<float>	s Standard deviation σ_t of the temporal Gaussian distribution that describes the decay of the optical generation rate outside the time interval WaveTime.
WaveTSlope	=<float>	s^{-1} Slope that characterizes the linear decay of the optical generation rate outside the time interval WaveTime.

Table 262   TMM() Transfer Matrix Method on page 625

IntensityPattern		(r) Choose type of intensity pattern.
	=Envelope	Compute the envelope of the optical intensity instead of the regular optical intensity.
	=StandingWave	* Compute the regular optical intensity without applying any algorithm that filters out oscillations on the wavelength scale.
LayerStackExtraction(	ComplexRefractiveIndex Threshold=<float>	0 Choose threshold value for layer creation when using ElementWise extraction mode.
	Medium(Table 244))	Specification of media surrounding the extracted layer structure.
	Mode=RegionWise | ElementWise	RegionWise Specify whether layer stack is created on a per-element or per-region basis.
	Position=(<float>*3)	Specify starting point of extraction line.
	WindowName=<string>	Reference to illumination window in Excitation section.
	WindowPosition=<ident>)	Center Specify starting point of extraction line in terms of a cardinal direction (North, South, East, West, NorthEast, SouthEast, NorthWest, SouthWest).
NodesPerWavelength	=<float>	Number of nodes per wavelength used for computation of optical field.
PropagationDirection	=Perpendicular | Refractive	Refractive Choose interpolation mode for 1D TMM solution.
RoughInterface		+ Flag interfaces as rough, that is, physics of rough interface scattering is applied.
Scattering(	AngularDiscretization=<int>	91 Angular discretization of interval $[-\pi/2, \pi/2]$ used in scattering solver.
	MaxNumberOfIterations=<int>	10 Break criterion for iterative scattering solver.
	Tolerance=<float>)	1e-3 Break criterion for iterative scattering solver.

Table 263   UserWindow in Physics{Optics(OpticalSolver(Raytracing(...)))}, User-Defined Window of Rays on page 600

NumberOfRays	=<int>	Set number of rays in file.
PolarizationVector	=Random	Generate random polarization for the user input rays.
	=ReadFromExcitation	Read the polarization from the Excitation section.
	=ReadFromFile	Read the polarization vectors from the user input ray file.
RaysFromFile	=<string>	Set file name of the user input rays.

Table 264   WidthExtraction() Accelerating Gain Calculations and LED Simulations on page 930

ChordWeight	=<float>	Specify chord weight for width extraction. Thickness Extraction on page 313
MinAngle	=(<float>, <float>)	Specify minimum angles for width extraction. Thickness Extraction on page 313
SideMaterial	=("mat1", ..., "matn")	Specify the materials adjoining the QW.
SideRegion	=("reg1", ..., "regn")	Specify the regions adjoining the QW.

LED

NOTE   LED simulations present unique challenges that require problem-specific model and numerics setups. Contact TCAD Support for advice if you are interested in simulating LEDs (see Contacting Your Local TCAD Support Team Directly on page xliii).

Table 265   LED() Chapter 34, p. 921

Bandstructure(	CrystalType=Zincblende | Wurtzite)	Zincblende Crystal structure of active region. Electronic Band Structure for Wurtzite Crystals on page 967
Broadening(	Table 266)	Activate gain-broadening models or nonlinear gain saturation model. Gain-Broadening Models on page 965, Simple Quantum-Well Subband Model on page 973
Optics(	Table 268)	Optics.
QWExtension	=AutoDetect	Autodetect width of quantum wells. The quantum-well region must be specified by the keyword Active. Radiative Recombination and Gain Coefficients on page 962
QWTransport		Use 'three-point' QW model with thermionic emission. Radiative Recombination and Gain Coefficients on page 962

Table 265   LED() Chapter 34, p. 921 (Continued)

SplitOff	=<float>	eV Spin-orbit split-off energy. Strain Effects on page 976
SponEmissionCoeff	(<ident> [(Table 341)])	Use PMI model <ident> for spontaneous emission. Importing Gain and Spontaneous Emission Data With PMI on page 982
SponIntegration	(<float>,<int>)	eV Energy integration range and number of discretization intervals for numeric integration (for LED simulations only). Spontaneous Emission Rate and Power on page 923
SponScaling	=<float>	Scaling factor for matrix element of spontaneous emission. Radiative Recombination and Gain Coefficients on page 962
StimEmissionCoeff	(<ident> [(Table 341)])	Use PMI model <ident> for stimulated emission. Importing Gain and Spontaneous Emission Data With PMI on page 982
StimScaling	=<float>	Scaling factor for matrix element of stimulated emission. Radiative Recombination and Gain Coefficients on page 962
Strain	(RefLatticeConst=<float>)	m Use strain model for quantum well with given reference lattice constant. Strain parameters are input in the parameter file. Strain Effects on page 976

Table 266   Broadening() Gain-Broadening Models on page 965

Gamma	=<float>	eV Broadening coefficient Γ.
Type	=CosHyper	Use hyperbolic-cosine broadening. Hyperbolic-Cosine Broadening on page 966
	=Landsberg	Use Landsberg broadening. Landsberg Broadening on page 966
	=Lorentzian	Use Lorentzian broadening. Lorentzian Broadening on page 965

Table 267   ClusterActive() in LED(Optics(RayTrace())) Clustering Active Vertices on page 937

ClusterQuantity	=Nodes	Clustering by recursive grouping of active vertices.
	=OpticalGridElement	Clustering by grouping active vertices in each active optical element.
	=PlaneArea	Clustering by evenly dividing up QW plane area and grouping active vertices in each area element.
NumberOfClusters	=<int>	Specify number of clusters, only for Nodes or PlaneArea clustering.

Table 268   Optics() in LED() LED Optics: Raytracing on page 931

RayTrace(	Table 271)	Raytracing.

Table 269   OutputLightToolsFarfieldRays() in LED(Optics(RayTrace())) Interfacing Far-Field Rays to LightTools on page 951

Filename	=<string>	Base file name of the LightTools® ray data file to be output.
SaveType	=Ascii	Choose ASCII format for LightTools ray data file.
	=Binary	Choose binary format for LightTools ray data file.
WavelengthDiscretization	=<int>	Number of discretization for the spectrum. The span of the spectrum is determined automatically.

Table 270   OutputLightToolsRays() in LED(Optics(RayTrace(Disable()))) Interfacing LED Starting Rays to LightTools® on page 941

IsotropyType	=InBuilt	Use the internal geodesic distribution of starting rays from each active emission vertex cluster.
	=Random	Use a random distribution of starting rays.
	=UserRays	Use the user input set of starting rays defined by the keyword SourceRaysFromFile (see Table 271).
RaysPerCluster	=<int>	Set number of starting rays in each active cluster.
SaveType	=Ascii	Choose ASCII format for LightTools ray data file.
	=Binary	Choose binary format for LightTools ray data file.
WavelengthDiscretization	=<int>	Number of discretization for the spectrum. The span of the spectrum is determined automatically.

Table 271   RayTrace() in LED(Optics()) LED Optics: Raytracing on page 931

ClusterActive(	Table 267)	Activate the clustering option. Clustering Active Vertices on page 937
CompactMemoryOption		Activate the compact memory model for LED raytracing. Will not work with the full photon-recycling model.
Coordinates	=Cartesian	*
	=Cylindrical	

Table 271   RayTrace() in LED(Optics()) LED Optics: Raytracing on page 931 (Continued)

`DebugLEDRadiation`	`(<string> <float1>` `<float2> <float3>)`	off Trace the origin of the output rays that are within the angles [`<float1>`,`<float2>`] (in degrees) and of minimum intensity specified by the `<float3>` parameter. In two dimensions, the angle is defined in the regular polar coordinates. In three dimensions, the angles are defined from the z-axis, as in θ in regular spherical coordinates. The results are output to the file specified by `<string>`.
`DepthLimit`	`=<int>`	5 Stop tracing the ray after passing through more than `<int>` material boundaries.
`Disable`		off Disable raytracing but still run LED simulation.
`Disable(OutputLightToolsRays(`	Table 270`))`	Output starting rays from active vertices to a LightTools ray data file. Interfacing LED Starting Rays to LightTools® on page 941
`EmissionType`	`(Anisotropic(` `Sine(<float>*3)` `Cosine(<float>*3)))`	
	`(Isotropic)`	*
`ExcludeHorizontalSource`	`(<float>)`	off Omit the source rays that are emitted within the horizontal angular zone specified by the `<float>` parameter (in degrees).
`LEDRadiationPara`	`(<float>, <int>)`	μm Observation radius and discretization of the observation circle or sphere.
`LEDSpectrum`	`(<float>*2 <int>)`	eV Starting and ending energy range, and number of subdivisions in that energy range.
`MinIntensity`	`=<float>`	1e-5 Stop tracing the ray when the intensity of a ray becomes less than `<float>` times the original intensity.
`MonteCarlo`		Activate Monte Carlo raytracing.
`MoveBoundaryStartRays`	`=<float>`	0 nm Shift the starting ray position at device boundary inwards. Recommended values are 1 to 5 nm.
`NonActiveAbsorptionOff`		Do not add nonactive region absorption as generation rate to continuity equation. Nonactive Region Absorption (Photon Recycling) on page 953
`ObservationCenter`	`=<vector>`	Fixed observation center for LED radiation. By default, center of device.
`OmitReflectedRays`		Discard all reflected rays in raytracing process.
`OmitWeakerRays`		Discard the weaker ray at a material interface. This is decided by comparing the reflectivity and transmittivity.
`OptGenScaling`	`=<float>`	Set a multiplication factor to the nonactive optical generation computed.

Table 271   RayTrace() in LED(Optics()) LED Optics: Raytracing on page 931 (Continued)

OutputLightToolsFarfieldRays(	Table 269)	Output far-field rays with embedded spectrum information into a LightTools ray data file. Interfacing Far-Field Rays to LightTools on page 951
PolarizationVector	=Random	Default. Automatically choose a random polarization vector that is perpendicular to the starting ray direction.
	=<vector>	Set a user-defined polarization vector.
Print		off Output all rays to the output .tdr file.
	(ActiveVertex(<int>))	off Output only ray paths emitted from this active vertex.
	(Skip(<int>))	1 Output every other <int> ray to the output .tdr file.
PrintRayInfo	(<string>)	off Print all indices and positions of starting rays into the file specified by <string>.
PrintSourceVertices	(<string>)	off Print the index and coordinates of all active vertices into the file specified by <string>.
ProgressMarkers	=<int>	5 Completion meter for raytracing.
RaysPerVertex	=<int>	10 Number of rays starting from each active source vertex. For 3D, the number of starting rays are constrained by 6, 18, 68, and so on. The number in the sequence is chosen such that RaysPerVertex is slightly larger or equal to it.
RaysRandomOffset		Randomize the angular shift of the starting rays.
	(RandomSeed=<int>)	Set a fixed random seed so that repeated simulations will yield the exact pseudorandom results.
RedistributeStoppedRays		Distribute the total accumulated power in terminated rays back into the raytree.
RetraceCRIchange	=<float>	Fractional change of the complex refractive index to force retracing of rays.
SourceRaysFromFile(	<string>)	Import a set of starting ray directions from the file name specified by <string>. The number of imported rays are specified by RaysPerVertex.
Staggered3DFarfieldGrid		Use the staggered 3D far-field collection sphere. Staggered 3D Grid LED Radiation Pattern on page 947
TraceSource	()	Retrace the source of the output rays to produce a map of the source regions that give the strongest ray output.
TurnOffTreeNodeCount		Disable counting the total number of nodes in the raytree.

