Semiconductor Module

User's Guide

COMSOL

Semiconductor Module User's Guide

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Introduction

This guide describes the Semiconductor Module, an add-on package for the COMSOL Multiphysics® modeling environment. The Semiconductor Module provides physics interfaces for modeling semiconductor devices as well as additional related functionality.

This chapter introduces the capabilities of this module with a summary of the physics interfaces. We will also show you where to find documentation and model examples. The last section is a brief overview with links to each chapter in this user's guide.

In this chapter:

• About the Semiconductor Module
• Overview of the User's Guide

About the Semiconductor Module

These topics are included in this section:

- Modeling Semiconductor Devices
- What Can the Semiconductor Module Do?
- The Semiconductor Module Physics Interface Guide
- Common Physics Interface and Feature Settings and Nodes
- The Semiconductor Module Study Capabilities by Physics Interface
- The Semiconductor Materials Database
- Where Do I Access the Documentation and Application Libraries?

🔍   The Physics Interfaces and Building a COMSOL Multiphysics Model in the *COMSOL Multiphysics Reference Manual*.

Modeling Semiconductor Devices

The invention of the *bipolar transistor* at Bell labs in the late 1940s and the subsequent development of field-effect devices and integrated circuits led to many of the important technological advancements of the second half of the 20th century. The widespread adoption of integrated circuits and the continuing efforts to improve the technology has motivated significant efforts to develop detailed models of devices. The semiconductor equations are highly nonlinear, so it is very difficult to develop detailed analytic solutions to them, and consequently numerical modeling has been important in the development of the technology. Multiphysics effects can often have important influences on semiconductor device performance. Device processing often occurs at high temperatures and consequently stresses can be introduced into the materials. Furthermore, high power devices can generate a significant amount of heat. The Semiconductor Module enables device level modeling on the COMSOL Multiphysics platform and helps easily create customized simulations involving multiple physical effects.

What Can the Semiconductor Module Do?

The Semiconductor Module is a collection of interfaces and predefined models for COMSOL Multiphysics, which can be used to model semiconductor devices.

It includes a dedicated physics interface to model semiconductor devices with the *drift-diffusion equations*, enhanced capabilities for modeling electrostatics, and an Electrical Circuits interface (with a SPICE import facility) that can be coupled to the device level models.

It also includes a dedicated physics interface to solve the single-particle Schrödinger Equation, for general quantum mechanical problems as well as quantum-confined semiconductor systems such as quantum wells, wires, and dots.

The included Applications Libraries contains a suite of models that demonstrate how to use the physics interfaces for modeling a range of practical devices. These models provide step-by-step instructions demonstrating how to use the physics interface to model practical devices.

The Semiconductor Module is well documented and includes a detailed outline of the underlying theory on which it is based. The software is uniquely transparent because the model equations are always visible. Furthermore, you have complete freedom to include phenomena that are not predefined in the Module with easy-to-enter user-defined expressions and equations.

The Semiconductor Module Physics Interface Guide

The Semiconductor Module extends the functionality of the physics interfaces of the base package for COMSOL Multiphysics. The details of the physics interfaces and study types for the Semiconductor Module are listed in the table below.

In the *COMSOL Multiphysics Reference Manual*:

- Studies and Solvers
- The Physics Interfaces
- For a list of all the core physics interfaces included with a COMSOL Multiphysics license, see Physics Interface Guide.

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
⚡ **AC/DC**				
Electrical Circuit		cir	Not space dependent	stationary; frequency domain; time dependent; small signal analysis, frequency domain
Electrostatics[1]		es	all dimensions	stationary; time dependent; stationary source sweep; eigenfrequency; frequency domain; small signal analysis, frequency domain
📟 **Semiconductor**				
Semiconductor		semi	all dimensions	small-signal analysis, frequency domain; stationary; time dependent; semiconductor equilibrium
Semiconductor Optoelectronics, Beam Envelopes[2]		—	3D, 2D, and 2D axisymmetric	frequency-stationary; frequency-transient; small-signal analysis, frequency domain
Semiconductor Optoelectronics, Frequency Domain[2]		—	3D, 2D, and 2D axisymmetric	frequency-stationary; frequency-transient; small-signal analysis, frequency domain
Schrödinger Equation		schr	all dimensions	eigenvalue; stationary; time dependent
Schrödinger-Poisson Equation		—	all dimensions	Schrödinger-Poisson

[1] This physics interface is included with the core COMSOL package but has added functionality for this module.

[2] Requires both the Wave Optics Module and the Semiconductor Module.

Common Physics Interface and Feature Settings and Nodes

There are several common settings and sections available for the physics interfaces and feature nodes. Some of these sections also have similar settings or are implemented in the same way no matter the physics interface or feature being used. There are also some physics feature nodes that display in COMSOL Multiphysics.

In each module's documentation, such as this one, only unique or extra information is included; standard information and procedures are centralized in the *COMSOL Multiphysics Reference Manual.*

> In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

The Semiconductor Module Study Capabilities by Physics Interface

Table 1-1 lists the physics interfaces specific to semiconductor modeling and this module. It includes the physical quantities solved for and the standard abbreviation each one uses. The physical quantities in these interfaces are:

- The *electric scalar potential*, V
- The *electron concentration*, N
- The *hole concentration*, P
- The *wave function*, psi

> Studies and Solvers in the *COMSOL Multiphysics Reference Manual.*

TABLE 1-1: SEMICONDUCTOR MODULE INTERFACE DEPENDENT VARIABLES AND PRESET STUDY OPTIONS

PHYSICS INTERFACE	NAME	DEPENDENT VARIABLES	STATIONARY	SEMICONDUCTOR EQUILIBRIUM	TIME DEPENDENT	EIGENFREQUENCY	FREQUENCY DOMAIN	SMALL SIGNAL ANALYSIS, FREQUENCY-DOMAIN	FREQUENCY STATIONARY	FREQUENCY TRANSIENT	EIGENVALUE	SCHRÖDINGER-POISSON
AC/DC												
Electrostatics	es	V	√		√	√	√	√				
Electrical Circuit	cir	none	√		√		√					
SEMICONDUCTOR												
Semiconductor	semi	V, N, P	√	√	√			√				
Semiconductor Optoelectronics, Beam Envelopes[1]	—	V, N, P E_1, E_2						√	√	√		
Semiconductor Optoelectronics, Frequency Domain[1]	—	V, N, P E						√	√	√		
Schrödinger Equation	schr	psi	√		√						√	
Schrödinger-Poisson Equation	schrp	V, psi										√

[1] Requires both the Wave Optics Module and the Semiconductor Module. These are also multiphysics interfaces.

The Semiconductor Materials Database

The Semiconductor Module includes an additional Semiconductors material database with material properties appropriate for several materials.

> For detailed information about materials and the Semiconductor Materials Database, see Materials in the *COMSOL Multiphysics Reference Manual*.

Where Do I Access the Documentation and Application Libraries?

A number of internet resources have more information about COMSOL, including licensing and technical information. The electronic documentation, topic-based (or context-based) help, and the application libraries are all accessed through the COMSOL Desktop.

> If you are reading the documentation as a PDF file on your computer, the blue links do not work to open an application or content referenced in a different guide. However, if you are using the Help system in COMSOL Multiphysics, these links work to open other modules, application examples, and documentation sets.

THE DOCUMENTATION AND ONLINE HELP

The *COMSOL Multiphysics Reference Manual* describes the core physics interfaces and functionality included with the COMSOL Multiphysics license. This book also has instructions about how to use COMSOL Multiphysics and how to access the electronic Documentation and Help content.

Opening Topic-Based Help

The Help window is useful as it is connected to the features in the COMSOL Desktop. To learn more about a node in the Model Builder, or a window on the Desktop, click to highlight a node or window, then press F1 to open the Help window, which then

displays information about that feature (or click a node in the Model Builder followed by the **Help** button (?). This is called *topic-based* (or *context) help*.

Win	To open the **Help** window: • In the **Model Builder**, **Application Builder**, or **Physics Builder** click a node or window and then press F1. • On any toolbar (for example, **Home**, **Definitions**, or **Geometry**), hover the mouse over a button (for example, **Add Physics** or **Build All**) and then press F1. • From the **File** menu, click **Help** (?). • In the upper-right corner of the COMSOL Desktop, click the **Help** (?) button.

Mac **Linux**	To open the **Help** window: • In the **Model Builder** or **Physics Builder** click a node or window and then press F1. • On the main toolbar, click the **Help** (?) button. • From the main menu, select **Help>Help**.

Opening the Documentation Window

Win	To open the **Documentation** window: • Press Ctrl+F1. • From the **File** menu select **Help>Documentation** (▮).

Mac **Linux**	To open the **Documentation** window: • Press Ctrl+F1. • On the main toolbar, click the **Documentation** (▮) button. • From the main menu, select **Help>Documentation**.

THE APPLICATION LIBRARIES WINDOW

Each model or application includes documentation with the theoretical background and step-by-step instructions to create a model or app. The models and applications are available in COMSOL Multiphysics as MPH files that you can open for further investigation. You can use the step-by-step instructions and the actual models as templates for your own modeling. In most models, SI units are used to describe the relevant properties, parameters, and dimensions, but other unit systems are available.

Once the Application Libraries window is opened, you can search by name or browse under a module folder name. Click to view a summary of the model or application and its properties, including options to open it or its associated PDF document.

🔍	The Application Libraries Window in the *COMSOL Multiphysics Reference Manual*.

Opening the Application Libraries Window
To open the **Application Libraries** window (▥):

Win	• From the **Home** toolbar, **Windows** menu, click (▥) **Applications Libraries**. • From the **File** menu select **Application Libraries**. To include the latest versions of model examples, from the **File>Help** menu, select (▥) **Update COMSOL Application Library**.

Mac Linux	Select **Application Libraries** from the main **File>** or **Windows>** menus. To include the latest versions of model examples, from the **Help** menu select (▥) **Update COMSOL Application Library**.

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email. You can also access technical support, software updates, license information, and other resources by registering for a COMSOL Access account.

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COMSOL website	www.comsol.com
Contact COMSOL	www.comsol.com/contact
COMSOL Access	www.comsol.com/access
Support Center	www.comsol.com/support
Product Download	www.comsol.com/product-download
Product Updates	www.comsol.com/support/updates
COMSOL Blog	www.comsol.com/blogs
Discussion Forum	www.comsol.com/community
Events	www.comsol.com/events
COMSOL Video Gallery	www.comsol.com/video
Support Knowledge Base	www.comsol.com/support/knowledgebase

Overview of the User's Guide

The *Semiconductor Module User's Guide* gets you started with semiconductor modeling using COMSOL Multiphysics. The information in this user's guide is specific to the Semiconductor Module. Instructions on how to use COMSOL Multiphysics in general are included in the *COMSOL Multiphysics Reference Manual*.

> 💡 As detailed in the section Where Do I Access the Documentation and Application Libraries? this information can also be searched from the COMSOL Multiphysics software **Help** menu.

TABLE OF CONTENTS AND INDEX

To help you navigate through this guide, see the Contents and Index.

MODELING SEMICONDUCTORS

The Modeling Guidelines chapter discusses topics including the Physics for Semiconductor Modeling, Connecting to Electrical Circuits, Defining the Carrier Mobility, Meshing, Solving, Quantum-Confined Systems, and many others.

THE SEMICONDUCTOR INTERFACE

The Semiconductor Branch Interface chapter includes physics feature information and describes the theory relating to The Semiconductor Interface. Topics include The Sommerfeld Model and the Density of States, Electrons in a Perturbed Periodic Potential, Equilibrium Carrier Concentrations, Band Gap Narrowing, and many others.

THE AC/DC BRANCH INTERFACES

The AC/DC Branch chapter includes physics feature information for The Electrostatics Interface and The Electrical Circuit Interface as well as theory is discussed.

THE SCHRÖDINGER EQUATION INTERFACE

The Schrödinger Equation Interfaces chapter describes the physics features and usage of The Schrödinger Equation Interface.

2

Modeling Guidelines

In this chapter:

- Physics for Semiconductor Modeling
- Finite Element and Finite Volume Discretization
- Defining the Carrier Mobility
- Doping
- Connecting to Electrical Circuits
- Nonisothermal Models
- SPICE Import and Export
- Small-Signal Analysis
- Meshing
- Solving
- Quantum-Confined Systems

Physics for Semiconductor Modeling

The physics of semiconductor devices is highly dependent on the size of the device. Over the last 50 years semiconductor devices have been progressively miniaturized enabling improvements in speed and reductions in power consumption. Nonetheless semiconductor devices are so ubiquitous that devices of larger sizes are still widely used for many applications. The Semiconductor Module is directed at these larger scale devices (with length scales of 100s of nm or more), which can still be modeled by a conventional drift-diffusion approach using partial differential equations. It is useful to note some of the important assumptions implicit to this approach:

- The relaxation-time approximation is used to describe the scattering process. This is a much simplified form of the scattering probability, which is elastic and isotropic.

- Magnetic fields are not included in the model.

- The carrier temperature is assumed to be equal to the *lattice* temperature and, consequently, the diffusion of hot carriers is not properly described.

- The energy bands are assumed to be parabolic. In reality the band structure is significantly altered in a complex manner in the vicinity of free surfaces or grain boundaries.

- Velocity overshoot, and other complex time-dependent conductivity phenomena, are not included in the model.

In addition to these intrinsic assumptions, The Semiconductor Interface allows you to make additional assumptions to simplify the solution process:

- For *nondegenerate semiconductors* it is possible to assume a *Maxwell-Boltzmann distribution* for the carrier energies at a given temperature, which reduces the nonlinearity of the semiconductor equations. If *degenerate semiconductors* are present within the model, or at lower temperatures, it is necessary to use *Fermi-Dirac statistics*.

- In *majority carrier* devices, it is often only necessary to solve for one of the carrier concentrations (the majority carrier). The *minority carrier concentration* is usually unimportant for the device operation and can be estimated by assuming the mass action law.

By default Maxwell-Boltzmann statistics are assumed by the Semiconductor interface and the interface explicitly solves for both the electron and hole concentrations.

The Semiconductor interface solves Poisson's equation in conjunction with continuity equations for the charge carriers. An important length scale to consider when modeling electrostatic fields in the presence of mobile carriers is the Debye length:

$$L_d = \sqrt{\frac{k_B T \varepsilon_0 \varepsilon_r}{q^2 N_{\text{ion}}}}$$

where k_B is Boltzmann's constant, T is the lattice temperature, ε_0 is the permittivity of free space, ε_r is the relative permittivity of the semiconductor, N_{ion} is the concentration of ionized donors or acceptors, and q is the electron charge. The Debye length is the length scale over which the electric field decays in the presence of mobile carriers; it is important to resolve this length scale with the mesh in semiconductor models.

Ⓠ | Theory for the Semiconductor Interface

Units of Band Gap and Electron Affinity

In the graphical user interface, the input for the band gap is actually "band gap divided by the elementary charge", so it takes on the unit of electric potential, but has the same numerical value as the band gap energy in eV. The same applies to the input for the electron affinity.

Finite Element and Finite Volume Discretization

The Semiconductor Interface includes linear and logarithmic finite element formulations and a finite volume formulation. The formulation used is selected in the Discretization section since the shape functions that can be used are directly related to the formulation employed. The finite volume formulation uses constant shape functions, whilst the two finite element formulations can use either linear or quadratic shape functions. In the different formulations the carrier concentration dependent variables (by default Ne and Ph) represent different quantities. In the linear finite element and finite volume formulations $Ne = N$ and $Ph = P$, where N is the electron concentration and P is the hole concentration. For the logarithmic finite element formulation $Ne = \ln(N)$ and $Ph = \ln(P)$. For the quasi-Fermi level formulation, the quasi-Fermi levels for the electrons and holes are the dependent variables.

Under **Discretization** you can select a **Formulation** (as in Figure 2-1). Each formulation has advantages and disadvantages.

> In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections (such as Discretization) and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.
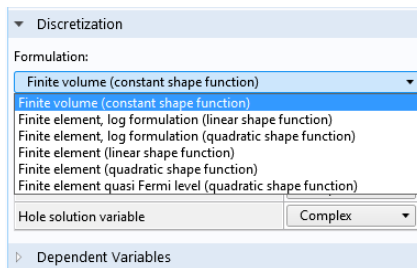
Figure 2-1: The Discretization section. Choose between a finite volume or a linear or quadratic finite element, or quasi-Fermi level formulation.

The finite volume discretization inherently conserves current. Consequently, it usually provides the most accurate result for the current density of the charge carriers. This is why it is the default setting. In order to enhance numerical stability, a Scharfetter-Gummel upwinding scheme is used for the charge carrier equations. Poisson's equation is discretized using a centered difference scheme. When doing multiphysics simulations it is important to realize that the shape functions are constant. Consequently, fluxes cannot be evaluated using spatial derivatives of the dependent variables (for example, expressions such as `d(V,x)` evaluate to zero as `V` is represented by a constant shape function within each element). Flux quantities such as fields and currents can be evaluated and used in equations (both within the Semiconductor interface and in other physics interfaces) if the predefined variables from Table 2-1 are used in expressions:

TABLE 2-1: SEMICONDUCTOR PREDEFINED VARIABLES

NAME	VARIABLE
Electric displacement field	`semi.D semi.Dx, semi.Dy, semi.Dz)`
Electron current density	`semi.Jn (semi.Jnx, semi.Jny, semi.Jnz)`
Hole current density	`semi.Jp (semi.Jpx, semi.Jpy, semi.Jpz)`
Electron drift current density	`semi.Jn_drift (semi.Jn_driftx, semi.Jn_drifty, semi.Jn_driftz)`
Hole drift current density	`semi.Jp_drift (semi.Jp_driftx, semi.Jp_drifty, semi.Jp_driftz)`
Electron diffusion current density	`semi.Jn_diff (semi.Jn_diffx, semi.Jn_diffy, semi.Jn_diffz)`
Hole diffusion current density	`semi.Jp_diff (semi.Jp_diffx, semi.Jp_diffy, semi.Jp_diffz)`
Electron thermal diffusion current density	`semi.Jn_th (semi.Jn_thx, semi.Jn_thy, semi.Jn_thz)`
Hole thermal diffusion current density	`semi.Jp_th (semi.Jp_thx, semi.Jp_thy, semi.Jp_thz)`

Any variables that involve expressions directly derived from the variables in Table 2-1 can also be used in expressions, for example, the electric field, `semi.E`, or the total current, `semi.J`.

The finite element formulation typically solves faster than the finite volume formulation. One reason is that, for an identical mesh, the finite element method with linear shape functions typically results in fewer degrees of freedom. In 2D, for triangular mesh elements, the number of degrees of freedom for the finite element method with linear shape functions is approximately half that for a finite volume

discretization. Coupling to other physics interfaces is straightforward and variables can be differentiated using the d operator. The finite element method is an energy conserving method and thus current conservation is not implicit in the technique. Current conservation for the linear formulation is poor and this formulation is provided primarily for reasons of backward compatibility. Current conservation in the log formulation is much better but still not as good as the finite volume method. In order to help with numerical stability a Galerkin least-squares stabilization method is included. This method usually enhances the ability to achieve a converged solution, particularly when using the linear formulation. However, it can be preferable to disable the stabilization, since the additional numerical diffusion the technique introduces can produce slightly unphysical results. As a result of the reduced gradients in the dependent variables obtained when using the log formulation, stabilization is often not required when using this technique.

It is also possible to solve a problem with the stabilization active and then use this solution as the initial condition in a separate study, where the stabilization is inactive. To turn the stabilization on or off, click the **Show** button ( ) and select **Stabilization**. Then click to select the **Streamline diffusion** check box or click to clear.

In the *COMSOL Multiphysics Reference Manual*:

- Numerical Stabilization
- Introduction to Solvers and Studies

The quasi-Fermi level formulation use the quasi-Fermi levels as the dependent variable, instead of the carrier concentrations. This formulation is advantageous in some cases, for example for near-equilibrium systems at very low temperatures.

Defining the Carrier Mobility

Realistic models for the carrier mobility are important to simulate semiconductor devices with a drift diffusion approach. The mobility is limited by scattering of the carriers within the material. Phenomena that can affect the mobility include:

- Phonons (L): thermally generated acoustic waves traveling through the crystal (scattering by phonons is frequently referred to as lattice scattering, which is somewhat confusing as the lattice itself never scatters the carriers unless perturbed from perfect periodicity).

- Ionized impurities (I): these begin to have an effect at doping levels above approximately 10^{15} cm^{-3} at room temperature.

- Carrier-carrier scattering (C)

- Neutral impurity scattering (N): this is important only at low temperatures, typically below 77 K.

- High field velocity saturation (E).

- Surface scattering (S): this includes effects such as interface charges, scattering by surface phonons, and so on. It is important in field effect devices, such as *field effect transistors*.

The Semiconductor Module includes several predefined mobility models, as well as user-defined models. These models are added as subnodes to the Semiconductor Material Model node.

	The letters in the above list (for example, L for phonons) are used to identify which effects a given predefined mobility model incorporates and appears in the name of the feature.

Both user-defined and predefined mobility models can be combined in arbitrary ways. Each mobility model defines an output electron and hole mobility. If appropriate (some filtering occurs in the predefined mobility models to prevent inappropriate combinations), the output mobility can be used as an input to other mobility models. User-defined mobility models accept any of the predefined mobility models as inputs and can be used as inputs for all the predefined mobility models that require an input. The model used within the simulation is selected for *electrons* and *holes* by changing the **Electron mobility** and the **Hole mobility** settings in the **Mobility Model** section of the

Semiconductor Material Model node, which by default uses a constant mobility obtained from the material properties.

It is important to understand that each type of mobility model subnode only defines mobility variables for electrons and holes that can be used by other models, or by the Semiconductor Material Model parent node. The mobility models for electrons and holes actually used in the simulation are determined by the selections or settings in the Semiconductor Material Model node (the parent node), which do not change when additional mobility model subnodes are added. In order to add a mobility model to a simulation, it is necessary to both add the sequence of mobility model subnodes to the Model Builder, and then to select the required final mobility for the electrons and holes in the Semiconductor Material Model parent node.

In order to implement field dependent mobility models it is usually necessary to add additional dependent variables for the field components used in the model (typically the electric field components parallel to or perpendicular to the current components). This is the approach taken in the Caughey-Thomas Mobility Model (E) and Lombardi Surface Mobility Model (S). Consequently, creating such mobility models is only recommended for advanced users.

- Mobility Models
- User-Defined Mobility Model
- Power Law Mobility Model (L)
- Arora Mobility Model (LI)
- Fletcher Mobility Model (C)

Doping

Specifying the doping distribution is critical to model semiconductor devices. COMSOL multiphysics includes a range of tools which enable any doping profile to be realized. This functionality is provided by the Analytic Doping Model and Geometric Doping Model.

In this section:

- Using the Analytic Doping Model
- Using the Geometric Doping Model
- Visualizing the Dopant Distribution
- Example of Multiple Superimposed Doping Profiles.

Using the Analytic Doping Model

The Analytic Doping Model makes it possible to express doping profiles as a function of the local coordinate system, which can be rotated with respect to the global coordinate system if required. This is suitable to achieve profiles that are convenient to define in relation to the coordinate axes. The dopant distribution can be defined using either the user defined or box methods.

ANALYTIC DOPING MODEL: USER DEFINED

A user-defined doping distribution can be used to specify a constant dopant density in a domain. Alternately a spatially varying doping profile can be specified; the doping profile is defined using the functions available within COMSOL Multiphysics. Any analytic expression, written in terms of the local coordinate system, is permitted. Figure 2-2 shows an example of a user-defined profile consisting of a Gaussian decay away from the lower boundary.

Doping distributions can also be imported from external files. This is useful when the required distribution cannot be defined analytically; for example, if the doping profile is output from an external diffusion simulation.

To import a doping profile using an interpolation function:

1 From the **Definitions** toolbar, click **Interpolation** ( ).

2 On the **Settings** window for **Interpolation** select **File** as the **Data source**.

3 Specify the **Filename** and the **Number of arguments**.

4 Once an interpolation function is defined, it can be used in an **Analytical Doping Model** feature. This is achieved by selecting a **User defined** dopant distribution and calling the interpolation function with the appropriate arguments.

🔍   Interpolation in the *COMSOL Multiphysics Reference Manual*.
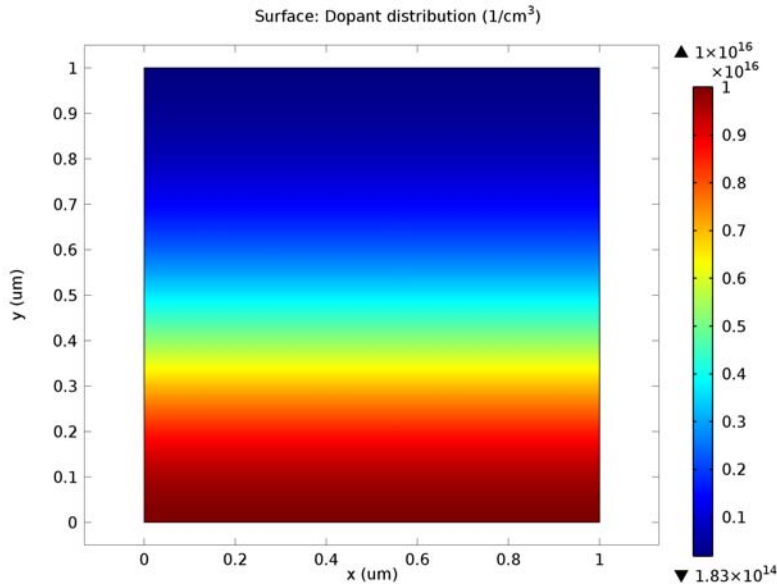
Figure 2-2: Example of a user-defined dopant distribution created using the Analytic Doping Model feature. The Analytic Doping Model feature is the appropriate doping feature as this distribution is trivial to express as a function of the coordinate axes.

ANALYTIC DOPING MODEL: BOX

The box method allows a block-shaped region of constant doping to be defined, along with a decay profile away from the region. This is useful for approximating some physical doping techniques, such as diffusion processes, which distribute dopants away from regions of high concentration resulting in characteristic decay profiles. The location of the region is defined by specifying either the corner or center coordinate using the global coordinate system. If a local rotated coordinate system is used within the feature, the orientation of the block rotates around this specified coordinate. A profile is selected from the **Dopant profile away from uniform region** list. The decay

length scale of the profile is controlled by either specifying a control length directly or by specifying a junction depth. The junction depth specifies the distance, from the boundary of the uniformly doped region, where the dopant concentration is equal to the value specified in the **Background doping concentration** input. This distance can be specified independently for each axis in the component geometry by selecting **Specify different length scales for each direction**. Figure 2-3 is an example of a doping profile created using this method. A rectangular region of uniform doping is specified in the top left of the geometry, and a Gaussian profile is selected away from this region with different junction depths in the x and y directions.

Surface: Dopant distribution (1/cm^3)
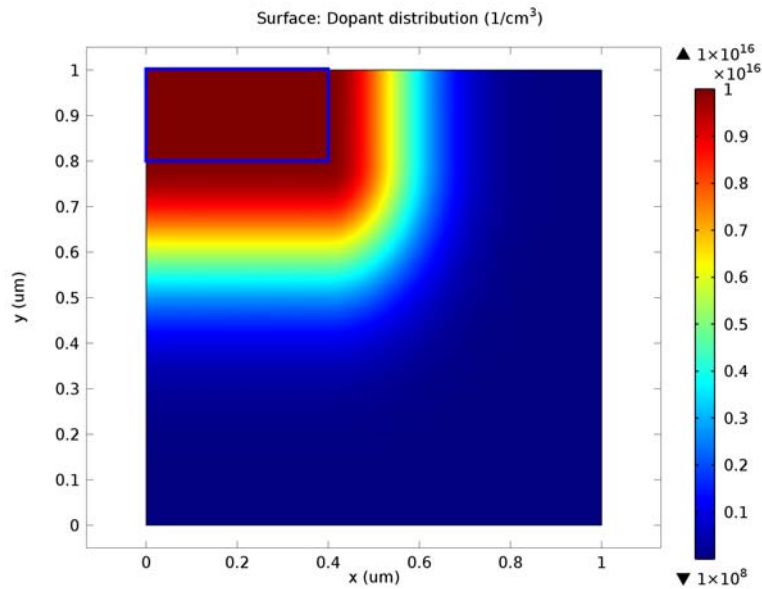
Figure 2-3: Example of a box doping distribution created using the Analytic Doping Model feature. This distribution is defined as a rectangle of constant doping located in the top left of the domain with a Gaussian decay profile away from the boundaries of this region. The region of uniform doping in the top left is outlined with a blue box.

Using the Geometric Doping Model

The Geometric Doping Model enables doping profiles to be expressed as a function of the distance from selected boundaries. This is suitable for cases where the profile wanted is more conveniently expressed in terms of the geometry than the coordinate axes. The boundaries from which the distance is calculated using the Boundary

Selection for Doping Profile node. The form of the profile is selected from the **Dopant profile away from the boundary** list. This list contains preset functions that enable several common profiles to be easily defined. A **User defined** option is also available that enables any expression to be manually entered.

GEOMETRIC DOPING MODEL: USER DEFINED

A user-defined profile can be used to specify any dopant distribution that is expressed as a function of the distance from boundaries in the geometry. This distance is available as `semi.gdm#.D` within COMSOL, where `#` indicates the number of the Geometric Doping Model feature. Figure 2-4 is an example doping profile that is created with the expression `1e16[1/cm^3]*exp(-(semi.gdm1.D/0.5[um])^2)`.
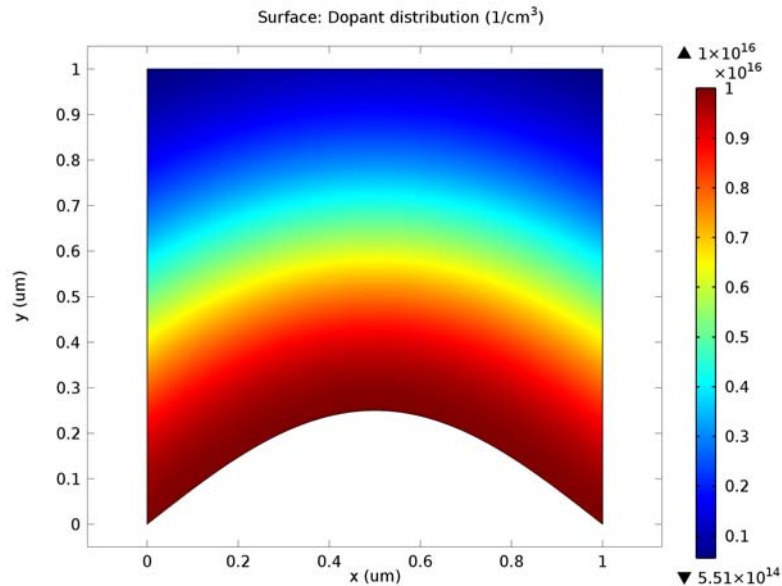
Figure 2-4: Example of a user-defined dopant distribution created using the Geometric Doping Model feature. The dopant concentration decays as a Gaussian away from the lower boundary. The Geometric Doping Model feature is the appropriate doping feature as it is more convenient to define this distribution in terms of the distance from the curved boundary than as a function of the coordinate system.

GEOMETRIC DOPING MODEL: PRESET PROFILES

The Geometric Doping Model makes Gaussian, linear, and error function profiles available as options in the **Dopant profile away from the boundary** list. When a preset option is selected, the dopant concentration at the boundary can be input along with a parameter to set the decay length scale of the profile. The decay length scale of the

profile is controlled by specifying a control length directly or by specifying a junction depth. The junction depth specifies the distance from the selected boundaries at which the dopant concentration is equal to the value specified in the **Background doping concentration** user input.