Table 271   RayTrace() in LED(Optics()) LED Optics: Raytracing on page 931 (Continued)

Wavelength	=<float>	nm Wavelength.
	=AutoPeak	Take wavelength at the peak of the spontaneous emission rate spectrum. LED Wavelength on page 927
	=AutoPeakPower	Take wavelength at the peak of the spontaneous emission power spectrum.
	=Effective	Wavelength computed such that total power = total rate x effective photon energy.

Mobility

Table 272   Mobility(), eMobility(), hMobility() Chapter 15, p. 317

BalMob		off Use ballistic mobility model. Ballistic Mobility Model on page 377
(	Fermi	off Use Fermi–Dirac correction in the ballistic mobility. Using the Ballistic Mobility Model on page 379
	Frensley	off Use Frensley rule for final mobility. Using the Ballistic Mobility Model on page 379
	KineticEnergy	off Use kinetic ballistic mobility model. Using the Ballistic Mobility Model on page 379
	Lch=<float>	10^7 nm Use explicit channel length in simple ballistic mobility. Using the Ballistic Mobility Model on page 379
	TempDep)	off Use temperature dependency in simple ballistic mobility. Using the Ballistic Mobility Model on page 379
CarrierCarrierScattering	(BrooksHerring)	off Use Brooks–Herring carrier–carrier scattering model. Carrier–Carrier Scattering on page 326
	(ConwellWeisskopf)	off Use Conwell–Weisskopf carrier–carrier scattering model. Carrier–Carrier Scattering on page 326
ConstantMobility		+ Use constant mobility if neither PhuMob nor DopingDependence is specified. Mobility due to Phonon Scattering on page 318
Diffusivity(	Table 273)	off Use non-Einstein diffusivity. Non-Einstein Diffusivity on page 376

Table 272   Mobility(), eMobility(), hMobility() Chapter 15, p. 317 (Continued)

DopingDependence(	<ident> [(Table 341)]	off PMI model <ident>. Doping-Dependent Mobility on page 1107
	Arora	off Use Arora doping-dependent mobility model. Doping-Dependent Mobility Degradation on page 318
	BalMob([Lch=<float>])	off Use low-field ballistic mobility model. Low-Field Ballistic Mobility Model on page 325
	Masetti	off Use Masetti doping-dependent mobility model. Doping-Dependent Mobility Degradation on page 318
	PhuMob [options on page 1461]	off Use Philips unified mobility model. Philips Unified Mobility Model on page 328
	PhuMob2	off Use an alternative Philips model.241 Using an Alternative Philips Model on page 329
	PMIModel(Table 318)	off Use PMI for MSC-dependent mobility. Multistate Configuration–Dependent Bulk Mobility on page 1113
	UniBo)	off Use University of Bologna doping-dependent mobility model. Doping-Dependent Mobility Degradation on page 318
eDiffusivity(	Table 273)	off Use non-Einstein electron diffusivity. Non-Einstein Diffusivity on page 376
eHighFieldSaturation(	Table 273)	off Electron high-field saturation. High-Field Saturation on page 361

Table 272   Mobility(), eMobility(), hMobility() Chapter 15, p. 317 (Continued)

Enormal(	<ident> [(Table 341)]	off PMI model <ident>. Mobility Degradation at Interfaces on page 1116
	Coulomb2D	off 'Two-dimensional' ionized impurity mobility degradation. Mobility Degradation Components due to Coulomb Scattering on page 347
	IALMob (Table 274)	off Inversion and accumulation layer mobility model. Mobility Degradation at Interfaces on page 332
	InterfaceCharge[(SurfaceName=<string>)]	off Negative and positive interface charge mobility degradation. Mobility Degradation Components due to Coulomb Scattering on page 347
	Lombardi (Table 275)	off Enhanced Lombardi model. Mobility Degradation at Interfaces on page 332
	Lombardi_highk	off Enhanced Lombardi model with high-k degradation. Mobility Degradation at Interfaces on page 332
	NegInterfaceCharge [(SurfaceName=<string>)]	off Negative interface charge mobility degradation. Mobility Degradation Components due to Coulomb Scattering on page 347
	PosInterfaceCharge [(SurfaceName=<string>)]	off Positive interface charge mobility degradation. Mobility Degradation Components due to Coulomb Scattering on page 347
	RCS	off Remote Coulomb scattering mobility degradation. Remote Coulomb Scattering Model on page 351
	RPS	off Remote phonon scattering mobility degradation. Remote Phonon Scattering Model on page 353
	UniBo)	off University of Bologna surface mobility model. Mobility Degradation at Interfaces on page 332
hDiffusivity(	Table 273)	off Use non-Einstein hole diffusivity. Non-Einstein Diffusivity on page 376
hHighFieldSaturation(	Table 273)	off Hole high-field saturation. High-Field Saturation on page 361
HighFieldSaturation(	Table 273)	off High-field saturation. High-Field Saturation on page 361
IncompleteIonization		off Incomplete ionization-dependent mobility. Incomplete Ionization–Dependent Mobility Models on page 382

Table 272 Mobility(), eMobility(), hMobility() Chapter 15, p. 317 (Continued)

PhuMob		off Philips unified mobility model. Philips Unified Mobility Model on page 328
(	Arsenic	* Use arsenic parameters. Table 56 on page 332
	Phosphorus)	Use phosphorus parameters. Table 56 on page 332
ThinLayer		off Thin-layer mobility model. Thin-Layer Mobility Model on page 356
(	ChordWeight=<float>	0 Weight of chord length. Thickness Extraction on page 313
	IALMob(Table 274)	Use the inversion and accumulation layer mobility model with the thin-layer mobility model. Thin-Layer Mobility Model on page 356
	Lombardi(Table 275)	* Use the enhanced Lombardi model with the thin-layer mobility model. Thin-Layer Mobility Model on page 356
	MinAngle=(<float>*2)	0 0 Angle constraints. Thickness Extraction on page 313
	Thickness=<float>)	µm Explicit thickness value.
ToCurrentEnormal	as Enormal	off Dependence on electric field normal to current. Mobility Degradation at Interfaces on page 332
Tunneling		– Tunneling correction to mobility. Eq. 233, p. 295

Table 273 HighFieldSaturation(), Diffusivity() High-Field Saturation on page 361

<ident>	[(Table 341)]	PMI model <ident>. High-Field Saturation Model on page 1125
AutoOrientation		– Use a parameter set based on the orientation of the nearest interface. Auto-Orientation for High-Field Saturation on page 363
CarrierTempDrive		Temperature driving force (default for hydrodynamic simulation). Hydrodynamic Driving Force on page 372
CarrierTempDriveBasic		Basic temperature driving force. Basic Model on page 367
CarrierTempDriveME		Meinerzhagen–Engl temperature driving force. Meinerzhagen–Engl Model on page 367
CarrierTempDrivePolynomial		Energy-dependent mobility model using an irrational polynomial. Energy-Dependent Mobility on page 772
CarrierTempDriveSpline		Energy-dependent mobility model using spline interpolation. Spline Interpolation on page 774
CaugheyThomas		* Use Canali–Hänsch model. Extended Canali Model on page 363
Eparallel		Use electric field parallel to current as driving force. Electric Field Parallel to the Current on page 370

Table 273   HighFieldSaturation(), Diffusivity() High-Field Saturation on page 361 (Continued)

`EparallelToInterface`		Use electric field parallel to the closest semiconductor–insulator interface as driving force. Electric Field Parallel to the Interface on page 371
`GradQuasiFermi`		* Use gradient of quasi-Fermi potential as driving force. For hydrodynamic simulations, default is `CarrierTempDrive`. Gradient of Quasi-Fermi Potential on page 370
`ParameterSetName`	`=<string>`	Name of parameter set to use. Named Parameter Sets for High-Field Saturation on page 362
`PFMob`		Use Poole–Frenkel mobility model. Poole–Frenkel Mobility (Organic Material Mobility) on page 382
`PMIModel(`	Table 318)	PMI model dependent on two fields. High-Field Saturation With Two Driving Forces on page 1134
`TransferredElectronEffect`		Use transferred electron model. Transferred Electron Model on page 364
`TransferredElectronEffect2`		Use an alternative transferred electron model. Transferred Electron Model 2 on page 365

Table 274   IALMob() Mobility Degradation at Interfaces on page 332

`AutoOrientation`		– Use a parameter set based on the orientation of the nearest interface. Auto-Orientation for IALMob on page 345
`ClusteringEverywhere`		– Use clustering formulas for all occurrences of N_A and N_D. Inversion and Accumulation Layer Mobility Model on page 337
`FullPhuMob`		+ Use the full `PhuMob` mobility expressions. Inversion and Accumulation Layer Mobility Model on page 337
`ParameterSetName`	`=<string>`	Name of `IALMob` parameter set. Named Parameter Sets for IALMob on page 344
`PhononCombination`	`=<0..2>`	1 Selects how 2D and 3D phonon mobility are combined. Inversion and Accumulation Layer Mobility Model on page 337

Table 275   Lombardi() Mobility Degradation at Interfaces on page 332

`AutoOrientation`		– Use a parameter set based on the orientation of the nearest interface. Auto-Orientation for Lombardi Model on page 337
`ParameterSetName`	`=<string>`	Name of `EnormalDependence` parameter set. Named Parameter Sets for Lombardi Model on page 336

Radiation Models

Table 276 AlphaParticle() Alpha Particles on page 666

Direction	=<vector>	! Direction of motion of the particle.
Energy	=<float>	! eV Energy of the alpha particle.
Location	=<vector>	! µm Point where the alpha particle enters the device (bidirectional track).
StartPoint	=<vector>	! µm Point where the alpha particle enters the device (one-directional track).
Time	=<float>	! s Time at which the charge generation peaks.

Table 277 HeavyIon() Heavy Ions on page 668

Direction	=<vector>	Direction of motion of the ion.
Exponential		* Use exponential shape for the spatial distribution $R(w)$.
Gaussian		Use Gaussian shape for the spatial distribution $R(w)$.
Length	=[<float>...]	Length l where `Wt_hi` and `Let_f` are specified (in cm by default or µm if the `PicoCoulomb` option is selected).
LET_f	=[<float>...]	Linear energy transfer (LET) function (in $pairs cm^{-3}$ by default or $pC µm^{-1}$ if the `PicoCoulomb` option is selected). Entries in the list match those in `Length`.
Location	=<vector>	µm Point where the heavy ion enters the device (bidirectional track).
PicoCoulomb		Switch units for `LET_f`, `Wt_hi`, and `Length`.
SpatialShape	=<ident> [(Table 341)]	PMI for spatial distribution function. Spatial Distribution Function on page 1257
StartPoint	=<vector>	µm Point where the heavy ion enters the device (one-directional track).
Time	=<float>	s Time at which the ion penetrates the device.
Wt_hi	=[<float>...]	Characteristic distance, $w_t(l)$ (in cm by default or µm if the `PicoCoulomb` option is selected). Entries in the list match those in `Length`.

Table 278   Radiation() Chapter 22, p. 665

Dose	=<float>	rad Total dose over exposure time.
DoseRate	=<float>	$\mathrm{rad\,s^{-1}}$ Dose rate.
DoseTime	=(<float>*2)	! s Exposure time.
DoseTSigma	=<float>	! s Standard deviation of rise and fall of dose rate over time.

Various

Table 279   Aniso() Chapter 28, p. 779

Avalanche		Use anisotropic avalanche generation. Anisotropic Avalanche Generation on page 791
direction	[(<System_Coord>)]	Crystal or simulation system coordinate.
	=(<float>*3)	Anisotropic direction. Anisotropic Direction on page 783
	=xAxis	Equivalent to direction=(1 0 0).
	=yAxis	Equivalent to direction=(0 1 0).
	=zAxis	Equivalent to direction=(0 0 1).
eAvalanche		Use anisotropic electron avalanche generation. Anisotropic Avalanche Generation on page 791
eMobility		Use self-consistent anisotropic mobility for electrons. Self-Consistent Anisotropic Mobility on page 789
eMobilityFactor	(Total)=<float>	Total anisotropic mobility factor for electrons. Total Anisotropic Mobility on page 789
eQuantumPotential		Use electron anisotropic density-gradient equation with tensor grid approximation. Using the Density Gradient Model on page 296
hAvalanche		Use anisotropic hole avalanche generation. Anisotropic Avalanche Generation on page 791
hMobility		Use self-consistent anisotropic mobility for holes. Self-Consistent Anisotropic Mobility on page 789
hMobilityFactor	(Total)=<float>	Total anisotropic mobility factor for holes. Total Anisotropic Mobility on page 789
hQuantumPotential		Use hole anisotropic density-gradient equation with tensor grid approximation. Using the Density Gradient Model on page 296

Table 279   Aniso() (Continued)

Mobility		Use self-consistent anisotropic mobility. Self-Consistent Anisotropic Mobility on page 789
Poisson		Use anisotropic electrical permittivity. Anisotropic Electrical Permittivity on page 793
Temperature		Use anisotropic thermal conductivity. Anisotropic Thermal Conductivity on page 794

Table 280   BandEdge() in RandomizedVariation() Band Edge Variations on page 699

Table 230		Statistical properties of the correlation.
Table 321		Spatial restriction of variation.
Amplitude_Chi	=<float>	eV Amplitude of affinity variation for exponential and Gaussian correlation.
Amplitude_Eg	=<float>	eV Amplitude of bandgap variation for exponential and Gaussian correlation.
Chi2Eg	=<float>	0 Correlation between affinity and band gap.
ChiComponent	=<0..1>	0 Named random field component for affinity randomization.
EgComponent	=<0..1>	1 Named random field component for bandgap randomization.
GrainChi	=(<float>...)	eV Grain affinity values.
GrainEg	=(<float>...)	eV Grain bandgap values.
GrainProbability	=(<float>...)	Probability for grain types.
Volume	=<string>	Named volume in which to activate the variation.

Table 281   BarrierType() in SingletExciton() Singlet Exciton Equation on page 235

Bandgap		* (i) Use bandgap difference as barrier.
CondBand		(i) Use conduction band-edge difference as barrier.
ValBand		(i) Use valence band-edge difference as barrier.

Table 282   Charge(()...) in Physics{} Insulator Fixed Charges

Conc	=<float>	$q\mathrm{cm}^{-3}$ (r) $q\mathrm{cm}^{-2}$ (i) Oxide or interface charge density.
Gaussian		(i) Gaussian distribution.
SpaceMid	=<vector>	µm (i) Charge distribution center.
SpaceSig	=<vector>	µm (i) Charge distribution width.
Uniform		* (i) Uniform distribution.

Table 283   ComplexRefractiveIndex() Complex Refractive Index Model on page 578

CarrierDep(	imag	Use carrier dependency of extinction coefficient. Carrier Dependency on page 580
	real)	Use carrier dependency of refractive index. Carrier Dependency on page 580
CRIModel(	Name=<string>)	Activate user-defined complex refractive index model. Complex Refractive Index Model Interface on page 586
GainDep	(real(lin))	Use linear gain dependency of refractive index. Gain Dependency on page 581
	(real(log))	Use logarithmic gain dependency of refractive index. Gain Dependency on page 581
TemperatureDep(	real)	Use temperature dependency of refractive index. Temperature Dependency on page 579
WavelengthDep(	imag	Use wavelength dependency of extinction coefficient. Wavelength Dependency on page 579
	real)	Use wavelength dependency of refractive index. Wavelength Dependency on page 579

Table 284   Conductivity() in RandomizedVariation() Metal Conductivity Variations on page 700

Table 230		Statistical properties of the correlation.
Table 321		Spatial restriction of variation.
`Amplitude`	`=<float>`	A/cmV Amplitude of conductivity variation for exponential and Gaussian correlation.
`GrainConductivity`	`=(<float>...)`	A/cmV Grain conductivity values.
`GrainProbability`	`=(<float>...)`	Probability for grain types.
`Volume`	`=<string>`	Named volume in which to activate the variation.

Table 285   DeterministicVariation() Deterministic Variations on page 703

`DopingVariation`	`<string>`(Table 288)	Deterministic Doping Variations on page 703
`GeometricVariation`	`<string>`(Table 301)	Deterministic Geometric Variations on page 705
`ParameterVariation`	`<string>`(Table 316)	Parameter Variations on page 706

Table 286   Doping() in Noise() Random Dopant Fluctuations on page 683

Table 321		Spatial restriction of fluctuations.
`BandgapNarrowing`		Include effect on bandgap narrowing.
`Mobility`		Include effect on mobility.
`Type`	`=Acceptor`	Only acceptors fluctuate.
	`=Donor`	Only donors fluctuate.
	`=Doping`	* All dopants fluctuate.

Table 287   Doping() in RandomizedVariation() Doping Variations on page 695

Table 321		Spatial restriction of variation.
BandgapNarrowing		+ Account for doping dependency of bandgap narrowing.
Mobility		+ Account for doping dependency of mobility.
Type	=Acceptor	Randomize acceptors only.
	=Donor	Randomize donors only.
	=Doping	* Randomize all dopants.

Table 288   DopingVariation() in DeterministicVariation() Deterministic Doping Variations on page 703

Table 321		Spatial restriction of variation.
Amplitude	=<vector>	μm Vectorial amplitude for gradient specification.
Amplitude_Abs	=<vector>	μm Vectorial amplitude for absolute gradient specification.
Amplitude_Iso	=<float>	μm Isotropic amplitude for gradient specification.
BandgapNarrowing		+ Account for doping dependency of bandgap narrowing.
Conc	=<float>	cm^{-3} Normalization concentration.
Factor	=<float>	1 Multiplier for variation.
Mobility		+ Account for doping dependency of mobility.
SFactor	=<string>	Dataset name for variation.
Type	=Acceptor	Apply variation to acceptor concentration.
	=Donor	Apply variation to donor concentration.
	=Doping	* Apply variation according to sign to acceptor or donors.

Table 289   DopingVariation() in RandomizedVariation() Doping Profile Variations on page 702

Table 230		Statistical properties of the correlation.
Table 321		Spatial restriction of variation.
`Amplitude`	`=<float>`	`0` µm Vectorial amplitude.
`Amplitude_Iso`	`=<float>`	`0` µm Isotropic amplitude.
`BandgapNarrowing`		+ Account for doping dependency of bandgap narrowing.
`Conc`	`=<float>`	`0` cm^{-3} Normalization concentration.
`Mobility`		+ Account for doping dependency of mobility.
`SFactor`	`=<string>`	! Dataset name for variation.
`Type`	`=Acceptor`	Apply variation to acceptor concentration.
	`=Donor`	Apply variation to donor concentration.
	`=Doping`	* Apply variation according to sign to acceptor or donors.

Table 290   EffectiveIntrinsicDensity() Band Gap and Electron Affinity on page 249

`BandGap`	`(<ident>` `[(Table 341)])`	Use PMI model `<ident>` to compute band gap E_g. Band Gap on page 1138
`BandGapNarrowing`	`(<ident>` `[(Table 341)])`	Use PMI model `<ident>` for bandgap narrowing. Bandgap Narrowing on page 1141
	`(BennettWilson)`	* Bennett–Wilson model.
	`(delAlamo)`	del Alamo model.
	`(JainRoulston)`	Jain–Roulston model.
	`(oldSlotboom)`	Old Slotboom model.
	`(Slotboom)`	Slotboom model.
	`(TableBGN)`	Table-based model.
`NoBandGapNarrowing`		No bandgap narrowing.
`NoFermi`		off Omit correction Eq. 178, p. 259 even when using Fermi statistics. Bandgap Narrowing With Fermi Statistics on page 259

Table 291   eLucky(), hLucky(), eFiegna(), hFiegna() Effective Field on page 742

`CarrierTempDrive`		Use field derived from temperature.
`CarrierTempPost`		Use field derived from postprocessed temperature.
`Eparallel`		* Use field parallel to interface.

Table 292   eNMP() Extended Nonradiative Multiphonon Model on page 513

`Conc`	`=<float>`	0 cm^{-2} Precursor concentration for the eNMP model.
`NumberOfSamples`	`=<int>`	0 Number of random samples.
`SFactor`	`=<ident> [(Table 341)]`	Name of the PMI model to compute the eNMP precursor concentration. Using the eNMP Model on page 516 and Space Factor on page 1190
	`=<string>`	Dataset for the spatial distribution of the eNMP precursor concentration. Using the eNMP Model on page 516

Table 293   Epsilon() in RandomizedVariation() Dielectric Constant Variations on page 701

Table 230		Statistical properties of the correlation.
Table 321		Spatial restriction of variation.
`Amplitude`	`=<float>`	1 Amplitude of relative dielectric constant variation for exponential and Gaussian correlation.
`GrainEpsilon`	`=(<float>...)`	1 Grain relative dielectric constant values.
`GrainProbability`	`=(<float>...)`	Probability for grain types.
`Volume`	`=<string>`	Named volume in which to activate the variation.