Figure 2-5 is an example profile that is created using a combination of an Analytic Doping Model and a Geometric Doping Model. The dopant concentration is constant within the top left domain, which is bounded by a curve. Away from this constant region the concentration decays with a Gaussian profile. The constant region is specified using a user-defined profile in an Analytic Doping Model. The Gaussian profile is achieved using a preset profile in a Geometric Doping Model with the curve as the selected boundary. This example shows how the Geometric Doping Model allows curves in the geometry to be easily incorporated into the dopant distribution, without the need to express the curves analytically in terms of the coordinate system.
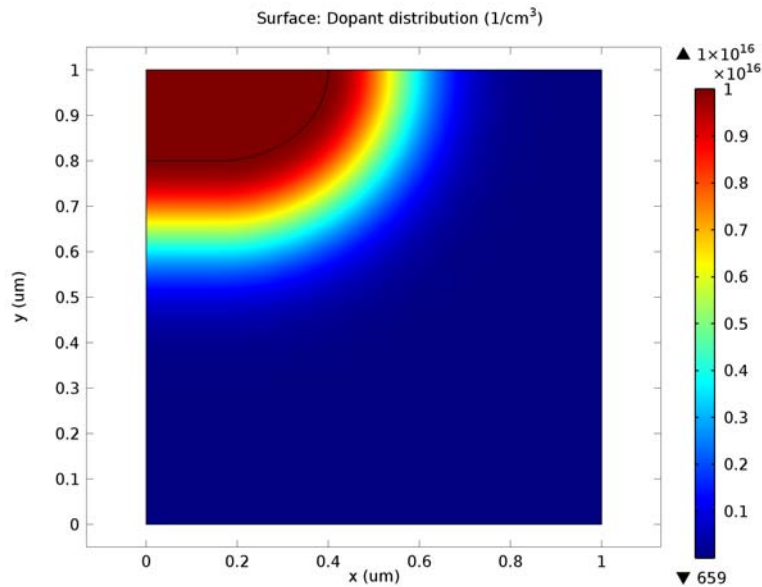
Figure 2-5: Example of a profile that uses the Geometric Doping Model feature to accommodate a curved boundary. An Analytic Doping Model feature is used to create a region of constant doping in the top left that is bounded by the curve. This curve is used as the selected boundary in the Geometric Doping Model feature to generate a Gaussian decay profile away from the constant region.

Visualizing the Dopant Distribution

To visualize the distribution, on the **Study** toolbar, click **Get Initial Value** ($\underset{t=0}{\cup}$). Then add a plot group and display the corresponding dopant density. The signed doping concentration, `semi.Nd-semi.Na` (positive for net donor doping and negative for net acceptor doping), gives the net doping and can be useful for visualizing the effect of different doping steps. If multiple doping features are superimposed, it is possible to visualize the total dopant concentration or to display the contribution from individual doping features.

🔍	Study and Computing the Initial Values in the *COMSOL Multiphysics Reference Manual*.

The `semi.Nd-semi.Na` expression shows the total net doping due to the sum of all doping features. To see the distribution from a single doping feature the corresponding node tag must be included in the plot variable.

📝	To select the node labels to display, on the **Model Builder** toolbar click **Model Builder Node Label** ☰.

The node tags are shown in curly brackets next to the nodes in the Model Builder. **Analytic Doping Model** features are tagged as `adm#` and **Geometric Doping Model** features are tagged as `gdm#`, where # corresponds to the number of the feature. The dopant concentration from each doping feature is available as `semi.<tag>.Na` for acceptor doping or `semi.<tag>.Nd` for donor doping. For example, `semi.adm1.Nd` for a donor distribution from the first **Analytic Doping Model** added to the component.

Example of Multiple Superimposed Doping Profiles

This example uses multiple Gaussian profiles to demonstrate how to create an intricate doping distribution using a combination of several doping features. Figure 2-6 shows the geometry along with a line graph of the dopant concentrations. The geometry shows the location of the contacts and the line cut along which the line graph is plotted.

To create the doping profile three Analytic Doping Model nodes and one Geometric Doping Model node are used. The line graph shows the total resultant dopant concentration as well as the individual contribution from each node.

> ⚠️ Care should be taken when specifying multiple doping profiles in the same domains as the resultant dopant concentration is the sum of all coincident doping models.
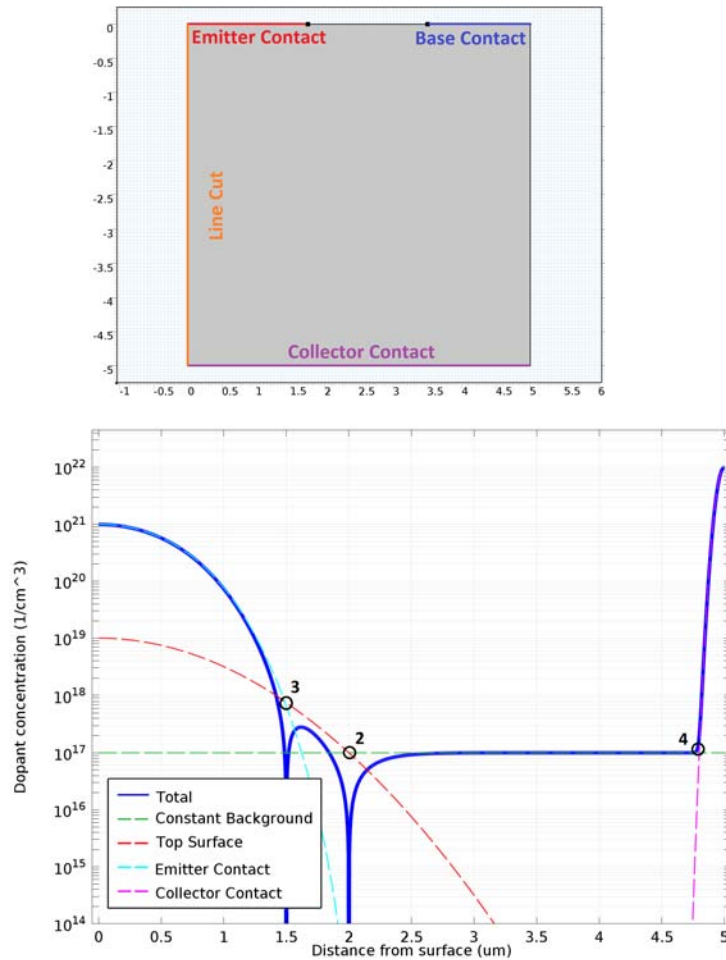
Figure 2-6: Top: Geometry in which the example dopant concentration is created. Bottom: Line graphs of the total doping distribution and the individual contributions from each of the steps in the instructions. The numbered circles highlight the overlap points of the different distributions due to the junction depth specified in the corresponding step.

To create the doping profile:

> The following example is similar to the model *Bipolar Transistor*, which is available in the Semiconductor Applications Libraries (**Semiconductor_Module/Devices/bipolar_transistor**).

1 Constant background: a constant *n-type* doping of 10^{17} cm^{-3} is added using an **Analytic Doping Model** that specifies a **User defined** profile with constant **Donor Concentration**.

2 Top surface: a **Box** dopant distribution that decays away from the top surface with a Gaussian profile is added using a second **Analytical Doping Model**. The uniformly doped region is set to cover the entire width of the model at the top surface but to have zero depth, thus the profile decays away from the surface.

- **Acceptor** doping is applied with a maximum concentration of 10^{19} cm^{-3}.

- The donor concentration defined in the previous step, semi.adm1.Nd, is selected for the **Background doping concentration**.

- The **Junction depth** is set to 2 µm below the top surface. Since the background doping is of a different type, semi.adm2.Na has equal magnitude to semi.adm1.Nd at this depth, as indicated by point **2** shown in Figure 2-6. Thus the overall contribution to semi.Nd-semi.Na due to the first two distributions is zero at a depth of 2 µm. This is an example of doping distribution into a constant background distribution of the opposite type.

3 Emitter contact: a **Geometric Doping Model** is used to define a Gaussian profile which decays away from the emitter contact.

- The boundary that represents the emitter contact is selected in **Boundary Selection for Doping Profile** node and a Gaussian **Dopant profile away from the boundary** is selected.

- The **Junction depth** is set to 1.5 µm.

- The **Background doping concentration** must account for the effect of *both* of the two preceding steps. To achieve this, choose a **User defined** background concentration and set it to semi.adm2.Na-semi.adm1.Nd. This causes the resulting distribution, semi.gdm1.Nd, to be equal magnitude to semi.adm2.Na

at the desired junction depth of 1.5 μm, as can be seen at point **3** labeled in Figure 2-6.

- This is an example that demonstrates the need to carefully consider the cumulative effects of coincident dopant distributions when placing junction depths.

4 Collector contact: another **Box** distribution is defined with a third **Analytic Doping Model**. This is used to create a Gaussian profile that decays away from the collector contact. The uniformly doped region is set to cover the entire width of the model at the bottom surface but to have zero depth.

- **Donor** doping is applied with a maximum concentration of 10^{22} cm^{-3}.

- The **Junction depth** is set to 0.2 μm, which produces a junction at a depth of 4.8 μm from the top surface.

- In this case the constant donor concentration defined in step 1 (10^{17} cm^{-3}), `semi.adm1.Nd`, is selected for the **Background doping concentration**. Since donors are being doped into donors the concentration due to this final distribution (`semi.adm3.Nd`) is 2×10^{17} cm^{-3} at the junction depth, which is double the background level as indicated a point **4** shown in Figure 2-6. This is because at the junction depth `semi.adm3.Nd` has equal magnitude to the constant background and, because it is the same doping type, the sum of the contribution from both distributions results in double the concentration. This is an example of doping one type into a constant background of the same type.

Connecting to Electrical Circuits

In this section:

- About Connecting Electrical Circuits to Physics Interfaces
- Connecting Electrical Circuits Using Predefined Couplings
- Connecting Electrical Circuits by User-Defined Couplings
- Solving
- Postprocessing

About Connecting Electrical Circuits to Physics Interfaces

This section describes the various ways electrical circuits can be connected to other physics interfaces in COMSOL Multiphysics. If you are not familiar with circuit modeling, it is recommended that you review the Theory for the Electrical Circuit Interface.

In general electrical circuits connect to other physics interfaces via one or more of three special circuit features:

- External I vs. U
- External U vs. I
- External I-Terminal

These features either accept a voltage measurement from the connecting non-circuit physics interface and return a current from a or the Electrical Circuit interface or the other way around.

> The "External" features are considered "ideal" current or voltage sources by the Electrical Circuit interface. Hence, you cannot connect them directly in parallel (voltage sources) or in series (current sources) with other ideal sources. This results in the error message *The DAE is structurally inconsistent*. A workaround is to provide a suitable parallel or series resistor, which can be tuned to minimize its influence on the results.

Connecting Electrical Circuits Using Predefined Couplings

In addition to these circuit features, interfaces in the AC/DC Module, RF Module, MEMS Module, Plasma Module, and Semiconductor Module (the modules that include the Electrical Circuit interface) also contain features that provide couplings to the Electrical Circuit interface by accepting a voltage or a current from one of the specific circuit features (External I vs. U, External U vs. I, and External I-Terminal).

This coupling is typically activated when:

• A choice is made in the **Settings** window for the non-circuit physics interface feature, which then announces (that is, includes) the coupling to the Electrical Circuit interface. Its voltage is then included to make it visible to the connecting circuit feature.

• A voltage that has been announced (that is, included) is selected in a feature node's **Settings** window.

These circuit connections are supported in Terminals.

Connecting Electrical Circuits by User-Defined Couplings

A more general way to connect a physics interface to the Electrical Circuit interface is to:

• Apply the voltage or current from the connecting "External" circuit feature as an excitation in the non-circuit physics interface.

• Define your own voltage or current measurement in the non-circuit physics interface using variables, coupling operators and so forth.

• In the **Settings** window for the Electrical Circuit interface feature, selecting the User-defined option and entering the name of the variable or expression using coupling operators defined in the previous step.

DETERMINING A CURRENT OR VOLTAGE VARIABLE NAME

To determine a current or voltage variable name, look at the **Dependent Variables** node under the **Study** node. To do this:

1 In the **Model Builder**, right-click the **Study** node and select **Show Default Solver**.

2 Expand the **Solver>Dependent Variables** node and click the state node, in this example, **Current through device R1 (comp1.currents)**. The variable name is shown in the **Settings** window for **State**.
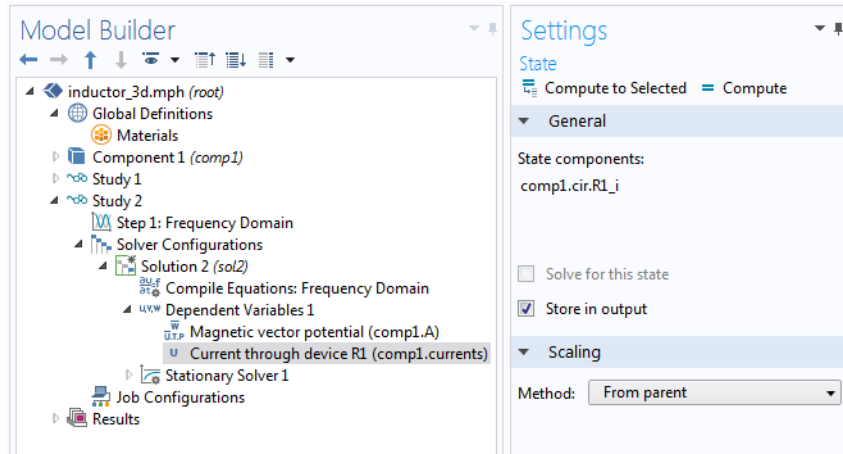
> Typically, voltage variables are named `cir.Xn_v` and current variables `cir.Xn_i`, where *n* is the "External" device number — 1, 2, and so on.

Solving

> Some modeling errors lead to the error message *The DAE is structurally inconsistent*, being displayed when solving. This typically occurs from having an open current loop, from connecting voltage sources in parallel, or connecting current sources in series.
>
> In this respect, the predefined coupling features are also treated as (ideal) voltage or current sources. The remedy is to close current loops and to connect resistors in series with voltage sources or in parallel with current sources.

Postprocessing

The Electrical Circuits interface, unlike most of the other physics interfaces, solves for a relatively large number of Global dependent variables (such as voltages and currents),

instead of solving for a few space-varying fields (such as temperature or displacement). For this reason, the Electrical Circuit interface does not provide default plots when computing a Study.

The physics interface defines a number of variables that can be used in postprocessing. All variables defined by the Electrical Circuit interface are of a global scope, and can be evaluated in a **Global Evaluation** node (under **Derived Values**). In addition, the time evolution or dependency on a parameter can be plotted in a **Global** plot (under a **ID Plot Group** node).

The physics interface defines a Node voltage variable for each electrical node in the circuit, with name `cir.v_name`, where `cir` is the physics interface Label and `<name>` is the node Name. For each two-pin component, the physics interface also defines variables containing the voltage across it and the current flowing through it.

ℚ	In the *COMSOL Multiphysics Reference Manual:* • Derived Values, Evaluation Groups, and Tables and Global Evaluation • Plot Groups and Plots and Global

Nonisothermal Models

The Semiconductor interface is designed to model nonisothermal devices. In order to model heat transfer in the device, an additional Heat Transfer in Solids interface should be added to the model. This physics interface can be used to model the heat transfer within the domain. Appropriate thermal boundary conditions must be added in addition to a heat source term that is coupled to the Semiconductor interface.

To add the heat source term, from the **Physics** toolbar, **Domain** menu, select **Heat Source**. Then click the **Heat Source 1** node and select **Total heat source (semi)** from the list of coupling variables in the **General source** Q list (note that if several heat sources or Semiconductor interfaces are added then the name of the heat source feature and the semiconductor heat source coupling variable is incremented accordingly). To couple the temperature computed by a heat transfer interface back into the Semiconductor interface, go to the **Model Inputs** section of the **Semiconductor Material Model 1** node. Under **Temperature**, T, select **Temperature (ht)**.

Currently COMSOL implements a simplified heat source term incorporating only Joule heating and the heat source due to recombination (see Ref. 26 for a detailed discussion of the appropriate heat source term to be used in semiconductor modeling). The heat source term Q is given by:

$$Q \ = \ \mathbf{E} \cdot \mathbf{J} + (E_g + 3k_B T)U$$

where U is the total recombination rate computed from summing all the recombination mechanisms. U is computed from the mean of the total electron and hole recombination rates $U = (U_n + U_p)/2$, which are almost always equal except in advanced models.