Table 294   eQuantumPotential() and hQuantumPotential() Density Gradient Quantization Model on page 294

`AnisoAxes`	`[(<System_Coord>)]`	Crystal or simulation system coordinate.
	`={<vector> <vector>}`	Two directions of anisotropy. Anisotropic Direction on page 783
`AutoOrientation`		off Use parameter set based on orientation of nearest interface. Auto-Orientation for Density Gradient on page 298
`BoundaryCondition`	`=Dirichlet`	(ci) Enforce homogeneous Dirichlet boundary conditions.
	`=Neumann`	(ci) Enforce homogeneous Neumann boundary conditions.

Table 294 eQuantumPotential() and hQuantumPotential() Density Gradient Quantization
Model on page 294 (Continued)

Density		– (r) Use Eq. 230, p. 294 instead of Eq. 231, p. 295.
direction	[(<System_Coord>)]	Crystal or simulation system coordinate.
	=(<float>*3)	Anisotropic direction. Anisotropic Direction on page 783
	=xAxis	Equivalent to direction=(1 0 0).
	=yAxis	Equivalent to direction=(0 1 0).
	=zAxis	Equivalent to direction=(0 0 1).
Gamma(	EffectiveMass	+ Quantization mass is density of states mass. Gamma Factor for Density Gradient Model on page 1283
	name=<string> [(Table 341)]	PMI for γ. Gamma Factor for Density Gradient Model on page 1283
Ignore		– (r) Compute, but do not apply quantum correction.
LocalModel	=<ident> [(Table 341)]	(r) Name of PMI for apparent band-edge shift. Chapter 14, p. 283, Apparent Band-Edge Shift on page 1144
	=SchenkBGN_elec	(r) Schenk bandgap narrowing model for electrons. Schenk Bandgap Narrowing Model on page 255
	=SchenkBGN_hole	(r) Schenk bandgap narrowing model for holes. Schenk Bandgap Narrowing Model on page 255
ParameterSetName	=<string>	Name of QuantumPotentialParameters parameter set. Named Parameter Sets for Density Gradient on page 298
Resolve		– (r) Use more accurate discretization of non-heterointerfaces.

Table 295 eSHEDistributionl(), hSHEDistribution() Spherical Harmonics Expansion Method
on page 746

AdjustImpurityScattering		+ Use an option to adjust impurity scattering to match the low-field mobility specified in the Physics section.
FullBand		– Use the full band structure with the default band-structure file.
	=<string>	! File name of the user-defined band-structure file.
RTA		– Use relaxation time approximation.

Table 296   ExternalSchroedinger() External 2D Schrödinger Solver on page 292

Carriers=(	Electron	Use quantum correction for electrons.
	Hole)	Use quantum correction for holes.
DampingLength	=<float>	0.005 µm Distance from volume enclosed by slices beyond which quantum correction is disabled.
MaxMismatch	=<float>	1e-4 µm Tolerance in matching of slice meshes and device mesh.
NumberOfSlices	=<2,>	* Number of slices.
SBandCommandFile	=<string>	Start Sentaurus Band Structure automatically, using this command file.
Volume	=<string>	Domain to which to restrict quantum corrections.

Table 297   GateCurrent() Chapter 24, p. 715, Chapter 25, p. 737

<ident>(	<carrier>... [Table 341])	(i) Use PMI model <ident> to compute hot-carrier injection. Hot-Carrier Injection on page 1230
DirectTunneling		(i) Schenk direct tunneling model. Direct Tunneling on page 718
eFiegna	[(Table 291)]	(i) Fiegna model for electrons. Fiegna Hot-Carrier Injection on page 743
eLucky	[(Table 291)]	(i) Lucky electron model. Classical Lucky Electron Injection on page 742
eSHEDistribution		(i) SHE distribution model for electrons. SHE Distribution Hot-Carrier Injection on page 744
Fowler		(i) Fowler–Nordheim tunneling. Fowler–Nordheim Tunneling on page 716
	(EVB)	(i) Fowler–Nordheim valence band tunneling of electrons. Fowler–Nordheim Tunneling on page 716
GateName	=<string>	(i) Electrode for monitoring gate current. Overview on page 737
hFiegna	[(Table 291)]	(i) Fiegna model for holes. Fiegna Hot-Carrier Injection on page 743
hLucky	[(Table 291)]	(i) Lucky hole model. Classical Lucky Electron Injection on page 742
hSHEDistribution		(i) SHE distribution model for holes. SHE Distribution Hot-Carrier Injection on page 744
InjectionRegion	=<string>	Regions to which hot carriers are injected. Destination of Injected Current on page 738
Interface		(i) Activate carrier injection with explicitly evaluated boundary conditions for continuity equations during a transient (Carrier Injection With Explicitly Evaluated Boundary Conditions for Continuity Equations on page 759) or if not in transient monitor interface current. Overview on page 737

Table 298   Gaussian() in IntensityDistribution() Spatial Intensity Function Excitation on page 568

Length	=(<float>,<float>)	Length of Gaussian decay, cannot specify together with Sigma.
PeakPosition	=(<float>,<float>)	Peak position of the Gaussian profile, in local coordinate of the defined shape function.
PeakWidth	=(<float>,<float>)	Width of the plateau of the modified Gaussian profile.
Scaling	=<float>	Scaling factor for the Gaussian profile.
Sigma	=(<float>,<float>)	Sigma of Gaussian decay, cannot specify together with Length.

Table 299   Geometric() in RandomizedVariation() Geometric Variations on page 698

Table 230		Statistical properties of the correlation.
Table 321		Spatial restriction of variation.
Amplitude	=<vector>	0 µm Vectorial amplitude for displacement.
Amplitude_Iso	=<float>	0 µm Isotropic amplitude for displacement.
Options	=<0..1>	0 Select approximation specific to insulator position variations.
Surface	=<string>	! Name of varying surface.
WeightDielectic	=<float>	0 Interpolation coefficient between two approximations of dielectric term.
WeightQuantumPotential	=<float>	0.5 Interpolation coefficient between two approximations for density-gradient quantum-correction term.

Table 300   GeometricFluctuations in Noise() Random Geometric Fluctuations on page 684

Table 321		Spatial restriction of variation.
Options	=<0..1>	0 Select approximation specific to insulator position variations.
WeightDielectic	=<float>	0 Interpolation coefficient between two approximations of dielectric term.
WeightQuantumPotential	=<float>	0.5 Interpolation coefficient between two approximations for density-gradient quantum-correction term.

Table 301   GeometricVariation() in DeterministicVariation() Deterministic Geometric Variations on page 705

Table 321		Spatial restriction of variation.
Amplitude	=<vector>	µm Vectorial amplitude for displacement.
Amplitude_Iso	=<float>	µm Isotropic amplitude for displacement.
Options	=<0..1>	0 Select approximation specific to insulator position variations.
Surface	=<string>	! Name of varying surface.
WeightDielectic	=<float>	0 Interpolation coefficient between two approximations of dielectric term.
WeightQuantumPotential	=<float>	0.5 Interpolation coefficient between two approximations for density-gradient quantum-correction term.

Table 302   HeatCapacity() Heat Capacity on page 899

<ident>	[(Table 341)]	PMI model <ident> for lattice heat capacity. Heat Capacity on page 1177
Constant		Constant lattice heat capacity.
PMIModel(	Table 318)	Use multistate configuration–dependent model.
TempDep		* Temperature-dependent lattice heat capacity.

Table 303   HydrogenAtom(), HydrogenIon(), HydrogenMolecule() in Hydrogen Transport on page 500

Alpha	=<ident>	Use PMI model for prefactor of the thermal diffusion term α_{td} .
Diffusivity	=<ident>	Use PMI model for $D_i \exp(-E_{di}/(kT))$.

Table 304   HydrogenDiffusion() Hydrogen Transport on page 500

HydrogenAtom(	Table 303)	Hydrogen atom specification.
HydrogenIon(	Table 303)	Hydrogen ion specification.
HydrogenMolecule(	Table 303)	Hydrogen molecule specification.
HydrogenReaction(	Table 305)	Reactions Between Mobile Elements on page 502

NOTE   In Table 305, d is 3 for bulk reactions and 2 for interface reactions.

Table 305   HydrogenReaction() Reactions Between Mobile Elements on page 502

FieldFromMaterial	=<string>	(i) Material where the electric field is obtained.
FieldFromRegion	=<string>	(i) Region where the electric field is obtained.
ForwardReactionCoef	=<float>	0 /cm^{d}s Forward reaction coefficient.
ForwardReactionEnergy	=<float>	0 eV Forward reaction activation energy.
ForwardReactionFieldCoef	=<float>	0 cm/V Forward reaction field coefficient.
LHSCoef		Define particle numbers to be removed.
(	Electron=<int>	0 Number of electrons to be removed.
	Hole=<int>	0 Number of holes to be removed.
	HydrogenAtom=<int>	0 Number of hydrogen atoms to be removed.
	HydrogenIon=<int>	0 Number of hydrogen ions to be removed.
	HydrogenMolecule=<int>)	0 Number of hydrogen molecules to be removed.
Material	=<string>	(i) Material where the recombination rate enters.
Region	=<string>	(i) Region where the recombination rate enters.
ReverseReactionCoef	=<float>	0 /cm^{d}s Reverse reaction coefficient.
ReverseReactionEnergy	=<float>	0 eV Reverse reaction activation energy.
ReverseReactionFieldCoef	=<float>	0 cm/V Reverse reaction field coefficient.
RHSCoef		Define particle numbers to be created.
(	Electron=<int>	0 Number of electrons to be created.
	Hole=<int>	0 Number of holes to be created.
	HydrogenAtom=<int>	0 Number of hydrogen atoms to be created.
	HydrogenIon=<int>	0 Number of hydrogen ions to be created.
	HydrogenMolecule=<int>)	0 Number of hydrogen molecules to be created.