Additional terms can be added to the heat source manually in the finite element method (the existing terms are available as the variable `semi.Q_tot`).

It is not straightforward to add these terms for the finite volume method, as they involve the derivatives of the dependent variables, which must be computed using appropriate expressions.

Some of the boundary conditions for the Semiconductor interface require an equilibrium reference temperature to be defined in order to correctly define the potentials with respect to the equilibrium Fermi energy.

To change this reference temperature click the **Show** button ( ) and select **Advanced Physics Options**. Then adjust the **Temperature reference for energy levels** (T_0) setting in the **Temperature Reference** section of the **Semiconductor** interface **Settings** window. The reference temperature should be within the range of validity of any temperature-dependent material properties used in the model.

When solving nonisothermal semiconductor models, a segregated solver should be used, with the temperature degree of freedom included in a separate segregated group from the carrier densities and the potential.

To add a segregated solver, click the study and from the **Study** toolbar, click **Show Default Solver** ( ) (this is not necessary if the **Solver Configurations** node is already visible in the Model Builder). Expand the Solver Configurations node until you can see either the **Stationary Solver 1** or the **Time-Dependent Solver 1** node (depending on whether the study is stationary or time-dependent). Right-click the node and select **Segregated**. Expand the resulting **Segregated 1** node and select the **Segregated Step** node. Then in the **General** settings section, delete the **Temperature (mod1.T)** variable from the list. Right-click the **Segregated 1** node and add a **Segregated Step**. In the **Settings** window for **Segregated Step 1**, add **Temperature (mod1.T)** to the list.

The node numbers given above can be altered if multiple studies or study steps are present in the model.

In the *COMSOL Multiphysics Reference Manual*:

• Introduction to Solvers and Studies
• Segregated and Segregated Step

SPICE Import and Export

SPICE Import

The circuit definition in COMSOL Multiphysics adheres to the SPICE format developed at the University of California, Berkeley (Ref. 1). SPICE netlists can be imported and the corresponding circuit nodes are generated in the COMSOL Multiphysics model. Most circuit simulators can export to this format or some version of it.

The Electrical Circuit interface supports the following device models:

TABLE 2-2: SUPPORTED SPICE DEVICE MODELS

STATEMENT	DEVICE MODEL
R	Resistor
C	Capacitor
L	Inductor
V	Voltage Source
I	Current Source
E	Voltage-Controlled Voltage Source
F	Current-Controlled Current Source
G	Voltage-Controlled Current Source
H	Current-Controlled Voltage Source
D	Diode
Q	NPN BJT and PNP BJT
M	n-Channel MOSFET and p-Channel MOSFET
X	Subcircuit Instance

Statements corresponding to multiple devices are resolved by parsing the associated `.model` statement. The physics interface also supports the `.subckt` statement, which is represented in COMSOL by a Subcircuit Definition node, and the `.include` statement. SPICE commands are interpreted case-insensitively. The statement defining each device is also interpreted as the **Device name**.

According to SPICE specification, the first line in the netlist file is assumed to be the title of the netlist and it is ignored by the parser.

SPICE Export

The **SPICE Export** functionality creates a SPICE netlist file containing a description of the circuit represented by the physics interface. This functionality can be accessed from the physics interface context menu (right-click the physics interface node and select **Export SPICE Netlist**). After specifying a file name, the circuit is exported and messages from the export process display in the **Messages** window. During the export process, a series of operations are performed:

- In order to avoid conflicts, each component must be identified by a unique **Device name**. If one or more components have the same device name, the export operation fails and an error message is displayed. All characters in a **Device name** that are not letters, digits or underscores are replaced by underscores.

- According to the SPICE specification, each circuit must have a node with name 0, which is assumed to be the only ground node. When exporting a circuit, any node with name 0 that is not connected to a **Ground** component is exported with a different node name. All nodes that are connected to a Ground components are exported as a merged node with name 0. The Messages window shows a log message if these operations are performed, showing the name of the renamed or merged nodes.

- All characters in node names that are not letters, digits or underscores are replaced by underscores.

- Some components (most notably, the **External** components used to couple to other physics interfaces) cannot be exported to a SPICE netlist. These components are ignored during the export process, and a message is shown in the Messages window. Note that this can change the exported circuit, since some components are then missing.

- Subcircuit definitions are added as `.subckt` statements in the netlist. Semiconductor devices (such as MOSFETs, BJTs, and diodes) are exported as a SPICE device with a corresponding `.model` statement.

The title of the exported netlist file is the model's filename, and the time, date, and version of COMSOL Multiphysics is added as a comment in the netlist file.

Reference

1. http://bwrc.eecs.berkeley.edu/Classes/IcBook/SPICE/

Small-Signal Analysis

COMSOL Multiphysics includes sophisticated and very general tools for small-signal analysis, which are available in the Semiconductor Module. Small signals are applied to features such as source, drain, or gate contacts by using the **Harmonic Perturbation** subfeature (a subnode in the Model Builder tree structure). This feature should be used in conjunction with the **Small-Signal Analysis, Frequency Domain** study. The Small-Signal Analysis, Frequency Domain study includes **Stationary** and **Frequency Domain, Perturbation** study steps. The Stationary study step is used to compute the linearization point for the equation system, which is the solution for the DC operating point in the absence of any AC signals. The Frequency Domain, Perturbation study step then computes the response of the system to small AC deviations from the linearization point, correctly accounting for nonlinearities in the equation system.

To specify an AC voltage (with a DC offset) applied, for example, to the Thin Insulator Gate feature, the DC voltage should be specified as usual by typing it into the **Voltage** user input in the **Terminal** section of the settings for the feature. Next add a **Harmonic Perturbation** subnode to the Thin Insulator Gate node.

> 📋 The **Harmonic Perturbation** subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar in the **Contextual** group.

The amplitude of the AC signal is typed into this **Harmonic Perturbation** feature. By default, the solution from a Small-Signal Analysis, Frequency Domain study contains both the Static (or DC) solution and the Harmonic Perturbation (or AC solution). When evaluating expressions in result analysis you can choose which part of the solution is displayed in the **Evaluate expression for** list (a range of other options are also available, which are described in the link below).

When evaluating the Harmonic Perturbation it is important that the **Compute differential** check box is selected so that COMSOL Multiphysics differentiates the solution at the linearizion point when evaluating the expression. The solutions to Harmonic Perturbation studies are in general complex valued, with the argument representing the phase of the signal. By default, the real part of the solution is plotted in graphs. Use the `imag` operator to obtain the imaginary part of a variable or an expression. To drive the system with several signals at different phases, enter complex-valued numbers into the Harmonic Perturbation subnode.

Care must be taken when computing quantities such as the transconductance and output conductance for a MOSFET. For example, if the drain is a Metal Contact with terminal name 1, then evaluating the global terminal current `semi.IO_1` for the Harmonic Perturbation (with the Compute differential check box selected) gives the (complex) perturbation in the drain current, $\delta I_{\mathrm{drain}}$. The output conductance is obtained by taking the absolute value of the perturbation and dividing by the amplitude of the voltage perturbation applied (for example `0.01[V]`). Thus the output conductance ($\mathrm{d}I_{\mathrm{drain}}/\mathrm{d}V_{\mathrm{drain}}$) is obtained by evaluating the quantity: `abs(semi.IO_1)/0.01[V]`. It is not possible to evaluate the output conductance by evaluating the perturbation part of the expression: `abs(semi.IO_1)/abs(semi.VO_1)` because COMSOL Multiphysics linearizes the expression entered, computing the quantity: $\delta I_{\mathrm{drain}}/V_{\mathrm{drain}}\text{-}(I_{\mathrm{drain}}/V_{\mathrm{drain}}{}^{2})\delta V_{\mathrm{drain}}$.

In the *COMSOL Multiphysics Reference Manual*:

- For details on the small-signal analysis study type see Frequency Domain Perturbation Study Step in the Studies and Solvers section.
- For details on postprocessing small signals see Results Analysis and Plots

Meshing

The mesh is an important component of any numerical model of a semiconductor device. When assessing a numerical solution it is always important to ensure that the results do not change significantly when the mesh is refined; this is sometimes referred to as *grid independence*. Different meshing strategies produce optimum results with the finite element and finite volume formulations of the semiconductor equations. The Semiconductor Module includes default mesh suggestions that automatically refine the mesh based on the physics features selected. These mesh suggestions are usually appropriate for both the finite element and the finite volume methods. In some cases manually tuning the default mesh improves performance and helps with the solution process.

The finite volume formulation works best in 2D when triangular elements are used. In 3D a swept mesh is currently required (tetrahedral elements are not currently supported for finite volumes in 3D). In this case it is best to mesh with a triangular mesh in the plane of the wafer surface and to sweep the mesh into the wafer. This is particularly important for gate contacts. Figure 2-7 shows some of the techniques that can be used when meshing gates for the finite volume discretization in 3D.

The finite element method (with either the log or linear formulation) works well with all the types of mesh elements available in COMSOL. It is also possible to use adaptive meshing to refine the mesh selectively in regions where the error in the solution is greatest. Adaptive mesh refinement can be added to a Stationary or Time Dependent study step by selecting the **Adaptation and error estimates** drop down menu in the **Adaptation and error estimates** section.

For details on the settings for adaptive meshing, see Adaptive Mesh Refinement in the *COMSOL Multiphysics Reference Manual.*

For finite elements it is particularly important to assess the dependence of the global current conservation on the mesh — this can give a good indication of the overall accuracy of the solution. If current conservation is still poor with a refined mesh tightening the solver tolerances can help (see Solving).
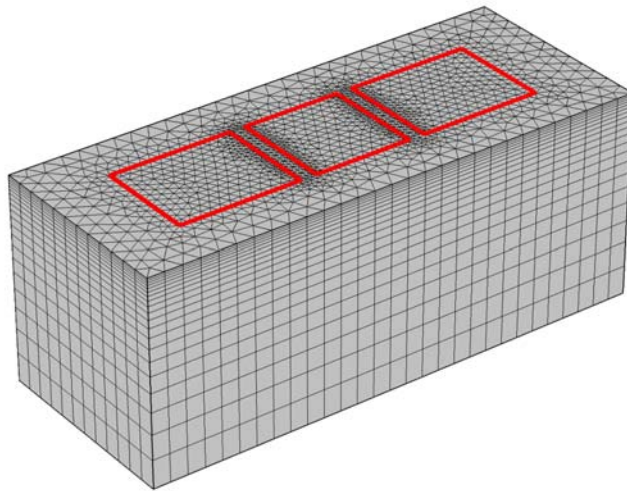
Figure 2-7: Example of a swept mesh appropriate for a gate contact in 3D. The mesh is swept in the direction perpendicular to the gate. The source (left), drain (right), and gate (center) contacts are highlighted in red. The mesh is refined in between the contacts, where the Gaussian profile drops off. A geometric sequence with an element ratio of 15 is used to sweep the mesh in the z-direction.

For both finite elements and finite volumes, increasing the mesh density in the vicinity of junctions is important. Note that the **Size** feature in the mesh sequence can be applied to boundaries, edges, and points, and if the settings are adjusted appropriately this feature can be used to produce a local refinement of the mesh.

For more details on setting up a mesh sequence see the Meshing chapter in the *COMSOL Multiphysics Reference Manual*.

Solving

The equations solved by the Semiconductor interface are highly nonlinear and are consequently difficult to solve in the absence of good initial conditions. The default initial conditions are good approximate guesses for the carrier concentration in the absence of applied voltages or currents. For stationary models when currents flow it is often necessary to ramp up the currents or voltages slowly to the desired operating point within the solver. To achieve this, ensure that the currents and voltages in the model are controlled by parameters and then use the **Auxiliary sweep** settings in the **Study Extensions** section of the **Stationary** study step. Then set up the voltage and current parameters so that these are swept up from zero. Note that you select the parameter on which the continuation solver should be used in the **Run continuation for** drop down menu. When performing multiple sweeps it is desirable to set the **Reuse solution for previous step** setting to **Auto**. Note also that the solution from one study can be used as the starting point for a second study by altering the settings in the **Values of Dependent Variables** section of the **Stationary** study step. To do this, select the **Initial values of variables solved for** check box, select **Solution** for the **Method**, and then select the appropriate solution from the **Study** list.

In addition to ramping up currents and voltages it is also possible to gradually introduce contributions to the equation system using the continuation solver. This is particularly useful when problems are highly nonlinear. When this approach is appropriate a **Continuation Settings** section is present in some of the semiconductor feature settings. By default **No continuation** is selected, which means that the equation contribution is as specified. For **User defined** an input for the **Continuation parameter** appears and this should be set to a parameter with values between 0 and 1 to determine the scaling of the equation contribution. Adding the name of a parameter to this setting and ramping it from 0 to 1 in the continuation solver will gradually introduce the contribution into the equation system. By choosing **Use interface continuation parameter** the continuation parameter is linked to the value of the interface-level continuation parameter specified in the **Continuation Settings** section of the Semiconductor interface's **Settings** window. This enables several features to be ramped up simultaneously. Finally it is possible to ramp up the dopant concentration, starting from a small fraction of that specified (or even zero) and gradually increasing the doping. By default the **Continuation Settings** for the doping features link to an interface-level doping continuation parameter that can be set up in the **Continuation Settings** section of the Semiconductor interface's **Settings** window. In turn this can be

linked to the interface level continuation parameter or specified separately. For the finite volume method the doping continuation parameter should be started at a small value (for example, 10^{-6}) rather than zero, as the continuation solver does not handle the transition from no doping to finite doping when this numerical method is used. The doping continuation can also be disabled or defined within each individual feature.

The nanowire_traps tutorial in the Application Libraries (**Semiconductor Module>Transistors>nanowire_traps**) provides a good example on using the continuation solver (through the Auxiliary sweep and the Continuation parameter as mentioned above) to ramp up a number of different nonlinear contributions to the model.

The **Semiconductor Equilibrium** study step can often provide a good initial condition for subsequent ramping up of applied voltages.

For time-dependent models it is recommended that the simulation is started in the manner described previously using a known solution to an appropriate stationary problem. The time-dependent effects can then be turned on during the simulation.

The pin_forward_recovery and pin_reverse_recovery tutorials in the Application Libraries (**Semiconductor Module>Device Building Blocks>pin_forward_recovery** and **pin_reverse_recovery**) provide good examples on using the equilibrium or stationary solution as the initial condition for the time-dependent study step.

In many cases the time-dependent solver performs better than the continuation solver for nonlinear stationary problems. By changing the **Equation** setting in the Semiconductor interface **Settings** window from the default (**Study controlled**) to **Stationary**, you can force the physics interface to use the stationary equation form even though the time dependent solver is used. Then parameters can be defined as functions of time, so that the applied currents and voltage, as well as nonlinear equation contributions and the doping, can be gradually turned on.

Using the correct solver tolerance for a problem is also important. The nonlinear solver tolerances are set up differently in 1D, 2D, and 3D to achieve a balance between solution speed and accuracy. For minority carrier devices it might be necessary to tighten the solver tolerances to ensure that the solution is converged to within sufficient accuracy. For a Stationary study the solver tolerance is adjusted in the

Stationary Solver node of the **Solver Configurations** branch (if this branch is not visible click the study and from the **Study** toolbar, click **Show Default Solver** (▐▐▬)). The **Relative tolerance** setting determines the fractional accuracy that the carrier concentrations are solved to. The Time-Dependent Solver has both relative and absolute tolerance settings. The relative tolerance setting is available on the **Time Dependent** study step in the **Study Settings** section. The absolute tolerance is set in the **Time-Dependent Solver** node on the **Solver Configurations** branch.