Table 306   IncompleteIonization() Chapter 13, p. 277

Dopants	=<string>	Restrict incomplete ionization to dopants named in <string>. Dopant names are separated by spaces.
Model(	<ident>(<string> [Table 341]))	Use PMI model <ident> for species named in <string>. Incomplete Ionization on page 1222
Split(	Doping=<string>	Dopant that is redistributed into multiple lattice sites. Multiple Lattice Sites on page 278
	Weights=(<float>...))	Occupation probabilities of the various lattice sites. Multiple Lattice Sites on page 278

Table 307   Mechanics() Mechanics Solver on page 890

binary	=<string>	Name of the Sentaurus Interconnect binary. Mechanics Solver on page 890
command	=<string>	Sentaurus Interconnect Tcl commands. Mechanics Solver on page 890
initial_structure	=<string>	Initial structure for first call of Sentaurus Interconnect. Mechanics Solver on page 890
parameter	=<string>	Sentaurus Interconnect parameters. Mechanics Solver on page 890

Table 308   MetalWorkfunction() Metal Workfunction on page 242

Randomize(	AtInsulatorInterface	off (r) Randomize workfunction at metal–insulator vertices only. Metal Workfunction Randomization on page 243
	AverageGrainSize=<float>	! (r) Average metal grain size. Metal Workfunction Randomization on page 243
	GrainProbability= (<float>...)	! (r) Probabilities that grains will have a certain workfunction value. Metal Workfunction Randomization on page 243
	GrainWorkfunction= (<float>...)	! eV (r) Workfunction values corresponding to the above probabilities. Metal Workfunction Randomization on page 243
	RandomSeed=<int>	Seed for the random number generator. Metal Workfunction Randomization on page 243
	UniformDistribution)	off (r) Attempt to evenly distribute uniformly sized grains. Metal Workfunction Randomization on page 243

Table 308   MetalWorkfunction() Metal Workfunction on page 242 (Continued)

SFactor	=\<string\>	Dataset for the spatial distribution of metal workfunction. Metal Workfunction on page 242
	=\<ident\> [(Table 341)]	Name of model to be used by the PMI to compute the spatial distribution of metal workfunction. Space Factor on page 1190
	[Factor=\<float\>]	! Scale factor for normalized SFactor values. Metal Workfunction on page 242
	[Offset=\<float\>]	! Offset for raw or normalized SFactor values. Metal Workfunction on page 242
Workfunction	=\<float\>	eV Metal workfunction. Metal Workfunction on page 242
	=(\<float\> \<float\>*3)...	eV , μm , μm , μm Metal workfunction–position quadruplets. Metal Workfunction on page 242

Table 309   Model(), options of stress-dependent models Chapter 31 on page 821

DeformationPotential		Linear deformation potential model for computing band structure. Deformation of Band Structure on page 826
(	ekp	$k \cdot p$ method for electron bands to account for shear strain components. Deformation of Band Structure on page 826
	hkp	6×6 $k \cdot p$ method for hole bands. Deformation of Band Structure on page 826
	Minimum	Compute conduction and valence band edges using minimum band energies. Deformation of Band Structure on page 826
	multivalley)	Compute conduction and valance band edges using Multivalley band structure. Using Deformation Potential Model on page 829
DOS(	eMass	Strained electron effective mass and DOS model. Strained Electron Effective Mass and DOS on page 831
	hMass	Strained hole effective mass and DOS model. Strained Hole Effective Mass and DOS on page 833
	hMass(AnalyticLTFit)	Strained hole effective mass and DOS model with analytic lattice temperature fit. Strained Hole Effective Mass and DOS on page 833
	hMass(NumericalIntegration))	Strained hole effective mass and DOS model with numeric integrations. Strained Hole Effective Mass and DOS on page 833

Table 309   Model(), options of stress-dependent models Chapter 31 on page 821
(Continued)

Mobility(	eFactor[(Table 322)]	Piezoresistive factor for electrons. Isotropic Factor Models on page 870
	eMinorityFactor=<float>	`1.0` Factor to scale stress effect for minority electrons. Stress Mobility Model for Minority Carriers on page 877
	eMinorityFactor(DopingThreshold=<float>)= <float>	`1.0` Factor to scale stress effect for minority electrons with no doping dependency. Stress Mobility Model for Minority Carriers on page 877
	eSaturationFactor=<float>	`1.0` Saturation factor for electrons. Dependency of Saturation Velocity on Stress on page 879
	eSubband(Doping)	Strain-induced subband model for electrons with doping dependency. Multivalley Electron Mobility Model on page 839
	eSubband(EffectiveMass)	Stress-induced change of the electron effective mass. Effective Mass on page 842
	eSubband(EffectiveMass(-Transport))	Exclude 2D inverse transport mass tensor transformation. Effective Mass on page 842
	eSubband(EffectiveMass(Transport<vector>))	Activate 1D inverse transport mass tensor transformation. Effective Mass on page 842
	eSubband(Fermi)	Strain-induced subband model for electrons with carrier concentration (Fermi statistics) dependency. Multivalley Electron Mobility Model on page 839
	eSubband(Scattering)	Strain-induced subband model for electrons with scattering. Intervalley Scattering on page 840
	eSubband(Scattering(MLDA))	Strain-induced subband model with interface scattering. Intervalley Scattering on page 840
	eSubband(-RelChDir110)	Use <100> channel direction in reference mobility. Using Multivalley Electron Mobility Model on page 846
	eSubband(-AutoOrientation)	Use full tensor reference mobility. Using Multivalley Electron Mobility Model on page 846
	eTensor[(Table 322)]	Piezoresistive tensor for electrons. Piezoresistance Mobility Model on page 859
	Factor[(Table 322)]	Piezoresistive factor for electrons and holes. Isotropic Factor Models on page 870
	hFactor[(Table 322)]	Piezoresistive factor for holes. Isotropic Factor Models on page 870
	hMinorityFactor=<float>)	`1.0` Factor to scale stress effect for minority holes. Stress Mobility Model for Minority Carriers on page 877

Table 309   Model(), options of stress-dependent models Chapter 31 on page 821
(Continued)

Mobility(	hMinorityFactor(DopingThreshold=<float>)= <float>	1.0 Factor to scale stress effect for minority holes with no doping dependency. Stress Mobility Model for Minority Carriers on page 877
	hSaturationFactor=<float>	1.0 Saturation factor for holes. Dependency of Saturation Velocity on Stress on page 879
	hSixband	Intel stress-induced model for holes. Intel Stress-Induced Hole Mobility Model on page 854
	hSixband(Doping)	Intel stress-induced model for holes with doping dependency. Intel Stress-Induced Hole Mobility Model on page 854
	hSixband(Fermi)	Intel stress-induced model for holes with carrier concentration (Fermi statistics) dependency. Intel Stress-Induced Hole Mobility Model on page 854
	hSubband(Doping)	Strain-induced subband model for holes with doping dependency. Multivalley Hole Mobility Model on page 849
	hSubband(EffectiveMass)	Stress-induced change of the holes effective mass. Effective Mass on page 849
	hSubband(EffectiveMass(Transport))	Activate 2D inverse transport mass tensor transformation. Effective Mass on page 849
	hSubband(EffectiveMass(Transport<vector>))	Activate 1D inverse transport mass tensor transformation. Effective Mass on page 849
	hSubband(Fermi)	Strain-induced subband model for holes with carrier concentration (Fermi statistics) dependency. Multivalley Hole Mobility Model on page 849
	hSubband(Scattering)	Strain-induced subband model for holes with bulk scattering. Scattering on page 850
	hSubband(Scattering(MLDA))	Strain-induced subband model for holes with interface scattering. Scattering on page 850
	hSubband(-RelChDir110)	Use <100> channel direction in reference mobility. Using Multivalley Hole Mobility Model on page 852
	hSubband(-AutoOrientation)	Use full tensor reference mobility. Using Multivalley Hole Mobility Model on page 852
	hTensor[(Table 322)]	Piezoresistive tensor for holes. Piezoresistance Mobility Model on page 859
	SaturationFactor=<float>	1.0 Saturation factor for electrons and holes. Dependency of Saturation Velocity on Stress on page 879
	Tensor[(Table 322)])	Piezoresistive tensor for electrons and holes. Piezoresistance Mobility Model on page 859

Table 310   MoleFraction() Mole-Fraction Specification on page 17

Grading((		Alternative way to specify grading; allows a nonzero mole fraction and different distance of grading from different parts of the boundaries.
	GrDistance=<float>	μm Distance in the direction normal to the specified interface, where linear interpolation of mole fractions from the constant value to the specified boundary mole fractions occurs.
	RegionInterface= (<string>*2)	Restrict this grading to the given interface (applied to all interfaces by default).
	xFraction=<[0,1]>	Boundary xMoleFraction.
	yFraction=<[0,1]>)...)	Boundary yMoleFraction.
GrDistance	=<float>	μm Distance in the direction normal to the boundaries of the specified regions where linear interpolation of mole fractions from the specified constant value to 0 occurs.
RegionName	=[<string>...]	List of regions where the mole-fraction specification will take effect.
	=<string>	Regions where the mole-fraction specification will take effect.
xFraction	=<[0,1]>	Constant value of xMoleFraction.
yFraction	=<[0,1]>	Constant value of yMoleFraction.

Table 311   MSConfig() Chapter 18, p. 473

BandEdgeShift(	<ident> [(Table 341)] [<int>])	Compute band-edge shifts for conduction and valence by PMI model <ident> with optional constructor argument <int>. Apparent Band-Edge Shift on page 483
Conc	=<float>	0 cm^{-d} Concentration of states ($d = 3$ for bulk; $d = 2$ for interface MSCs).
eBandEdgeShift(	<ident> [(Table 341)] [<int>])	Compute band-edge shift for conduction band by PMI model <ident> with optional constructor argument <int>. Apparent Band-Edge Shift on page 483
Elimination		+ Switch solving algorithm.
hBandEdgeShift(	<ident> [(Table 341)] [<int>])	Compute band-edge shift for valence band by PMI model <ident> with optional constructor argument <int>. Apparent Band-Edge Shift on page 483
Name	=<string>	! Identifier of MSConfig.

Table 311   MSConfig() Chapter 18, p. 473 (Continued)

State(		! Define a state (at least two required).
	Charge=<int>	0 Number of positive elementary charges.
	Hydrogen=<int>	0 Number of hydrogen atoms.
	Name=<string>)	! Identifier of state.
Transition(	Table 324)	! Define a transition.

Table 312   NBTI() Two-Stage NBTI Degradation Model on page 509

Conc	=<float>	0 cm^{-2} Concentration of NBTI traps.
NumberOfSamples	=<int>	0 Number of random samples.
hSHEDistribution		– Use hole-energy distribution function.