When modeling nonisothermal semiconductor devices, the solver settings must be adjusted so that the temperature degree of freedom is in a separate segregated group from the carrier densities and the potential. To do this, click the study and from the **Study** toolbar, click **Show Default Solver** (▐▐▬) (this step is not necessary if the **Solver Configurations** node is already visible in the model tree). Then expand the Solver Configurations node until you can see either the **Stationary Solver 1** or the **Time-Dependent Solver 1** node (depending on whether the study is stationary or time-dependent). Right-click this node and select **Segregated**. Expand the resulting **Segregated 1** node and select the **Segregated Step** node. Then in the **General** settings for this node, delete the **Temperature (mod1.T)** variable from the list. Next right-click the **Segregated 1** node and select **Segregated Step**. In the settings for the resulting **Segregated Step 1** node, add **Temperature (mod1.T)** to the list. Note that the node numbers given above can be altered if multiple studies or study steps are present in the model.

For coupled optoelectronic models, it is better to first solve only the wave optics part, and then solve the fully coupled problem in the following study step.

	In the *COMSOL Multiphysics Reference Manual*:
⊙	• Introduction to Solvers and Studies • Study and Study Step Types • Computing a Solution • Solution Operation Nodes and Solvers

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Quantum-Confined Systems

The Schrödinger Equation Interface enables the simulation of quantum-confined systems such as quantum wells, wires, and dots. The single-particle Schrödinger Equation is solved for the electron or hole wave function under the assumption of the envelope function approximation.

The Schrödinger-Poisson Equation Multiphysics Interface creates a bidirectional coupling between an **Electrostatics** physics interface and a **Schrödinger Equation** physics interface, to model charge carriers in quantum-confined systems. The electric potential from the Electrostatics contributes to the potential energy term in the Schrödinger Equation. A statistically weighted sum of the probability densities from the eigenstates of the Schrödinger Equation contributes to the space charge density in the Electrostatics. All spatial dimensions (1D, 1D axial symmetry, 2D, 2D axial symmetry, and 3D) are supported. A dedicated Schrödinger-Poisson Study Step is available for automated generation of self-consistent iterations in the solver sequence.

3

Semiconductor Branch Interface

This chapter describes the physics interfaces found under the **Semiconductor** branch (icon). (except the **Schrödinger Equation** interface, which is covered in a separate chapter.)

In this chapter:

The Semiconductor Interface

The **Semiconductor (semi)** interface ( ), found under the **Semiconductor** branch ( ) when adding a physics interface, solves Poisson's equation for the electric potential and the drift-diffusion equations for electrons and holes in a semiconductor material. The default domain feature is the **Semiconductor Material Model**, which adds these equations to the domain, solving for the electric potential and dependent variables related to the electron and hole concentrations.

When this physics interface is added, these default nodes are also added to the Model Builder—**Semiconductor Material Model**, **Insulation**, **Zero Charge**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and Generation-Recombination models. You can also right-click **Semiconductor** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `semi`.

THICKNESS (1D/2D MODELS)

Enter the **Out-of-plane thickness** d (SI unit: m) (2D components), or **Cross-section area** A (SI unit: m^2) (1D components), or **Vertical height** d (SI unit: m) (1D axisymmetric components).

MODEL PROPERTIES

Use **Model properties** to set the carrier statistics and solution variables in the model.

Carrier Statistics

Select an option from the **Carrier statistics** list — **Maxwell-Boltzmann** (the default) or **Fermi-Dirac**.

- Maxwell-Boltzmann statistics apply when both the electron and hole quasi-Fermi levels are within the band gap and at least several k_BT away from the band edges.

- Fermi-Dirac statistics are required to simulate degenerate semiconductors. Fermi-Dirac statistics should be used when one or more of the quasi-Fermi levels are close to a band edge or even within the band.

Solution

Select an option from the **Solution** list — **Electrons and holes** (the default) to solve for both, or **Majority carriers only** to solve the drift diffusion equations for only one of the carriers, computing the concentration of the other carrier by means of the mass action law: $np=n_i^2$. For **Majority carriers only** also select the **Majority carriers** — **Electrons** (the default) or **Holes**.

CONTINUATION SETTINGS

Enter the **Interface continuation parameter** C_p (dimensionless). The default is 1.

Select a **Doping and trap density continuation** — **No continuation** (the default), **Use interface continuation parameter**, or **User defined**. For **User defined** enter a value for the **Doping and trap density continuation parameter** C_p (dimensionless). The default is 1.

REFERENCE TEMPERATURE

To display this section, click the **Show** button (👁) and select **Advanced Physics Options**. Enter a **Reference temperature for energy levels** T_0 (SI unit: K). The default is 293.15 K.

💡	The reference temperature is the temperature at which the equilibrium Fermi level is defined. The equilibrium Fermi level is the Fermi-level of the material when there are no applied voltages or currents and when the temperature is uniform throughout the model at the reference temperature. All potentials within the band diagram (for example the electron and hole Fermi-levels and the conduction and valence bands) are measured with respect to the equilibrium Fermi-level (which corresponds to 0 eV).

DISCRETIZATION

To see all settings available in this section, click the **Show** button ( ) and select **Advanced Physics Options**. Use this section to change the discretization of the semiconductor equations.

Select a **Formulation** — **Finite volume (constant shape function)** (the default), **Finite element, log formulation (linear shape function)**, **Finite element, log formulation (quadratic shape function)**, **Finite element (linear shape function)**, **Finite element (quadratic shape function)**, or **Finite element quasi Fermi level (quadratic shape function)**.

The Finite volume discretization is the default, and provides the best current conservation. The Finite element, log formulation uses fewer degrees of freedom (with a linear shape function) and can be more suitable for certain types of problem. The two Finite element discretization settings are provided mainly for backward compatibility and are not recommended for most purposes. The quasi-Fermi level formulation can be suitable for some systems, such as those at very low temperatures. Also specify the **Value type when using splitting of complex variables** — **Real** or **Complex** (the default).

STABILIZATION

To display the section: Click the **Show** button ( ) and select **Stabilization**. Then under **Discretization**, select one of these options to further define this section: **Finite element, log formulation (linear shape function)**, **Finite element, log formulation (quadratic shape function), Finite element (linear)**, or **Finite element (quadratic)**.

Streamline diffusion is on by default when the Discretization is set to Finite element. When Streamline diffusion is active additional contributions to the equation system are added which improve the numerical stability. This, however, can add unphysical artificial diffusion to the problem, which can perturb the carrier densities if they take very small values. While streamline diffusion is usually required for the **Finite element** (linear/quadratic) discretizations, the finite element, log formulation (linear/ quadratic shape function) discretizations usually work without it.

OPTIMAL AVERAGING FOR THE DIFFUSION ENHANCEMENT FACTORS GN GP

To display the section click the **Show** button ( ) and select **Advanced Physics Options**. This section is only applicable and visible for the Fermi-Dirac statistics with the Finite volume discretization. By selecting the check box, the computed current density is most consistent with the limiting case of equilibrium condition (zero current density).

The dependent variable (field variable) is for the **Electric potential** V, **Electron concentration** N_e, and/or **Hole concentration** P_h depending on the selected **Solution** (**Electron and holes** or **Majority carrier only**) under Model Properties. For the quasi-Fermi level formulation, the dependent variable for the electrons or holes is their quasi-Fermi level instead of their concentration. The name of the dependent variable can be changed but the names of fields and dependent variables must be unique within a model.

🔍	• Finite Element and Finite Volume Discretization • Domain, Edge, Boundary, Pair, and Point Nodes for the Semiconductor Interface • Theory for the Semiconductor Interface

Domain, Edge, Boundary, Pair, and Point Nodes for the Semiconductor Interface

The Semiconductor Interface has these domain, edge, boundary, pair, and point nodes available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking the main physics interface node to access the context menu (all users).

💡	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

❗	In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

🔍	• The Semiconductor Interface • Theory for the Semiconductor Interface

These nodes and subnodes are described in this section and listed in alphabetical order:

- Analytic Doping Model
- Analytic Trap Density
- Arora Mobility Model (LI)
- Auger Recombination
- Boundary Selection for Doping Profile
- Boundary Selection for Trap Density Profile
- Caughey-Thomas Mobility Model (E)
- Continuity/Heterojunction
- Continuous Energy Levels (Domains)
- Continuous Energy Levels (Boundaries)
- Direct Recombination
- Discrete Energy Level (Boundaries)
- Discrete Energy Level (Domains)
- Fletcher Mobility Model (C)
- Floating Gate

- Geometric Doping Model
- Geometric Trap Density
- Impact Ionization Generation
- Indirect Optical Transitions
- Initial Values
- Insulation
- Insulator Interface
- Lombardi Surface Mobility Model (S)
- Metal Contact
- Optical Transitions
- Power Law Mobility Model (L)
- Semiconductor Material Model
- Thin Insulator Gate
- Trap-Assisted Recombination
- User-Defined Generation
- User-Defined Mobility Model
- User-Defined Recombination
- WKB Tunneling Model, Electrons
- WKB Tunneling Model, Holes

These nodes and subnodes are described for The Electrostatics Interface:

- Change Cross Section
- Change Thickness (Out-of-Plane)
- Charge Conservation
- Distributed Capacitance
- Electric Displacement Field
- Electric Potential
- External Surface Charge Accumulation
- Floating Potential
- Ground

- Line Charge
- Line Charge (on Axis)
- Line Charge (Out-of-Plane)
- Periodic Condition
- Point Charge
- Point Charge (on Axis)
- Space Charge Density
- Surface Charge Density
- Terminal
- Zero Charge

Semiconductor Material Model

Use the **Semiconductor Material Model** to set the physical and transport properties of the semiconducting material. The following subnodes are available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

- User-Defined Mobility Model
- Power Law Mobility Model (L)
- Arora Mobility Model (LI)
- Fletcher Mobility Model (C)
- Caughey-Thomas Mobility Model (E)
- Lombardi Surface Mobility Model (S)

| 🔍 | See the theory in The Semiclassical Model. |

MATERIAL PROPERTIES

For each of the following, the default is taken **From material**. For **User defined** enter a value or expression in the text field.

- **Relative permittivity** ε_r (dimensionless). For **User defined**, also select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic**.

- **Band gap** $E_{g,0}$ (SI unit: V). The band gap is the energy difference between the conduction and valence band at equilibrium (independent of doping). The input is actually the band gap energy divided by the elementary charge. Therefore it takes on the unit of electric potential, and its numerical value is the same as the band gap energy in eV. The default is 1.12 V.

- **Electron affinity** χ_0 (SI unit: V). The electron affinity is the difference in energy between the vacuum level and the conduction band at equilibrium. The input is actually the electron affinity divided by the elementary charge. Therefore it takes on the unit of electric potential, and its numerical value is the same as the electron affinity in eV. The default is 4.05 V.

- **Effective density of states, valence band** N_v (SI unit: $1/m^3$). The default is 2.66×10^{19} $1/cm^3$.

- **Effective density of states, conduction band** N_c (SI unit: $1/m^3$). The default is 2.86×10^{19} $1/cm^3$.

SEMICONDUCTOR EQUILIBRIUM STUDY SETTINGS

To display this section, which only applies for the **Semiconductor Equilibrium** study step, click the **Show** button ( ) and select **Advanced Physics Options**.

The default **Equilibrium condition** is **Bias voltage**, suitable for situations where there is a well-defined bias electric potential for the domain, for example, given by a metal contact. Enter a **Bias voltage** $V_{0,\text{bias}}$ (SI unit: V). The default is 0 V. All metal contacts attached to the domain will be set to the specified value of $V_{0,\text{bias}}$ for the **Semiconductor Equilibrium** study step.

The other option for **Equilibrium condition** is **Total charge**, suitable for situations where there is a well-defined total charge for the domain, for example, if the domain is insulated on all its exterior boundaries by dielectric material and/or thin insulator gate. Enter a **Total charge** $Q_{0,\text{tot}}$ (SI unit: C). The default is 0 C. In this case, the electric potential of the system still needs to be constrained, for example, by a **Terminal** or an **Electric Potential** boundary condition attached to a dielectric domain, or a **Thin Insulator Gate** boundary condition attached to the **Semiconductor Material Model** domain. If there are also metal contacts attached to the semiconductor domain, then

the bias voltage on those contacts will be set to a value that is consistent with the specified total charge $Q_{0,\text{tot}}$.

> If there are two separate **Semiconductor Material Model** nodes, one assigned to each of two adjacent domains, then care must be taken when specifying the above settings, to ensure that the two domains are at the same equilibrium electric potential, for example, set the **Bias voltage** of the two domains to the same value.

MOBILITY MODEL

These settings determine the mobility values actually used by the Semiconductor interface. The defaults take constant values **From material**. For **User defined** manually define the electron and hole mobilities.

- **Electron mobility** μ_n (SI unit: m^2/(V·s)).
- **Hole mobility** μ_p (SI unit: m^2/(V·s)).

If mobility model subfeatures are added to the material model it is possible to select the output of these mobility models to be used as the mobility by changing the feature input from the appropriate model.

> See the theory in Mobility Models.

BAND GAP NARROWING

Band gap narrowing effects occur at high doping levels. To apply band gap narrowing, select an option from the **Band gap narrowing** list—**None** (the default), **Slotboom**, **Jain-Roulston model**, or **User defined**. Enter values or expressions for the following:

> The Band Gap Narrowing theory section also describes these options.

Slotboom

This option applies Slotboom's empirical model for the band gap narrowing. The model computes the band gap narrowing according to the equation:

$$\Delta E_g = E_{ref}\left(\ln\left(\frac{N_I}{N_{ref}}\right) + \sqrt{\left[\ln\left(\frac{N_I}{N_{ref}}\right)\right]^2 + \frac{1}{2}} \right)$$

where $N_I = N_d + N_a$ and the other parameters are material properties. The fraction of the band gap narrowing taken up by the conduction band is defined directly as a material property by default.

For each of the following model properties the default takes values **From material**, or for **User defined** enter a different value or expression. There are additional options also available for each.

- **Conduction band fraction** α (dimensionless). The default is 0.5.
- **Band gap narrowing reference energy** E_{ref} (SI unit: V). The default is 0.00692 V.
- **Band gap narrowing reference concentration** N_{ref} (SI unit: $1/m^3$). The default is 1.3×10^{17} $1/cm^3$.

Jain-Roulston Model

This option applies the physics-based model of Jain and Roulston for the band gap narrowing. Coefficients for the model are available for a wide range of III-V materials, as well as for silicon and germanium. The band gap narrowing is given by:

$$\Delta E_g = \begin{cases} A_n\left(\frac{N_d}{N_{ref}}\right)^{\frac{1}{3}} + B_n\left(\frac{N_d}{N_{ref}}\right)^{\frac{1}{4}} + C_n\left(\frac{N_d}{N_{ref}}\right)^{\frac{1}{2}} & N_d \geq N_a \\[2em] A_p\left(\frac{N_a}{N_{ref}}\right)^{\frac{1}{3}} + B_p\left(\frac{N_a}{N_{ref}}\right)^{\frac{1}{4}} + C_p\left(\frac{N_a}{N_{ref}}\right)^{\frac{1}{2}} & N_d < N_a \end{cases}$$

where A_n, A_p, B_n, B_p, C_n, and C_p are material properties (with the same units as the band gap) and N_{ref} is a reference doping level (SI unit: $1/m^3$). The fraction of the band gap narrowing taken up by the conduction band is defined directly as a material property by default.

For each of the following properties the default takes values **From material**, or for **User defined** enter a different value or expression. There are additional options available for each.

- **Conduction band fraction** α (dimensionless). The default is 0.5.
- **Jain-Roulston coefficient (n-type), A** (A_n) (SI unit: V). The default is 10e-9 V.
- **Jain-Roulston coefficient (n-type), B** (B_n) (SI unit: V). The default is 3e-7 V.

- **Jain-Roulston coefficient (n-type), C** (C_n) (SI unit: V). The default is 10e-12 V.
- **Jain-Roulston coefficient (p-type), A** (A_p) (SI unit: V). The default is 10e-9 V.
- **Jain-Roulston coefficient (p-type), B** (B_p) (SI unit: V). The default is 3e-7 V.
- **Jain-Roulston coefficient (p-type), C** (C_p) (SI unit: V). The default is 10e-12 V.
- **Band gap narrowing reference concentration** N_{ref} (SI unit: $1/\text{m}^3$). The default is 1.3×10^{17} $1/\text{cm}^3$.

User Defined

Enter a value or expression for **Band gap narrowing voltage** ΔE_g (SI unit: V). The default is 0 V, which represents the amount of band narrowing. Usually a function of the dopant concentrations should be specified.

Enter a value or expression for **Conduction band fraction** α (dimensionless). In general, the change in the band-gap energy can be taken up by a decrease in the conduction band energy and an increase in the valence band energy. The parameter α determines what fraction of the change is taken up by the conduction band. When band-gap narrowing is active $E_c \rightarrow E_c - \alpha \Delta E_g$ and $E_c \rightarrow E_c + (1-\alpha)\Delta E_g$. The default value of α is 1.

DOPANT IONIZATION

This section determines the ionization of the donors and acceptors. Specify the **Dopant ionization** — **Complete ionization** (the default) or **Incomplete ionization**. For **Incomplete ionization**, select an **Ionization model** — **Standard** (the default) or **User defined**.

For **Standard** enter values or expressions for the following:

- **Relative donor energy (below conduction band)** ΔE_d (SI unit: V). The default is 0.05 V.
- **Relative acceptor energy (above valence band)** ΔE_d (SI unit: V). The default is 0.05 V.
- **Donor degeneracy factor** g_d (dimensionless). The default is 2.
- **Acceptor degeneracy factor** g_d (dimensionless). The default is 4.

For **User defined** enter values or expressions for the following:

- **Donor ionization fraction** N_d^+/N_d (dimensionless). The default is 1.
- **Acceptor ionization fraction** N_a^-/N_a (dimensionless). The default is 1.

| ! | Incomplete ionization cannot be used together with the mobility models. |

	See the theory in Incomplete Ionization.

Optical Transitions

The **Optical Transitions** feature adds stimulated and spontaneous emission generation/ recombination rates to the semiconductor and computes the corresponding changes in the complex refractive index or relative permittivity.

OPTICAL TRANSITIONS

Select a **Frequency domain representation** — **Extra dimension** (the default) or **No extra dimension**. This setting determines whether an extra dimension is added to represent the frequency domain. The use of an extra dimension typically makes the problem faster to solve, but it means that additional memory is required. An extra dimension also allows quantities such as the stimulated emission power to be visualized as a function of frequency.

Select a **Transitions model** — **Direct band gap model** (the default) or **User defined**.

Direct Band Gap Model

The **Direct band gap model** uses a two-band model to represent a direct band gap semiconductor, as described in Optical Transitions in the Theory for the Semiconductor Interface.

Select the **Spontaneous emission** check box to compute the recombination due to spontaneous emission. Select the **Stimulated absorption and emission** check box to add the stimulated emission generation or recombination terms. Both check boxes are selected by default.

User Defined

The **User defined** transitions model allows arbitrary specification of the recombination and generation rates due to spontaneous and stimulated emission, and can also be used to compute the Kramers-Kronig integral for the stimulated emission contribution to the change in the real part of the dielectric constant or the refractive index.

For this model enter the:

- **Net generation rate from stimulated processes**, G_{stim} (SI unit: $1/(\text{m}^3 \cdot \text{s})$).

- **Net generation rate from stimulated processes, reference material**, $G^{\mathrm{ref}}{}_{\mathrm{stim}}$ (SI unit: $1/(\mathrm{m}^3 {\cdot} \mathrm{s})$). This rate is used when performing the Kramers–Kronig integral to compute the change in the real part of the dielectric constant or refractive index.

- **Spontaneous emission recombination rate**, R_{spon} (SI unit: $1/(\mathrm{m}^3 {\cdot} \mathrm{s})$).

TRANSITION MATRIX ELEMENT

This section is available when the **Direct band gap model** is selected as the **Transitions model**.

Select how to define the **Matrix element** — **From spontaneous lifetime** (the default), **Momentum matrix element**, **Dipole matrix element**, or **Kane 4-band model**.

Based on the options chosen enter:

- The spontaneous lifetime, τ_{spon} (SI unit: s). The default is 2 ns.
- The momentum matrix element, $|M_{12}{}^{av}|^2$, (SI unit: $\mathrm{kg}^2 {\cdot} \mathrm{m}^2 / \mathrm{s}^2$). The default is $0 \ \mathrm{kg}^2 {\cdot} \mathrm{m}^2 / \mathrm{s}^2$.
- The dipole matrix element, $|\mu_{12}{}^{av}|^2$, (SI unit: $\mathrm{m}^2 {\cdot} \mathrm{s}^2 {\cdot} \mathrm{A}^2$). The default is $0 \ \mathrm{m}^2 {\cdot} \mathrm{s}^2 {\cdot} \mathrm{A}^2$.

For the **Kane 4-band model** enter the **Kane 4-band model parameters**:

- **Electron effective mass**: Select **From band structure properties** (the default, defined in the corresponding section), **From density of states** (converted from N_c, which is defined on the Semiconductor Material Model domain feature), or **User defined**. For **User defined** enter the ratio of the effective mass to the electron mass $m_e{}^*/m_e$ (dimensionless). The default is 0.053.

- **Band gap**: Select **From band structure properties** (defined in the corresponding section), **From semiconductor material model** (defined in the Semiconductor Material Model node), or **User defined**. For **User defined** enter the band gap E_g (SI unit: V). The default is 0.341 V.

- **Valence band spin orbital splitting** Δ (SI unit: V). The default is 0.341 V.

> The matrix element can be dependent on the excitation angular frequency if desired. Any function of the angular frequency can be used, but the angular frequency should take the form: `semi.ot1.omega` (for interface tag `semi` and feature tag `ot1`).

BAND STRUCTURE PROPERTIES

This section is available when the **Direct band gap model** is selected for the **Transitions model**.

- Select an **Electron effective mass** m_e^* — **From density of states** (the default, which is converted from N_c, defined on the Semiconductor Material Model domain feature), or **User defined**. For **User defined** enter the ratio of the electron effective mass to the electron mass m_e^*/m_e (dimensionless). The default is 0.063.

- Select a **Hole effective mass** m_h^* — **From density of states** (the default, which is converted from N_v, defined on the Semiconductor Material Model domain feature), or **User defined**. For **User defined** enter the ratio of the hole effective mass to the electron mass m_h^*/m_e (dimensionless). The default is 0.51.

- Select a **Band gap** E_g — **From semiconductor material model** (defined in the material properties section of the Semiconductor Material Model domain feature) or **User defined**. For **User defined** enter the band gap E_g (SI unit: V). The default is 1.424 V.

OPTICAL EXCITATION FREQUENCY

This section is available when the excitation frequency is needed to calculate the stimulated emission rate or the matrix element and when the feature is not coupled to an Electromagnetic Waves interface.

Select an **Excitation frequency** f_0 — **From study** (the default), **User-defined frequency**, or **User-defined wavelength**.

- For **User-defined frequency**, enter the excitation frequency, f_0 (SI unit: Hz). The default is 344 GHz.

- For **User-defined wavelength**, enter the wavelength, λ_0 (SI unit: m). The default is 870 nm.

OPTICAL INTENSITY

This section is available in the absence of a multiphysics coupling when the **Direct band gap model** is selected for the **Transitions model** and when the **Stimulated absorption and emission** check box is selected. It is used to define the intensity of the optical field that is driving the stimulated emission. Enter the **Electric field norm**, E_0 (SI unit: V/m). The default is 500 V/m.

OPTICAL MATERIAL PROPERTIES

Select the **Electric displacement field model** — **Refractive index** (the default) or **Relative permittivity**.

Refractive Index

For **Refractive index** the default **Refractive index** n and **Refractive index, imaginary part** k take values **From material**. For **User defined** select **Isotropic** (for **Diagonal** the average of the diagonal elements are taken).

> ⚠ The time-harmonic sign convention used in COMSOL Multiphysics requires that a lossy material has a negative imaginary part of the refractive index.

Relative Permittivity

The default **Relative permittivity (real part)** ε' and **Relative permittivity (imaginary part)** ε'' take values **From material**. For **User defined** select **Isotropic** (for **Diagonal** the average of the diagonal elements are taken).

> ⚠ The time-harmonic sign convention used in COMSOL requires that a lossy material has a negative imaginary part of the relative permittivity.

OPTICAL OUTPUTS

Select the **Compute change in real part of susceptibility** check box to compute the change in the real part of the susceptibility (or permittivity/refractive index) using a Kramers–Kronig integral.

INTEGRAL PROPERTIES

The settings in this section determine the range and resolution of the numerical scheme used to compute integrals over the frequency domain.

The **Frequency domain integral discretization factor** (dimensionless) is an integer related to the discretization of the of the frequency domain. A higher number indicates a finer mesh in the extra dimension (if present) or smaller steps in the numerical integration (if no extra dimension is used). The default is 6.

The **Frequency domain integral lower limit** specifies the lower limit used in frequency domain integrals in units of $\hbar\omega_0$ (if **Stimulated absorption and emission** is enabled, or user defined is chosen — ω_0 is the excitation angular frequency) or in units of the band gap (if only spontaneous emission is chosen). The lower limit should be less than the band gap. The default is 0.5.

The **Frequency domain integral upper limit** specifies the upper limit used in frequency domain integrals in units of $\hbar\omega_0$ (if **Stimulated absorption and emission** is enabled, or

user defined is chosen — ω_0 is the excitation angular frequency) or in units of the band gap (if only spontaneous emission is chosen). The upper limit should be chosen so that the processes of interest are negligible above it. The default is 3.

The **Kramers-Kronig integral pole region width** specifies the total width of the pole region around the excitation frequency in units of $\hbar\omega_0$ (if **Stimulated absorption and emission** is enabled, or user defined is chosen — ω_0 is the excitation angular frequency) or in units of the band gap (if only spontaneous emission is chosen). It should be chosen so that the change in the susceptibility or the change in the absorption coefficient is linear to a good accuracy across the region. The default is 0.01.

Indirect Optical Transitions

The **Indirect Optical Transitions** feature adds an empirical absorption model for silicon to enable easy simulation of optical absorption in photovoltaic devices. The model uses the data from Ref. 44 to obtain the frequency-dependent real and imaginary components of the refractive index of silicon. Alternately, you can choose to specify a user-defined absorption via either supplying an absorption coefficient or the imaginary part of the refractive index — this enables the feature to be used for other materials for which this data is known. The photogeneration due to absorbed photons is then added into the model via a term that contributes to the carrier generation rate. If a multiphysics coupling between the Semiconductor interface and an Electromagnetic Waves interface is active, the refractive index data from the Indirect Optical Transitions feature is automatically used by the Electromagnetic Waves interface for calculating wave propagation. Also, the frequency and magnitude of the electromagnetic wave, which are required in order to calculate the absorption rate, are obtained automatically from the Electromagnetic Waves interface. If multiphysics coupling is not used, these quantities can be specified directly within the Indirect Optical Transitions feature.

TRANSITIONS MODEL

Select a **Transitions model**—**Empirical silicon absorption (Green and Keevers)** (the default) or **User-defined absorption**.

- **Empirical silicon absorption (Green and Keevers)**: This option automatically obtains the frequency-dependent real and imaginary components of the refractive index and computes the absorption and associate carrier generation. This model is most appropriate for intrinsic silicon at temperatures around 300 K.

- **User-defined absorption**: This option enables the user to specify the absorption. The photogeneration rate is then computed and the extra carriers are added to the model

automatically via an extra generation term. You can either supply the imaginary part of the refractive index or the absorption coefficient.

SPECIFY ABSORPTION

This section is available when **User-defined absorption** is selected as the transitions model.

Select an option from the **Specify absorption** list — **Absorption coefficient** (the default) or **Refractive index**. Then enter the following as required:

- **Imaginary part of refractive index** n (dimensionless).
- **Absorption coefficient** α (SI unit: 1/m).
- **Real part of the refractive index** k (dimensionless).

OPTICAL EXCITATION FREQUENCY

This section is available if a multiphysics coupling is not used. It enables the frequency of the electromagnetic wave to be specified. If the **Empirical silicon absorption (Green and Keevers)** transition model is selected, this frequency is used to look up the corresponding refractive index data. For both transition model options the frequency is used in calculating the photogeneration rate.

Select an **Excitation frequency** — **From study** (the default), **User-defined frequency**, or **User-defined wavelength**.

- For **User-defined frequency**, enter the excitation frequency, f_0 (SI unit: Hz). The default is 375 GHz.
- For **User-defined wavelength**, enter the wavelength, λ_0 (SI unit: m). The default is 800 nm.

OPTICAL INTENSITY

This section is available if a multiphysics coupling is not used. It enables the magnitude of the electromagnetic wave to be specified.

Enter the **Electric field norm**, E_0 (SI unit: V/m).

Insulation

The **Insulation** node is the default boundary condition. It specifies the zero normal flux condition at the selected boundaries, that is, setting the normal component of the electron current, hole current, and electric displacement field to zero.

	The functionality of the **Surface traps** check box in versions prior to 5.4 has been replaced and expanded by the Trap-Assisted Surface Recombination boundary condition.

Continuity/Heterojunction

The **Continuity/Heterojunction** node is added by default to all interior boundaries in a model. When the material properties are continuous across the boundary the feature has no effect. If there is a discontinuity in the material properties across the boundary then the feature includes the equations required to model a heterojunction.

CONTINUATION SETTINGS

These settings are the same as for Fletcher Mobility Model (C).

	The **Continuation Settings** do not scale the equation contributions for the **Continuous Quasi-Fermi** level option.

HETEROJUNCTION

Select a **Continuity model** — **Continuous quasi-Fermi levels** (the default) or **Thermionic emission**. The **Continuous quasi-Fermi levels** model enforces continuity of both quasi-Fermi levels at the boundary. The **Thermionic emission** model adds thermionic emission of the carriers over the boundary to the model.

EXTRA CURRENT CONTRIBUTION

This section appears if the **Continuity model** is set to **Thermionic emission** (See the section Heterojunction above).

Select an option for the **Extra electron current** drop-down menu:

1 **No extra current** (the default)

2 **WKB tunneling model** Computes the extra current contribution using the WKB approximation for tunneling. For this option to work, the user needs to manually

add a WKB Tunneling Model, Electrons sub-node to specify the tunneling parameters.

3 User-defined extra current fraction Computes the extra current contribution using the user-defined extra current fraction entered into the input field **Extra current fraction, electrons** that appears when this option is selected.

Select an option for the **Extra hole current** drop-down menu, which has a set of options analogous to the ones for electrons described above. For the option **WKB tunneling model** to work, remember to add a WKB Tunneling Model, Holes sub-node.

Q
- Solving in the Modeling Guidelines chapter.
- Boundary Conditions and Continuity/Heterojunction

WKB Tunneling Model, Electrons

This sub-node is available when the option **WKB tunneling model** is selected for a heterojunction or Schottky contact. Add this sub-node to compute the contribution to the electron current density from tunneling, using the WKB approximation.

POTENTIAL BARRIER DOMAIN SELECTION
Select a domain adjacent to the boundary selection of this sub-node, where the potential barrier is located and electrons tunnel across the domain.

📋
When drawing the geometry for the device model, consider adding a thin layer of domain adjacent to the heterojunction or Schottky contact, where you plan to use the WKB tunneling feature.

OPPOSITE BOUNDARY SELECTION
Select a boundary on the opposite side of the **Potential Barrier Domain Selection** from the boundary selection of this sub-node. These two boundary selections are each at the upstream and downstream of the electric field line. In other words, if an electron tunnel into the boundary selection of the sub-node, it emerges out of the **Opposite Boundary Selection**.

WKB TUNNELING MODEL, ELECTRONS

In this section, enter the electron effective mass and one or more coordinates depending on the space dimension of the model.

- For **Effective mass**, enter the electron effective mass m (SI unit: kg). The default is the free electron mass me_const.

- For **Field line coordinate**, enter an appropriate variable flc (SI unit: m) that is (approximately) proportional to the arc length along the electric field line across the potential barrier domain selection. The default is the first coordinate of the global coordinate system. The variable should be valid within the potential barrier domain selection and its isosurfaces should be approximately parallel to the equipotential surfaces in the domain.