Table 313   Noise() Chapter 23, p. 675

BandEdgeFluctuations	<string> (Table 321)	Band edge fluctuations. Random Band Edge Fluctuations on page 688
ConductivityFluctuations	<string> (Table 321)	Metal conductivity fluctuations. Random Metal Conductivity Fluctuations on page 689
DiffusionNoise(	Table 321	Diffusion noise, spatially restricted Diffusion Noise on page 681
	e_h_Temperature	Noise temperatures are the respective carrier temperatures.
	eTemperature	Noise temperature is electron temperature for electrons, lattice temperature for holes.
	hTemperature	Noise temperature is lattice temperature for electrons, hole temperature for holes.
	LatticeTemperature)	* Noise temperature is lattice temperature.
Doping(	Table 286)	Random dopant fluctuations
EpsilonFluctuations	<string> (Table 321)	Dielectric constant fluctuations. Random Dielectric Constant Fluctuations on page 690
FlickerGRNoise(	Table 321)	Bulk flicker noise. Bulk Flicker Noise on page 682
GeometricFluctuations	<string> (Table 300)	Geometric fluctuations for surface <string>. Random Geometric Fluctuations on page 684

Table 313   Noise() Chapter 23, p. 675 (Continued)

MonopolarGRNoise(	Table 321)	Equivalent monopolar noise. Equivalent Monopolar Generation–Recombination Noise on page 682
TrapConcentration(	Table 321)	Trap concentration fluctuations. Random Trap Concentration Fluctuations on page 687
Traps(	Table 321)	Trapping noise. Trapping Noise on page 682
WorkfunctionFluctuations	<string> (Table 321)	Workfunction fluctuations for surface <string>. Random Workfunction Fluctuations on page 687

Table 314   Optics() Transfer Matrix Method on page 625 and Beam Propagation Method on page 647

Table 268		Optics standalone.
BPMScalar(	Table 237)	Scalar beam propagation method (BPM) solver. Beam Propagation Method on page 647
TMM(	Table 262)	Transfer matrix method (TMM) solver. Transfer Matrix Method on page 625

Table 315   Optics() Specifying the Type of Optical Generation Computation on page 534

ComplexRefractiveIndex(	Table 283)	Complex refractive index models. Complex Refractive Index Model on page 578
Excitation		Specification of excitation parameters. Setting the Excitation Parameters on page 560
(	Intensity=<float>	Wcm^{-2}
	Phi=<float>	0 deg Angle between projection of propagation direction on xy plane and x-axis.
	Polarization=<float>	0 [0,1] Definition of polarization as in Using Transfer Matrix Method on page 630.
	Polarization=<ident>	TM Transverse electric (TE) or transverse magnetic (TM) polarized light.
	PolarizationAngle=<float>	0 deg Angle between H-field and $z \times \hat{k}$ used for vectorial solvers only.
	Theta=<float>	0 deg Angle between propagation direction and z-axis.
	Wavelength=<float>)	µm
	Window(Table 326)	

Table 315   Optics() Specifying the Type of Optical Generation Computation on page 534
(Continued)

OpticalGeneration(	Table 247)	Optical generation models. Specifying the Type of Optical Generation Computation on page 534
OpticalSolver		Specification of optical solver method. Specifying the Optical Solver on page 554
(	BPM (Table 237)	
	Composite	Composite Method on page 656
	FDTD (Table 241)	
	FromFile (Table 242)	
	OptBeam (Table 246)	
	RayTracing (Table 253)	Raytracer on page 593
	TMM (Table 262))	Note that `Excitation` section must not be defined in `TMM` section. Using Transfer Matrix Method on page 630
Verbosity	=<int>	`1` Verbosity level for optical solver output. A verbosity level of `0` suppresses all optical solver output.

Table 316   ParameterVariation() in DeterministicVariation() Parameter Variations on
page 706

Factor	=<float>	`1` 1 Multiplier for original parameter value.
Material	=<string>	Material location of varied parameter.
MaterialInterface	=<string>	Material interface location of varied parameter.
Model	=<string>	! Model to which varied parameter belongs.
Parameter	=<string>	! Name of the varied parameter.
Region	=<string>	Region location of varied parameter.
RegionInterface	=<string>	Region interface location of varied parameter.
Summand=	=<float>	`0` Summand to original parameter value.
Value=	=<float>	Modified parameter value.

Table 317   Piezo() Chapter 31, p. 821

Model(	(Table 309)	Stress-dependent models. Deformation of Band Structure on page 826 to Mobility Modeling on page 838
OriKddX	=<vector>	(1 0 0) Miller indices of the stress system relative to the simulation system.
OriKddY	=<vector>	(0 1 0) Miller indices of the stress system relative to the simulation system.
Strain	=(<float>*6)	Components xx, yy, zz, yz, xz, xy of strain tensor.
	=Hooke	Use Hooke's law to compute strain tensor from stress tensor. Eq. 937, p. 822
	=LoadFromFile	Load strain from Piezo file specified in File section.
Stress	=(<float>*6)	Pa Components xx, yy, zz, yz, xz, xy of stress tensor.
	=<ident> [(Table 341)]	Use PMI model <ident> to compute stress. Stress on page 1186

Table 318   PMIModel() Multistate Configuration–Dependent Bulk Mobility on page 1113, High-Field Saturation With Two Driving Forces on page 1134, Multistate Configuration–Dependent Thermal Conductivity on page 1173, Multistate Configuration–Dependent Heat Capacity on page 1180

Index	=<int>	0 Number passed to and interpreted by PMI model.
MSConfig	=<string>	"" Name of multistate configuration on which PMI depends.
Name	=<string>	! Name of PMI model.
String	=<string>	"" String passed to and interpreted by PMI model.
Table 341		PMI parameters.

Table 319   RandomizedVariation() in Physics{} Statistical Impedance Field Method on page 691

BandEdge	<string> (Table 280)	– Band Edge Variations on page 699
Conductivity	<string> (Table 284)	– Metal Conductivity Variations on page 700
Doping(	Table 287)	– Doping Variations on page 695
DopingVariation	<string> (Table 289)	– Doping Profile Variations on page 702
Epsilon	<string> (Table 293)	– Dielectric Constant Variations on page 701
Geometric	<string> (Table 299)	– Geometric Variations on page 698

Table 319   RandomizedVariation() in Physics{} Statistical Impedance Field Method on page 691 (Continued)

TrapConcentration(	Table 321)	– Trap Concentration Variations on page 696
Workfunction	`<string>` (Table 327)	– Workfunction Variations on page 697

Table 320   Schroedinger() 1D Schrödinger Solver on page 285

DensityTail	=Extrapolate	* Use estimate for lowest noncomputed subband energy as $E_{\mathrm{max,\,v}}$. Eq. 228, p. 291
	=MaxEnergy	Use highest computed subband energy as $E_{\mathrm{max,\,v}}$. Eq. 228, p. 291
eDensityCorrection		+ Activate electron quantization model in the quantum well. 1D Schrödinger Solver on page 285
Electron		– Solve Schrödinger equation for electrons.
EnergyInterval	`[(<carrier>)]=<float>`	`0` eV Highest energy to which eigensolutions are computed, measured from the lowest interior potential point on the nonlocal line on which the Schrödinger equation is solved. When `0`, only bound solutions are computed. Using 1D Schrödinger on page 287
Error	`[(<carrier>)]=<(0,)>`	`1e-5` eV Precision target for eigenenergies. Using 1D Schrödinger on page 287
hDensityCorrection		+ Activate hole quantization model in the quantum well. 1D Schrödinger Solver on page 285
Hole		– Solve Schrödinger equation for holes.
MaxSolutions	`[(<carrier>)]=<0..>`	`5` Maximum number of eigensolutions computed per ladder. Using 1D Schrödinger on page 287
Polarization	`= TE │ TM │ Mixed`	`TE` Set the polarization used for the computation of the optical transition matrix element. Optical Transition Matrix Element for Wurtzite Crystals on page 971
PolarizationFactor	`=<[0,1]>`	`1` Set the polarization factor used for the computation of the optical transition matrix element in mixed polarization simulations. Optical Transition Matrix Element for Wurtzite Crystals on page 971
Smooth	`=<float>`	`0` cm Length (measured from end of nonlocal line) over which to blend from classical to quantum density.

Table 321   Spatial restriction Energetic and Spatial Distribution of Traps on page 450,
Options Common to sIFM Variations on page 692

SpaceMid	=<vector>	(0 0 0) μm Center of spatial distribution.
SpaceSig	=<vector>	(1e100 1e100 1e100) μm Width of spatial distribution.
SpatialShape	=Gaussian	Use Gaussian shape function.
	=Uniform	* Use Uniform shape function.

Table 322   Tensor(), eTensor(), hTensor() Piezoresistance Mobility Model on page 859,
Factor(), eFactor(), hFactor() Isotropic Factor Models on page 870

<ident>	[(Table 341)]	Use PMI model <ident> to compute piezoresistive prefactors (first-order piezoresistance tensor model only). Piezoresistive Coefficients on page 1237
		Use PMI model <ident> to compute a mobility enhancement stress factor (isotropic factor model only). Mobility Stress Factor on page 1193
ApplyToMobilityComponents		– Apply the Factor model enhancement to individual mobility components. Factor Models Applied to Mobility Components on page 876
AutoOrientation		off Use parameter set based on orientation of nearest interface. Auto-Orientation for Piezoresistance on page 863 and Isotropic Factor Model Options on page 876
ChannelDirection	=<1..3>	1 Channel direction (Factor models only). Isotropic Factor Models on page 870
EffectiveStressModel		Use the effective stress Factor model. Effective Stress Model on page 872
	(AxisAlignedNormals)	off Use axis-aligned normals for the effective stress calculation. Effective Stress on page 873
Enormal		off Use piezoresistive prefactors (first-order piezoresistance tensor model only). Enormal- and MoleFraction-Dependent Piezo Coefficients on page 863
FirstOrder		* Use the first-order piezoresistance model. Piezoresistance Mobility Model on page 859
Kanda		off Include temperature and doping dependency. Doping and Temperature Dependency on page 860
ParameterSetName	=<string>	Name of Piezoresistance or EffectiveStressModel parameter set. Named Parameter Sets for Piezoresistance on page 863 and Isotropic Factor Model Options on page 876

Table 322   Tensor(), eTensor(), hTensor() Piezoresistance Mobility Model on page 859,
Factor(), eFactor(), hFactor() Isotropic Factor Models on page 870 (Continued)

SecondOrder		Use the second-order piezoresistance model. Piezoresistance Mobility Model on page 859
SFactor	=`<string>`	Dataset for the spatial distribution of the mobility enhancement factor. SFactor Dataset or PMI Model on page 876
	=`<ident>` `[(Table 341)]`	Name of model to be used by the PMI to compute the spatial distribution of the mobility enhancement factor. SFactor Dataset or PMI Model on page 876 and Space Factor on page 1190

Table 323   ThermalConductivity() Thermal Conductivity on page 901

`<ident>`	`[(Table 341)]`	Use PMI model `<ident>` for thermal conductivity. Thermal Conductivity on page 1167
Constant	Conductivity	Use constant conductivity.
	Resistivity	Use constant resistivity.
Formula		Use the built-in strategy for thermal conductivity. Thermal Conductivity on page 1167
PMIModel(	Table 318)	Use multistate configuration–dependent model.
TempDep	Conductivity	Use Eq. 1044, p. 901.
	Resistivity	Use Eq. 1043, p. 901.

Table 324   Transition() in MSConfig() Chapter 18, p. 473

CEModel(	`<ident>` `[(Table 341)]` `[<int>])`	! Use `PMI_TrapCaptureEmission` model `<ident>` with optional constructor argument `<int>`.
FieldFromInsulator		– Use the insulator electric field instead of the semiconductor electric field for the MSCs defined at the semiconductor–insulator interface.
From	=`<string>`	! Interacting state.
Name	=`<string>`	! Identifier of transitions.
Reservoirs(		List of reservoirs for particle conservation.
	`<string>`(Particles= `<int>`)...	Reservoir `<string>` and number of involved particles `<int>`.
To	=`<string>`	! Reference state.

> **NOTE** In Table 325, $d = 3$ for bulk traps and $d = 2$ for interface traps.

Table 325 Traps(()...) Chapter 17, p. 449, Chapter 19, p. 489

Table 321		Spatial restriction of trap distribution.
Acceptor		Acceptor trap type. Trap Types on page 450
ActEnergy	=<float>	eV Equilibrium activation energy of hydrogen on Si-H bonds, ε_A^0 . Chapter 19, p. 489
Add2TotalDoping(		Include the trap concentration in the acceptor, donor, and total doping concentrations used to compute mobility, lifetimes, and so on. Doping Specification on page 11
	ChargedTraps)	Include the charged trap concentration in the acceptor or donor doping concentrations used to compute mobility. Doping Specification on page 11
BarrierTunnelingEnhan	=(<float>*4)	(1 1 1 1) 1, 1, 1, 1 Barrier tunneling enhancement parameters for the Degradation model depassivation constant, δ_{BTe}, ρ_{BTe}, δ_{BTh}, and ρ_{BTh} . Reaction Enhancement Factors on page 493
BondConc	=<float>	cm^{-d} Total silicon dangling bond concentration N . Chapter 19, p. 489
BondConcSFactor	=<ident> [(Table 341)]	Name of model to be used by the PMI to compute the spatial distribution of bond concentration. Space Factor on page 1190
	=<string>	Dataset for the spatial distribution of bond concentration. Using the Trap Degradation Model on page 495
CBRate	=<ident> [(Table 341)]	Use PMI <ident> to compute electron capture and emission rate for conduction band.
	=(<ident> [(Table 341)] <int>)	Use PMI <ident> with constructor argument <int> to compute electron capture and emission rate for conduction band. Trap Capture and Emission Rates on page 1200
Conc	=<float>	cm^{-d} or $eV^{-1}cm^{-d}$ Concentration or the peak density of the trap distribution. Energetic and Spatial Distribution of Traps on page 450
Coupled	=Off	* Disable trap coupling.
	=Tunneling	Couple traps by tunneling. Trap-to-Trap Tunneling on page 461
CritConc	=<float>	cm^{-d} Critical concentration N_{crit} , default $0.1N$. Chapter 19, p. 489
CurrentEnhan	=(<float>*4)	(0 1 0 1) 1, 1, 1, 1 Parameters of the tunneling and hot carrier–dependent terms of the depassivation constant, δ_{Tun}, ρ_{Tun}, δ_{HC}, and ρ_{HC} . Reaction Enhancement Factors on page 493

Table 325 Traps(()...) Chapter 17, p. 449, Chapter 19, p. 489 (Continued)

Cutoff	=BandGap	Truncate trap energy distribution to plain band gap at 300 K. Energetic and Spatial Distribution of Traps on page 450
	=EffectiveBandgap	* Truncate trap energy distribution to effective bandgap at 300 K.
	=None	Do not truncate trap energy distribution.
	=Simple	Use a legacy truncation of trap energy distribution.
Degradation		Use degradation model based on kinetic equation. Chapter 19, p. 489
	(PowerLaw)	Use degradation model based on power law. Chapter 19, p. 489
DePasCoef	=<float>	s^{-1} Depassivation coefficient ν_0 at the passivation conditions (the equilibrium at the passivation temperature T_0). Chapter 19, p. 489
DiffusionEnhan	=(6*<float>)	cm cm^{2}s^{-1} eV cms^{-1} cm^{-3} 1 Parameters of hydrogen diffusion in oxide, x_P , D_0 , ε_H , k_P , N_H^0 , and N_{ox} in Eq. 551, p. 492, Chapter 19, p. 489.
DirectTunnelingEnhan	=(<float>*4)	(1 1 1 1) 1 , 1 , 1 , 1 Direct tunneling enhancement parameters for the Degradation model depassivation constant, δ_{DTe} , ρ_{DTe} , δ_{DTh} , and ρ_{DTh} . Reaction Enhancement Factors on page 493
Donor		Donor trap type. Trap Types on page 450
eBarrierTunneling(	NonLocal=<string>	Use nonlocal tunneling from the conduction band at reference surface of all connected unnamed, and all listed, connected named nonlocal meshes. Tunneling and Traps on page 463
	TwoBand)	Use two-band dispersion. WKB Tunneling Probability on page 729
eConstEmissionRate	=<float>	s^{-1} Constant electron emission rate term to the conduction band e_{const}^n . Local Trap Capture and Emission on page 457
eGfactor	=<float>	Electron degeneracy factor g_n . Trap Occupation Dynamics on page 455
eHCSDegradation		Use the hot-carrier stress (HCS) degradation model for electrons. Hot-Carrier Stress Degradation Model on page 519
(	BondDispersion	+ Use bond dispersion. Bond Dispersion on page 523
	SHE)	- Use the carrier distribution function from SHE. Spherical Harmonics Expansion Option on page 522
eJfactor	=<float>	Electron J-model factor g_n^J . Local Trap Capture and Emission on page 457
ElectricField	[(<carrier>)]	Field-dependent model for cross sections. J-Model Cross Sections on page 458

Table 325 Traps(()...) Chapter 17, p. 449, Chapter 19, p. 489 (Continued)

`EnergyMid`	`=<float>`	eV Central energy E_0 of the trap distribution. Eq. 502, p. 450
`EnergyShift`	`=<ident> [(Table 341)]`	Use PMI `<ident>` to compute trap energy shift.
	`=(<ident> [(Table 341)] <int>)`	Use PMI `<ident>` with constructor argument `<int>` to compute trap energy shift. Energetic and Spatial Distribution of Traps on page 450, Trap Energy Shift on page 1205
`EnergySig`	`=<(0,)>`	eV Width E_S of the trap distribution. Eq. 502, p. 450
`eNeutral`		Electron trap type. Trap Types on page 450
`eSHEDistribution`	`=(<float>*6)`	$(0\ 0\ 0\ 0\ 1\ 1)\ (\mathrm{cm}^2\mathrm{A}^{-1})^{\rho_{SHE}}$, eV , eV , eV , 1 , 1 Parameters of the electron energy–dependent terms of the depassivation constant, δ_{SHE} , ε_{th} , ε_a , $\delta_\perp$, $\rho_\perp$, and ρ_{SHE} . Trap Degradation Model on page 490
`Exponential`		Exponential energetic distribution. Energetic and Spatial Distribution of Traps on page 450, Eq. 502, p. 450
`eXsection`	`=<[0,)>`	cm^2 Electron capture cross section σ_n^0 . Local Trap Capture and Emission on page 457
`FieldEnhan`	`=(<float>*4)`	$(0\ 1\ 0\ 1)\ \mathrm{eVcm}^{\rho_{//}}\mathrm{V}^{-\rho_{//}}$, 1 , $\mathrm{eVcm}^{\rho_\perp}\mathrm{V}^{-\rho_\perp}$, 1 Parameters of the electric field–dependent terms of the Si-H bond energy and the activation energy, $\delta_{//}$, $\rho_{//}$, $\delta_\perp$, and $\rho_\perp$. Chapter 19, p. 489
`FixedCharge`		Fixed charge. Trap Types on page 450
`FowlerNordheimEnhan`	`=(<float>*4)`	$(1\ 1)\ 1$, 1 Fowler–Nordheim tunneling enhancement parameters for the `Degradation` model depassivation constant, δ_{FN} , and ρ_{FN} . Reaction Enhancement Factors on page 493
`fromCondBand`		Zero point for E_0 is conduction band. Eq. 503, p. 451
`fromMidBandGap`		Zero point for E_0 is intrinsic energy. Eq. 503, p. 451
`fromValBand`		Zero point for E_0 is valence band. Eq. 503, p. 451
`Gaussian`		Gaussian energetic distribution. Energetic and Spatial Distribution of Traps on page 450, Eq. 502, p. 450
`hBarrierTunneling(`	`NonLocal=<string>`	Use nonlocal tunneling from the valence band at reference surface of all connected unnamed, and all listed, connected named nonlocal meshes. Tunneling and Traps on page 463
	`TwoBand)`	Use two-band dispersion. WKB Tunneling Probability on page 729
`hConstEmissionRate`	`=<float>`	s^{-1} Constant hole emission rate to the valence band e_{const}^p . Local Trap Capture and Emission on page 457
`hGfactor`	`=<float>`	Hole degeneracy factor g_p . Trap Occupation Dynamics on page 455

Table 325   Traps(()...) Chapter 17, p. 449, Chapter 19, p. 489 (Continued)

hHCSDegradation		Use the HCS degradation model for holes. Hot-Carrier Stress Degradation Model on page 519
(	BondDispersion	+ Use bond dispersion. Bond Dispersion on page 523
	SHE)	- Use the carrier distribution function from SHE. Spherical Harmonics Expansion Option on page 522
hJfactor	=<float>	Hole J-model factor g_p^J. Local Trap Capture and Emission on page 457
hNeutral		Hole trap type. Trap Types on page 450
hSHEDistribution	=(<float>*6)	$(0\ 0\ 0\ 0\ 1\ 1)\ (cm^2 A^{-1})^{\rho_{SHE}}$, eV, eV, eV, 1, 1 Parameters of the hole energy–dependent terms of the depassivation constant, δ_{SHE}, ε_{th}, ε_a, $\delta_\perp$, $\rho_\perp$, and ρ_{SHE}. Trap Degradation Model on page 490
HuangRhys	=<[0,)>	Huang–Rhys factor. Tunneling and Traps on page 463
hXsection	=<[0,)>	cm^2 Hole capture cross section σ_p^0. Local Trap Capture and Emission on page 457
Level		Trap with single energy level. Energetic and Spatial Distribution of Traps on page 450, Eq. 502, p. 450
Location	=(<vector>...)	μm Locations of traps coupled by tunneling. Trap-to-Trap Tunneling on page 461
Makram-Ebeid	[(<carrier> <simpleCapt>)]	Use Makram–Ebeid–Lannoo model. Local Capture and Emission Rates Based on Makram-Ebeid–Lannoo Phonon-Assisted Tunnel Ionization Model on page 459
Material	=<string>	(i) Material to which energy specification refers. Energetic and Spatial Distribution of Traps on page 450
Name	=<string>	Identifier for trap.
PasCoef	=<float>	s^{-1} Passivation coefficient γ_0. By default, computed automatically to provide the equilibrium, $\nu_0 N_{hb}^0 / (N - N_{hb}^0)$. Chapter 19, p. 489
PasTemp	=<float>	300 K Passivation temperature T_0. Chapter 19, p. 489
PasVolume	=<float>	0 $cm^2|cm^3$ Passivation volume Ω. Chapter 19, p. 489
PhononEnergy	=<[0,)>	eV Phonon energy for inelastic tunneling. Tunneling and Traps on page 463

Table 325 Traps(()...) Chapter 17, p. 449, Chapter 19, p. 489 (Continued)