📄   In general a Curvilinear Coordinates physics interface can be used to compute the (approximated) electric field line coordinate, or each of the boundary coordinates below. See the Application Libraries example **Semiconductor_Module/Verification_Examples/heterojunction_tunneling**

- For 2D and 3D components, enter **Boundary coordinate** $bndc$ (SI unit: m). The default is the second coordinate of the global coordinate system. See below for more details.

- For 2D axisymmetry and 3D components, enter **Boundary coordinate 2** $bndc2$ (SI unit: m). The default is the Z coordinate of the global coordinate system. For this input and the input for $bndc$ above, enter an appropriate variable that can be used to form the boundary coordinate system of the boundary selection of the sub-node. The variable should be valid within the potential barrier domain selection and its isosurfaces should be approximately parallel to the electric field lines in the domain .

📄   For the formulation used in the WKB Tunneling Model sub-nodes, see the theory section WKB Tunneling Model.

WKB Tunneling Model, Holes

Add this sub-node to compute the contribution to the hole current density from tunneling, using the WKB approximation.

The settings of this sub-node is analogous to the ones for the sub-node WKB Tunneling Model, Electrons described above.

Initial Values

The **Initial Values** node provides initial values for the electric potential V, electron concentration, and the hole concentration that serve as an initial condition for a transient simulation or as an initial guess for the nonlinear solver in other studies.

INITIAL VALUES

Select an option from the **Specify initial values** list — **Automatic** (the default), **Equilibrium (carriers and potential)**, **Equilibrium (carriers)**, **Intrinsic (carriers and potential)**, **Intrinsic (carriers)**, or **User defined**.

	The **Automatic** setting varies based on the **Discretization** settings for the physics interface. If **Finite volume (constant shape function)** is selected, then equilibrium conditions are used. If any of the **Finite element** discretizations are selected, then the intrinsic concentrations are used.

Then depending on the choice, enter a value or expression or keep the defaults as follows:

- For **Equilibrium (carriers)** or **Intrinsic (carriers)** the default **Electric potential** V (SI unit: V) is –4 V. The carrier concentrations are automatically set to the equilibrium or intrinsic values.

- For **User defined** the default **Electric potential** V (SI unit: V) is –4 V, the default **Electron concentration** N (SI unit: $1/m^3$) is semi.n_init, and the default **Hole concentration** P (SI unit: $1/m^3$) is semi.p_init. For quasi-Fermi level formulation, the default user-defined quasi-Fermi levels are 0 V.

User-Defined Mobility Model

The **User-Defined Mobility Model** subnode is available from the context menu (right-click the Semiconductor Material Model parent node) or from the **Physics** toolbar, **Attributes** menu. This can be used to define a mobility model using expressions based on, for example, the temperature and the dopant concentrations.

DOMAIN SELECTION

	Usually the mobility model selection should not be changed from that of the parent Semiconductor Material Model.

Enter a value in the **Electron input mobility** $\mu_{n,in}$ (SI unit: m^2/(V·s)) text field. This parameter is used to define an input mobility that can be edited in the Electron mobility text field. The default **Electron input mobility** is for silicon at equilibrium, that is, 1448 cm^2/(V·s). Any electron input mobility from other mobility models added to the Semiconductor Material Model can be chosen from the list.

Enter a value in the **Hole input mobility** $\mu_{p,in}$ (SI unit: m^2/(V·s)) text field. This parameter is used to define an input mobility that can be edited in the Hole mobility field. The default **Hole input mobility** is for silicon at equilibrium, that is, 473 cm^2/(V·s). Any hole input mobility from other mobility models added to the Semiconductor Material Model can be chosen from the list.

The **Electron mobility** $\mu_{0,n}$ (SI unit: m^2/(V·s)) field defines the output electron mobility. The default value is taken from Electron input mobility. Any valid mathematical expression can be used to modify the default value.

The **Hole mobility** $\mu_{0,p}$ (SI unit: m^2/(V·s)) field defines the output hole mobility. The default value is taken from Hole input mobility. Any valid mathematical expression can be used to modify the default value.

| Q | Mobility Models and Theory for the User-defined Mobility Model |

Power Law Mobility Model (L)

The **Power Law Mobility Model (L)** subnode is available from the context menu (right-click the Semiconductor Material Model parent node) or from the **Physics** toolbar, **Attributes** menu. This model incorporates the effect of lattice or phonon scattering into the electron and hole mobilities for the material (the 'L' given in brackets indicates lattice scattering). The equations for the mobility model are shown in the **Equation** section.

DOMAIN SELECTION

| ! | Usually the mobility model selection should not be changed from that of the parent Semiconductor Material Model. |

The default **Reference temperature** T_{ref} (SI unit: K) is taken **From material**. For **User defined** enter a value in the text field. The default is 300 K.

ELECTRON PARAMETERS

For each of the following properties the default takes values **From material** or for **User defined** enter a different value or expression in the text field.

- **Electron mobility reference** $\mu_{n,0}$ (SI unit: m^2/(V·s)). The default value is for silicon (1448 cm^2/(V·s)). This value represents the zero field mobility at equilibrium.

- **Electron exponent** α_n (dimensionless). The default for silicon is 2.33.

HOLE PARAMETERS

For each of the following properties the default takes values **From material** or for **User defined** enter a different value or expression in the text field.

- **Hole mobility reference** $\mu_{p,0}$ (SI unit: m^2/(V·s)). The default value is for silicon (473 cm^2/(V·s)). This value represents the zero field mobility at equilibrium.

- **Hole exponent** α_p (dimensionless). The default value is for silicon (2.23).

> Mobility Models and Theory for the Power Law Mobility Model (L)

Fletcher Mobility Model (C)

The **Fletcher Mobility Model (C)** subnode is available from the context menu (right-click the Semiconductor Material Model parent node) or from the **Physics** toolbar, **Attributes** menu. Use this to add carrier-carrier scattering to an existing mobility model (or to a constant input mobility). The 'C' in brackets indicates the model includes carrier-carrier scattering only. It accepts input mobilities of type L or LI, as well as user-defined input mobilities. The set of equations defining the Fletcher mobility model is shown in the **Equation** section.

DOMAIN SELECTION

> ! Usually the mobility model selection should not be changed from that of the parent Semiconductor Material Model.

CONTINUATION SETTINGS

The continuation settings enable the equation contributions for the feature to be gradually introduced into the model.

The **Continuation type** defaults to **No continuation**, which means that the equation contribution is added in the usual way.

The continuity feature allows the equation contribution to be weighted by an external parameter: the value should be between 0 and 1. Then you can sweep this parameter with the continuity solver.

Selecting **User defined** allows the parameter to be specified within the feature or select **Use interface level continuation parameter** to specify the parameter on the physics interface level.

- For **User defined** enter a **Continuation parameter** C_p (dimensionless) between 0 and 1 to determine the scaling of the equation contribution. Generally the parameter is ramped from 0 to 1 in a continuation study.

- For **Use interface continuation parameter**, the continuation parameter is linked to the value of the continuation parameter specified in the Continuation Settings section for The Semiconductor Interface. This enables several features to be introduced simultaneously into the equation system with a single setting controlling it all.

🔍　　Solving

INPUT MOBILITIES

The **Electron input mobility** $\mu_{n,in}$ (SI unit: m^2/(V·s)) parameter is used to define an input mobility to which carrier-carrier scattering is added. The default value is **User defined** and is a room temperature mobility for silicon, that is, 1448 cm^2/(V·s).

The **Hole input mobility** $\mu_{p,in}$ (SI unit: m^2/(V·s)) parameter is used to define an input mobility to which carrier-carrier scattering is added. The default value is **User defined**, and is for silicon at equilibrium, that is, 473 cm^2/(V·s).

📋　　Other mobility models of type L (Power Law Mobility Model (L)) or LI (Arora Mobility Model (LI) as well as User-Defined Mobility Model input mobilities can be used as the **Electron input mobility** and **Hole input mobility**.

For each of the following properties the default takes values **From material** or for **User defined** enter a different value or expression in the text field.

- **Reference temperature** T_{ref} (SI unit: K). The default is 300 K.

- **Fletcher mobility coefficient1** F_1 (SI unit: $1/(\text{m.V·s})$). The default is for silicon ($1.04\text{e}21$ $1/(\text{cm-V·s})$).

- **Fletcher mobility coefficient2** F_2 (SI unit: $1/(\text{m}^2)$). The default is for silicon ($7.45\text{e}12$ $1/\text{cm}^{-2}$).

🔍	Mobility Models and Theory for the Fletcher Mobility Model (C)

Caughey-Thomas Mobility Model (E)

The **Caughey-Thomas Mobility Model (E)** subnode is available from the context menu (right-click the Semiconductor Material Model parent node) or from the **Physics** toolbar, **Attributes** menu. It adds a high field correction to an existing mobility model. The 'E' in brackets indicates the model includes high field effects only. It accepts input mobilities of type L, I, C, or S as well as user-defined input mobilities. The set of equations defining the Caughey-Thomas mobility model is shown in the **Equation** section.

DOMAIN SELECTION

❗	Usually the mobility model selection should not be changed from that of the parent Semiconductor Material Model.

CONTINUATION SETTINGS

These settings are the same as for Fletcher Mobility Model (C).

❗	The continuation solver should be used in most cases with the Caughey-Thomas mobility model.

$\textcircled{?}$	Solving

INPUT MOBILITIES

The **Electron input mobility** $\mu_{n,in}$ (SI unit: m^2/(V·s)) parameter is used to define the input mobility to which high field velocity saturation is added. The default is **User defined** for silicon at equilibrium, 1448 cm^2/(V·s).

The **Hole input mobility** $\mu_{p,in}$ (SI unit: m^2/(V·s)) defines the input mobility to which high field velocity saturation is added. The default is **User defined** for silicon at equilibrium, 473 cm^2/(V·s).

📋	Any other **Electron input mobility** and **Hole input mobility** from mobility models of the Semiconductor Material Model can be chosen.

GENERAL PARAMETERS

The default **Reference temperature** T_{ref} (SI unit: K) is taken **From material**. For **User defined** enter a different value in the text field. The default is 300 K.

ELECTRON PARAMETERS

The default for each of the following is taken **From material**. For **User defined** enter a different value in the text field.

- **Electron alpha coefficient** $\alpha_{n,0}$ (dimensionless). The default is 1.11.
- **Electron saturation velocity** $v_{n,0}$ (SI unit: m/s). The default is 1×10^7 cm/s.
- **Electron alpha exponent** $\beta_{n,1}$ (dimensionless). The default is 0.66.
- **Electron velocity saturation exponent** $\beta_{n,2}$ (dimensionless). The default is −0.87.

HOLE PARAMETERS

- **Hole alpha coefficient** $\alpha_{p,0}$ (dimensionless). The default is 1.21.
- **Hole saturation velocity** $v_{p,0}$ (SI unit: m/s). The default is 8.37×10^6 cm/s.

- **Hole alpha exponent** $\beta_{p,1}$ (dimensionless). The default is 0.17.
- **Hole velocity saturation exponent** $\beta_{p,2}$ (dimensionless). The default is −0.52.

Q	Mobility Models and Theory for the Caughey-Thomas Mobility Model (E)

Lombardi Surface Mobility Model (S)

The **Lombardi Surface Mobility Model (S)** subnode is available from the context menu (right-click the Semiconductor Material Model parent node) or from the **Physics** toolbar, **Attributes** menu. It changes an input mobility to account for surface effects, particularly surface roughness and scattering due to acoustic phonons. The 'S' in brackets indicates the model includes surface effects only. The mobility model accepts input mobilities of type L, LI, or C as well as user-defined input mobilities.

The set of equations defining the Lombardi Surface mobility model is shown in the **Equation** section.

DOMAIN SELECTION

!	Usually the mobility model selection should not be changed from that of the parent Semiconductor Material Model.

CONTINUATION SETTINGS

These settings are the same as for Fletcher Mobility Model (C).

!	The continuation solver should be used in most cases with the Lombardi Surface mobility model.

Q	Solving

Lombardi Surface Mobility shows how to use the continuity solver and how to set up the solver in the most efficient manner when using this mobility model. Application Library path: **Semiconductor_Module/Devices/lombardi_surface_mobility**

INPUT MOBILITIES

The **Electron input mobility** $\mu_{n,\text{in}}$ (SI unit: $\text{m}^2/(\text{V·s})$) parameter is used to define an input mobility. The default is **User defined** for silicon at equilibrium, $1448\ \text{cm}^2/(\text{V·s})$.

The **Hole input mobility** $\mu_{p,\text{in}}$ (SI unit: $\text{m}^2/(\text{V·s})$) defines an input mobility. The default is **User defined** for silicon at equilibrium $473\ \text{cm}^2/(\text{V·s})$.

Other mobility models of type L (Power Law Mobility Model (L)), LI (Arora Mobility Model (LI), C Fletcher Mobility Model (C), or User-Defined Mobility Model input mobilities can be used as the **Electron input mobility** and **Hole input mobility**.

GENERAL PARAMETERS

The default for each of the following is taken **From material**. For **User defined** enter a different value or expression in the text field.

- **Reference temperature** T_{ref} (SI unit: K). The default is 1 K.
- **Electric field reference** E_{ref} (SI unit: V/m). The default is 1 V/cm.
- **Doping concentration reference** N_{ref} (SI unit: $1/\text{m}^3$). The default is $1\ 1/\text{cm}^3$.

ELECTRON PARAMETERS

The default for each of the following is taken **From material**. For **User defined** enter a different value or expression in the text field.

- **Electron delta coefficient** δ_n (SI unit: V/s). The default is 5.82×10^{14} V/s.
- **Electron mobility reference** $\mu_{n,1}$ (SI unit: $\text{m}^2/(\text{V·s})$). The default is $4.75 \times 10^7\ \text{cm}^2/(\text{V·s})$.
- **Electron mobility reference** $\mu_{n,2}$ (SI unit: $\text{m}^2/(\text{V·s})$). The default is $1.74 \times 10^5\ \text{cm}^2/(\text{V·s})$.
- **Electron alpha coefficient** α_n (SI unit: 1). The default is 0.125.

HOLE PARAMETERS

- **Hole delta coefficient** δ_p (SI unit: V/s). The default is 2.05×10^{14} V/s.

- **Hole mobility reference** $\mu_{p,1}$ (SI unit: m^2/(V·s)). The default is 9.93×10^7 cm^2/(V·s)
- **Hole mobility reference** $\mu_{p,2}$ (SI unit: m^2/(V·s)). The default is 8.84×10^5 cm^2/(V·s)
- **Hole alpha coefficient** α_p (SI unit: 1). The default is 0.0317.

ADVANCED

To display this section, click the **Show** button (👁) and select **Advanced Physics Options**. Enter a **Current density activation threshold** J_{tol} (SI unit: A/m^2). The default is 1×10^6 A/m^2.

🔍	Mobility Models and Theory for the Lombardi Surface Mobility Model (S)

Arora Mobility Model (LI)

The **Arora Mobility Model (LI)** subnode is available from the context menu (right-click the Semiconductor Material Model parent node) or from the **Physics** toolbar, **Attributes** menu. Use it to simulate the effect of phonon/lattice and impurity scattering on the electron and hole mobilities in the semiconducting material (the 'L' in brackets indicates the model includes lattice scattering and the 'I' indicates the model includes impurity scattering). The Arora mobility model is empirical and involves many parameters. The set of equations defining the model is shown in the **Equation** section.

DOMAIN SELECTION

❗	Usually the mobility model selection should not be changed from that of the parent Semiconductor Material Model.

GENERAL PARAMETERS

For each of the following properties the default takes values **From material**, or for **User defined** enter a different value or expression in the text field.

- **Reference temperature** T_{ref} (SI unit: K). The default is 300 K.
- **Alpha coefficient** α_0 (dimensionless). The default is for silicon 0.88.
- **Mobility reference minimum exponent** β_1 (dimensionless). The default is for silicon –0.57.

- **Mobility reference exponent** β_2 (dimensionless). The default is for silicon −2.33.
- **Impurity concentration reference exponent** β_3 (dimensionless). The default is for silicon 2.4.
- **Alpha coefficient exponent** β_4 (dimensionless). The default is for silicon −0.146.

ELECTRON PARAMETERS

For each of the following properties the default takes values **From material**, or for **User defined** enter a different value or expression in the text field.