PooleFrenkel		Use Poole–Frenkel model for exchange with conduction or valence band, depending on trap type. Poole–Frenkel Model for Cross Sections on page 458
	(Electron)	Use Poole–Frenkel model for exchange with conduction band, irrespective of trap type.
	(Hole)	Use Poole–Frenkel model for exchange with valence band, irrespective of trap type.
PowerEnhan	=(<float>*3)	(0 0 0) 1, V^{-1}cm, V^{-1}cm Parameters in the chemical potential for kinetic equation degradation and the power for degradation by power law, β_0, $\beta_{//}$, and $\beta_{\perp}$. Chapter 19, p. 489
Randomize	[=<int>]	Randomize traps. Trap Randomization on page 454
Reference	=BandGap	Refer trap energies to band edges excluding bandgap narrowing. Energetic and Spatial Distribution of Traps on page 450
	=EffectiveBandgap	* Refer trap energies to effective band edges.
ReferencePoint	=<vector>	Coordinate where to take the data for EnergyShift.
Region	=<string>	(i) Region to which energy specification refers. Energetic and Spatial Distribution of Traps on page 450
SFactor	=<string>	Dataset for the spatial distribution of the traps. Energetic and Spatial Distribution of Traps on page 450
	=<ident> [(Table 341)]	Name of model to be used by the PMI to compute the spatial trap distribution. Space Factor on page 1190
SimpleCapt		– Restrict field enhancement of trapping to the emission rates. Local Trap Capture and Emission on page 457
SingleTrap		Use a single trap. Specifying Single Traps on page 453
Table	=(<float>*2...)	eV $\text{eV}^{-1}\text{cm}^{-d}$ Pairs of energy and concentration of a tabular approximation to a trap distribution. Energetic and Spatial Distribution of Traps on page 450, Eq. 502
TrapVolume	=<[0,)>	μm^3 Interaction volume for nonlocal tunneling. Tunneling and Traps on page 463
Tunneling(	Hurkx[(<carrier>)])	Use Hurkx trap-assisted tunneling model. Hurkx Model for Cross Sections on page 458
Uniform		Uniform energetic distribution. Energetic and Spatial Distribution of Traps on page 450, Eq. 502, p. 450

Table 325   Traps(()...) Chapter 17, p. 449, Chapter 19, p. 489 (Continued)

| VBRate | =<ident> [(Table 341)] | Use PMI <ident> to compute hole capture and emission rate for valence band. |
| | =(<ident> [(Table 341)] <int>) | Use PMI <ident> with constructor argument <int> to compute hole capture and emission rate for valence band. Trap Capture and Emission Rates on page 1200 |

Table 326   Window Illumination Window on page 562

Circle(	Radius=<float>)	
IntensityDistribution(	Gaussian(Table 298))	Specify spatial intensity profile. Spatial Intensity Function Excitation on page 568
Line(	Dx=<float>	
	X1=<float>	
	X2=<float>)	
Origin	=(<float>*3)	Global location of window origin.
OriginAnchor	=<ident>	Center Origin anchor of illumination window in terms of cardinal direction (North, South, East, West, NorthEast, SouthEast, NorthWest, SouthWest).
Polygon(	(<float>*2)*n	Specification of simple polygon using several vertices.
	((<float>*2)*n)*m)	Specification of complex polygon using several loops of vertices.
Rectangle(	Dx=<float>	
	Dy=<float>	
	Corner1=(<float>*2)	
	Corner2=(<float>*2))	
RotationAngles	=(<float>*3)	Angles specifying global orientation of window coordinate system.

Table 326   Window Illumination Window on page 562 (Continued)

WeightedAPDintegration		– Switch on weighted absorbed photon density (APD) integration. Accurate Absorbed Photon Density for 1D Optical Solvers on page 575
(	`Mode= Auto | Full | Simple`	`Auto` Set integration mode of APD. Options are: `Auto`: Mixed wireframe and 1D integration. `Full`: Wireframe integration. `Simple`: One-dimensional integration.
	`NumberOfCellsPerLayer= <int>`	`100` Set the number of wireframe cells per layer.
	`NumberOfTransverseCells PerDirection=<int>`	`200` Wireframe discretization parameter of the illumination window plane.
	`PrintInfo)`	Print detailed information about wireframe integration.
XDirection	`=(<float>*3)`	`(1, 0, 0)` Direction of x-axis.
YDirection	`=(<float>*3)`	`(0, 1, 0)` Direction of y-axis.

Table 327   Workfunction() in RandomizedVariation() Workfunction Variations on page 697

Table 230		Statistical properties of the correlation.
Table 321		Spatial restriction of variation.
Amplitude	`=<float>`	eV Amplitude of workfunction variation for exponential and Gaussian correlation.
GrainProbability	`=(<(0,)>...)`	Probability for grain orientation.
GrainWorkfunction	`=(<float>...)`	eV Grain workfunctions.
Surface	`=<string>`	! Surface of variation. Workfunction Variations on page 697

Plotting

Table 328   Plot{} Device Plots on page 122

Table 178		Scalar plot data. Device Plots on page 122
Table 178/Element		Scalar plot datasets defined on elements.
Table 178/RegionInterface		Scalar plot data on region interfaces; supported for just a few datasets. Interface Plots on page 125
Table 178/Tensor		Tensorial plot data. Device Plots on page 122
Table 179/Vector		Vectorial plot data. Device Plots on page 122
Table 180/SpecialVector		Special vectorial plot data; supported for the SHE distribution data. SHE Distribution Hot-Carrier Injection on page 744
Table 332		Occupation rates of MSConfig states. Specifying Multistate Configurations on page 475
DatasetsFromGrid		Copy datasets from TDR grid file. What to Plot on page 122
	(<ident>...)	Datasets to be copied.

Table 329   Average(), Integrate(), Maximum(), and Minimum() Tracking Additional Data in the Current File on page 110

Table 339		Sample over location.
Coordinates		Print coordinates where maximum, minimum, or average occurs.
DopingWell	<vector>	Sample over well, defined by point in the well.
Everywhere		Sample over entire device.
Insulator		Sample over all insulator regions of the device.
Name	=<string>	Name for sampled data to be used in output.
Semiconductor		Sample over all semiconductor regions of the device.
Window[	<vector> <vector>]	Sample over the window, defined by two specified corners.

Table 330   CurrentPlot{} Tracking Additional Data in the Current File on page 110

`<vector>`		µm Print data at coordinate `<vertex>`.
`Average(`	Table 329)	Print average over given domain.
`Device`	`=<string>`	Name of the device for which the parameter will be plotted.
`Integrate(`	Table 329)	Print integral over given domain.
`Material`	`=<string>`	Name of material for which the parameter will be plotted if it has been specified for a particular material.
`MaterialInterface`	`=<string>`	Name of material interface for which the parameter will be plotted if it has been specified for a particular material interface.
`Maximum(`	Table 329)	Print maximum in given domain.
`Minimum(`	Table 329)	Print minimum in given domain.
`Model`	`=<string>`	Select a model for printing of parameters.
`ModelParameter`	`=<string>`	Select model parameter for plotting when using unified interface for optical generation computation. Parameter Ramping on page 573
`OpticalDevice`	`=<string>`	Name of the optical device for which the parameter will be plotted.
`Parameter`	`=<string>`	Print parameter `<string>`.
`Region`	`=<string>`	Name of the region for which the parameter will be plotted if it has been specified for a particular region.
`RegionInterface`	`=<string>`	Name of the region interface for which the parameter will be plotted if it has been specified for a particular region interface.

Table 331   GainPlot{}

`Intervals`	`=<int>`	Number of points to plot for each gain curve.
`Range`	`=(<float>*2)`	eV Energy range of the gain plot.
	`=Auto`	Automatically find the energy range.

Table 332   MSConfig in Plot{} Specifying Multistate Configurations on page 475

`MSConfig`		All state occupations of all `MSConfig`.
	`(<string>)`	All state occupations of `MSConfig` `<string>`.
	`(<string1> <string2>)`	Occupation of state `<string2>` of MSConfig `<string1>`.

Table 333   NoisePlot{} Noise Output Data on page 710

Table 178	Scalar plot data.
Table 179/Vector	Vector plot data.
AllLNS	All used local noise sources.
AllLNVSD	All used local noise voltage spectral densities.
AllLNVXVSD	All use local noise voltage cross-correlation spectral densities.
GreenFunctions	All used Green's functions and their gradients.

Table 334   NonLocalPlot{} Visualizing Data Defined on Nonlocal Meshes on page 148

Table 178		Scalar data.
EigenEnergy(		Eigenenergies. 1D Schrödinger Solver on page 285
	Electron[(Number=<int>)]	Restrict output to [<int> lowest] electron eigensolutions.
	Hole[(Number=<int>)])	Restrict output to [<int> lowest] hole eigensolutions.
OverlapIntegral		Overlap integrals. 1D Schrödinger Solver on page 285
WaveFunction(		Wavefunctions. 1D Schrödinger Solver on page 285
	Electron[(Number=<int>)]	Restrict output to [<int> lowest] electron eigensolutions.
	Hole[(Number=<int>)])	Restrict output to [<int> lowest] hole eigensolutions.

Table 335   TensorPlot(){} Visualizing Results on Native Tensor Grid on page 655

Name	=<string>	! Name of tensor plot. The file name for the TensorPlot given in the File section is appended by this name.
OutputLevel	=maximum	For bidirectional BPM, tensor plots are generated not only for the final solution, but also after every iteration if maximum is specified.
Xconst	=<float>	µm X-coordinate.
Xmax	=<float>	µm Maximum x-coordinate.
Xmin	=<float>	µm Minimum x-coordinate.
Yconst	=<float>	µm Y-coordinate.
Ymax	=<float>	µm Maximum y-coordinate.
Ymin	=<float>	µm Minimum y-coordinate.
Zconst	=<float>	µm Z-coordinate.

Table 335 TensorPlot(){} Visualizing Results on Native Tensor Grid on page 655 (Continued)

Zmax	=<float>	μm Maximum z-coordinate.
Zmin	=<float>	μm Minimum z-coordinate.

Various

Table 336 Locations, all

Table 337		Bulk location.
Table 338		Interface location.
Electrode	=<string>	Name of an electrode that must exist in the device.

Table 337 Locations, bulk (dimension is that of the device)

Material	=<string>	Name of a material.
Region	=<string>	Name of a region that must exist in the device.

Table 338 Locations, interface (dimension is one less than that of the device)

MaterialInterface	=<string>	Material interface of the form "<ident1>/<ident2>", with <ident1> and <ident2> as the names of materials.
RegionInterface	=<string>	Region interface of the form "<ident1>/<ident2>", with <ident1> and <ident2> as the names of regions that must exist in the device and must have a common interface.

Table 339 Locations, noncontact

Table 337	Bulk location.
Table 338	Interface location.

Table 340 Optics() in Physics{}

Table 268		Optics standalone.

Table 340   Optics() in Physics{} (Continued)

BPMScalar(	Table 237)	Scalar beam propagation method (BPM) solver. Beam Propagation Method on page 647
TMM(	Table 237)	Transfer matrix method (TMM) solver. Transfer Matrix Method on page 625

Table 341   PMI parameters Command File of Sentaurus Device on page 1065

<ident>	=<float>	Scalar floating-point parameter.
	=<string>	Scalar string parameter.
	=(<float>...)	Vector of floating-point parameters.
	=(<string>...)	Vector of string parameters.

G: Command File Overview
Various