- **Electron mobility reference** $\mu_{n,0}{}^{\text{ref}}$ (SI unit: $m^2/(V{\cdot}s)$). The default value is for silicon (1252 cm$^2/(V{\cdot}s)$).
- **Electron mobility minimum reference** $\mu_{n,}{}^{\text{ref}}{}_{\min}$ (SI unit: $m^2/(V{\cdot}s)$). The default value is for silicon (88 cm$^2/(V{\cdot}s)$).
- **Electron reference impurity concentration** $N_{n,}{}^{\text{ref}}{}_0$ (SI unit: $1/m^3$). The default value is for silicon ($1.26e17$ $1/$cm^3).

HOLE PARAMETERS

For each of the following properties the default takes values **From material**, or for **User defined** enter a different value or expression in the text field.

- **Hole mobility reference** $\mu_{p,0}{}^{\text{ref}}$ (SI unit: $m^2/(V{\cdot}s)$. The default value is for silicon (407 cm$^2/(V{\cdot}s)$.
- **Hole mobility minimum reference** $\mu_{p,}{}^{\text{ref}}{}_{\min}$ (SI unit: $m^2/(V{\cdot}s)$). The default value is for silicon (54.3 cm$^2/(V{\cdot}s)$).
- **Hole reference impurity concentration** $N_{p,}{}^{\text{ref}}{}_0$ (SI unit: $1/m^3$). The default value is for silicon ($2.35e17$ $1/$cm^3).

Mobility Models and Theory for the Arora Mobility Model (LI)

Analytic Doping Model

Use the **Analytic Doping Model** to set the doping type and concentration within a Semiconductor Material Model domain. The concentration is defined as a function of the local coordinate system, making this doping method suitable for profiles that are convenient to express in terms of the coordinate axes.

In some cases it is desirable to increase the doping from zero or a low value to that required in the simulation during the solution process. This can improve the convergence of the simulation significantly. The continuity settings allow the dopant densities to be weighted by an external parameter, whose value should be between 0 and 1.

- By default the **Continuation type** is set to **Use interface continuation parameter**. This means that the continuity settings are determined by the **Doping and trap density continuation** in the Continuation Settings section for The Semiconductor Interface.

- To introduce the doping from a specific feature independently of the other features, select **User defined** and manually enter the **Continuation parameter**. This should be set to a dimensionless parameter that is swept from zero to 1 using the continuation solver.

- To disable the continuation for a particular doping feature select **No continuation** for the **Continuation type**.

	For the finite volume method it is recommended that a zero value of the parameter is avoided. Instead, start with a small value (for example, 1e-6) and increase the value of the parameter gradually to 1. The continuation solver usually does not manage the transition from zero to finite doping when the finite volume method is used.

	Solving

DISTRIBUTION

Choose the type of dopant distribution to apply on the selected domains from the **Distribution** list: **User defined** (the default) to enable any expression to be used to define the dopant distribution, or **Box** to create a block-shaped region of uniform doping away from which the concentration decays to a background level according to a specified profile. The Profile of the distribution away from the uniform region is selected from a list of preset functions.

IMPURITY

Choose an **Impurity type** to set the species of the dopants—**Acceptor doping (p-type)** (the default) or **Donor doping (n-type)**. Once the impurity type is selected, enter a value

or expression for the **Acceptor concentration** N_{A0} or **Donor concentration** N_{D0} (SI unit: $1/\mathrm{m}^3$).

For a **User defined** Distribution input, you can use any expression in terms of the coordinate system. This expression then defines the dopant concentration through the selected domains (if a constant value is entered this simply assigns a uniform concentration to all selected domains). For a **Box** distribution, a constant value must be entered and this sets the concentration within the region of uniform doping. The default value for both distributions is a constant value of $1 \cdot 10^{16}$ cm^3.

UNIFORM REGION

This section is available when **Box** is selected under **Distribution**. It is used to define the location and size of the region of uniform doping.

Set the position of the region using the **Base** list. Select **Corner** (the default) or **Center**.

The **Base position** r_0 (SI unit: m) vector sets the location of the region. When **Corner** is selected it describes the coordinate of the lower left front corner of the region, and when **Center** is selected it describes the coordinate of the center of the region. The default value is at the origin of the coordinate system.

> 📋 It is possible to set the height, width, or depth of the region to zero. In 2D, for example, setting the height of the region to zero results in a line of constant doping away from which the profile function decays.

The extent of the region is defined with the **Width**, **Depth**, and **Height** inputs. Only the inputs relevant to the dimension of the component to which the feature belongs are displayed, for example, in a 2D component only the **Width** and **Depth** are available.

- **Width** W (SI unit: m). This is the extent of the region in the direction parallel to the local x-axes.
- **Depth** D (SI unit: m). This is the extent of the region in the direction parallel to the local y-axes.
- **Height** H (SI unit: m). This is the extent of the region in the direction parallel to the local z-axes.

The default value is 0 for each dimension.

This section is available when **Box** is selected under **Distribution**. Select a **Profile away from uniform region** — **Gaussian** (the default), **Linear**, or **Error function (erf)**.

Then select an option from the **Specify profile length scale** list — **Junction depth** (available for all profiles), **Decay length** (available for a Gaussian), **Gradient** (available for **Linear**), or **Argument factor** (available for **Error function (erf)**).

By default, the **Specify different length scales for each direction** check box is not selected. It is possible to specify a different profile length scale in each coordinate direction when this check box is selected.

Junction Depth

For **Junction depth** enter a value for the **Junction depth** d_j (SI unit: m, default value is 1 μm) to specify the location at which the profile concentration drops to equal the **Background doping concentration** N_b (SI unit: $1/m^3$). The default background concentration is **User defined** with a doping concentration of $1 \cdot 10^{15}$ $1/cm^3$. Alternately, the doping distribution from another Analytic Doping Model or Geometric Doping Model can be used as the background concentration.

Each profile has a profile-specific parameter to directly control the length scale of the decay.

Decay Length — for Gaussian profile

For **Decay length** enter a value for the **Decay length** l_j of the Gaussian decay. (SI unit: m, default value is 1 μm).

Gradient—for Linear profile

For **Gradient** enter a value for the **Gradient** N_{grad} of the Linear profile (SI unit: $1/m^4$, default value is $-1 \cdot 10^{20}$ $1/cm^4$).

Argument Factor — for Error function (erf) profile

For **Argument factor** enter a value for the **Argument factor** m (SI unit: $1/m$, default value is 1 $(1/μm)$) to specify the factor by which the coordinate values are multiplied before being operated on by the **erf** function.

As when the **Junction depth** option is used, by default the **Specify different length scales for each direction** check box is not selected. Select it to specify a different profile length scale in each coordinate direction.

Geometric Doping Model

Use the **Geometric Doping Model** to define a dopant distribution in terms of the distance from selected boundaries. This is convenient when specifying distributions which are not easily expressed in terms of the coordinate system. For example, if a profile is defined in terms of the distance from a surface then it may not need to have its expression modified if the geometry is altered. This feature also allows any user defined decay profile away from the selected boundaries, which is suitable for cases where none of the preset decay functions available in the Analytic Doping Model are appropriate.

A default Boundary Selection for Doping Profile is added where the boundaries from which the distance is calculated can be specified.

CONTINUATION SETTINGS

These settings are the same as for Analytic Doping Model.

DISTRIBUTION

Select an option from the **Profile away from the boundary** list — **Gaussian** (the default), **Linear**, **Error function (erf)**, or **User defined**.

IMPURITY

For **Gaussian**, **Linear**, or **Error function (erf)** profiles, select the **Impurity type**—**Acceptor doping** (the default) or **Donor doping**. Then specify the maximum doping concentration of the distribution; this is the concentration of the dopants at the selected boundaries.

- For **Acceptor doping** specify the **Acceptor concentration at boundary** N_{A0} (SI unit: $1/m^3$) of the electron acceptor impurities. The default value is 1×10^{16} $1/cm^3$.
- For **Donor doping** specify the **Donor concentration at boundary** N_{D0} (SI unit: $1/m^3$) of the electron donor impurities. The default value is 1×10^{16} $1/cm^3$.

For **User defined** profiles select the **Dopant type** — **Acceptor doping** (the default) or **Donor doping**. Then enter an expression for **Define profile as a function of the distance,**

D, from the boundaries *N(D)* (SI unit $1/\text{m}^3$). The distance from the selected boundaries is available as variable `semi.gdm#.D`, which can be used in an expression to define the doping profile. The default expression gives an example of a Gaussian profile defined using this variable.

P R O F I L E

For the **Gaussian**, **Linear**, and **Error function (erf)** profiles it is necessary to specify the length scale of the profile decay. The **Profile** section allows the length scale of the profile to be controlled. As with the Analytic Doping Model, the length scale can be controlled either by entering a junction depth or via a profile-specific length scale parameter. See Analytic Doping Model, under **Profile** for the settings for more details.

- Doped Semiconductors
- Doping and Using the Geometric Doping Model
- Specifying the Dopant Distribution and Theory for the Geometric Doping Model

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Boundary Selection for Doping Profile

A default **Boundary Selection for Doping Profile** is added to the Geometric Doping Model. This node enables the boundaries from which the distance is calculated to be selected. Any internal or external boundary that bounds, or is within, the domains to which the corresponding **Geometric Doping Model** is applied can be selected.

- Doped Semiconductors
- Doping
- Specifying the Dopant Distribution

Analytic Trap Density

Use the **Analytic Trap Density** node to specify the density of traps within the domain. This feature enables a density to be defined by an expression written in terms of the local coordinate system. Alternately, it enables a region of uniform trap density which decays into a background density with one of three preset profile functions to be created. The trap density can be used in conjunction with a Trap-Assisted

Recombination feature to specify recombination via trapping sites whose density varies in space. The available options are similar to the Analytic Doping Model feature.

CONTINUATION SETTINGS

In some cases it is desirable to increase the trapping from zero or a low value to that required in the simulation during the solution process. This can improve the convergence of the problem significantly. The continuity settings allow the trap densities to be weighted by an external parameter whose value should be between 0 and 1. By default the **Continuation type** is set to **Use interface continuation parameter**. This means that the continuity settings are determined by the **Doping and trap density continuation** in the Continuation Settings section for The Semiconductor Interface. To introduce the trapping from a specific feature independently of the other features, select **User defined** and manually enter the **Continuation parameter**. This should be set to a dimensionless parameter that is swept from zero to 1 using the continuation solver.

To disable the continuation for a particular trapping feature select **No continuation** for the **Continuation type**. The effect of the traps can also be ramped on using the continuation feature within the trap-assisted recombination feature.

🔍	Solving

DISTRIBUTION

Select a **Distribution** — **User defined** (the default) or **Box**.

IMPURITY

Select an **Impurity type** to give the conductivity type of the selected semiconductor material — **Donor traps** (the default), **Acceptor traps**, **Neutral electron traps**, or **Neutral hole traps**.

📋	The **Impurity type** setting has no effect if a neutral level is used within the Trap-Assisted Recombination feature(s).

For any selection, enter a **Trap density** N_{t0} (SI unit: $1/m^3$). The default value is $1 \times 10^{16} \ 1/cm^3$.

This section is available when **Box** is selected under **Distribution**. See Analytic Doping Model for these settings.

This section is available when **Box** is selected under **Distribution**. Select a **Profile away from uniform region** — **Gaussian** (the default), **Linear**, or **Error function (erf)**.

By default, the **Specify different length scales for each direction** check box is not selected. It is possible to specify a different profile length scales in each coordinate direction when this check box is selected.

Based on the selected profile above, enter one of the following:

- **Decay length** l_d (SI unit: m, default value is 1 μm) (Gaussian profiles).
- **Gradient** N_{grad} (SI unit: $1/\mathrm{m}^4$, default value is -1×10^{20} $1/\mathrm{cm}^4$) (Linear profiles).
- **Argument factor** m (SI unit: $1/\mathrm{m}$, default value is 1 ($1/\mu\mathrm{m}$)) to specify the factor by which the coordinate values are multiplied before being operated on by the `erf()` function (Error function (erf) profiles).

Geometric Trap Density

Use the **Geometric Trap Density** node to specify the density of traps within the domain. This feature enables the trap density to be entered as a function of the distance from selected boundaries. In addition to enabling a fully user-defined trap density to be entered, three preset density profiles are also available. The trap density can be used in conjunction with a Trap-Assisted Recombination feature to specify recombination via trapping sites whose density varies in space. The available options are similar to the Geometric Doping Model feature.

These settings are the same as for Analytic Doping Model.

Select an option from the **Profile away from the boundary** list — **Gaussian** (the default), **Linear**, **Error function (erf)**, or **User defined**.

IMPURITY

Select an **Impurity type** to give the conductivity type of the selected semiconductor material — **Donor traps** (the default), **Acceptor traps**, **Neutral electron traps**, or **Neutral hole traps**.

	The **Impurity type** setting has no effect if a neutral level is used within the Trap-Assisted Recombination feature(s).

For **Gaussian**, **Linear**, or **Error function (erf)** distribution profiles, enter a **Trap density at boundary** N_{t0} (SI unit: $1/m^3$). The default value is 1×10^{16} $1/cm^3$.

For a **User defined** profile, enter a value to **Define profile as a function of the distance, D, from the boundaries** $N(D)$ (SI unit $1/m^3$).

PROFILE

This section is available for **Gaussian**, **Linear**, or **Error function (erf)** distribution profiles. Based on the profile selection enter one of the following:

- **Decay length** l_d (SI unit: m, default value is 1 μm) (Gaussian profiles).
- **Gradient** N_{grad} (SI unit: $1/m^4$, default value is -1×10^{20} $1/cm^4$) (Linear profiles).
- **Argument factor** m (SI unit: $1/m$, default value is 1 ($1/\mu m$)) to specify the factor by which the coordinate values are multiplied before being operated on by the erf() function (Error function (erf) profiles).

Boundary Selection for Trap Density Profile

A default **Boundary Selection for Trap Density Profile** is added to the Geometric Trap Density. This node enables the boundaries from which the distance is calculated to be selected. Any internal or external boundary that bounds, or is within, the domains to which the corresponding **Geometric Trap Density** is applied can be selected.

Trap-Assisted Recombination

	This feature is an expanded version of the original Shockley-Read-Hall Recombination feature, with new options to allow for more detailed modeling of traps.

Use the **Trap-Assisted Recombination** model to set the electron and hole recombination rates in indirect band-gap semiconductors such as silicon under low electric fields. Select this option from the **Generation-Recombination** submenu.

🔍 | Recombination and Generation and Theory for Trap-Assisted Recombination: Shockley-Read-Hall Recombination

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TRAP-ASSISTED RECOMBINATION

Select a **Domain trapping model**:

- **Shockley-Read-Hall model** (the default). This option corresponds to the original Shockley-Read-Hall model for steady state recombination via states located at the midgap.

- **Explicit trap distribution**. This option allows the specification of a number of discrete traps or a continuous density of trap states at energies within the band-gap. Degrees of freedom are added to the equation system to represent the occupancy of traps at a particular energy.

📄 | When **Explicit trap distribution** is selected as the **Domain trapping model**, the Discrete Energy Level (Domains) subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

SHOCKLEY-READ-HALL RECOMBINATION

This section is available when **Shockley-Read-Hall model** is selected as the **Domain trapping model**:

The Shockley-Read-Hall recombination rate is defined as:

$$R_n = R_p = \frac{np - n_{i,mod}^2}{\tau_p(n + n_1) + \tau_n(p + p_1)}$$

with

$$n_{i,mod} = \gamma_n \gamma_p \sqrt{N_{c0}N_{v0}} \exp\left(-\frac{E_g - \Delta E_g}{2V_{th}}\right)$$

$$n_1 = \gamma_n \sqrt{N_{c0} N_{v0}} \exp\left(-\frac{E_g - \Delta E_g}{2 V_{th}}\right) \exp\left(\frac{\Delta E_t}{V_{th}}\right)$$

$$p_1 = \gamma_p \gamma_p \sqrt{N_{c0} N_{v0}} \exp\left(-\frac{E_g - \Delta E_g}{2 V_{th}}\right) \exp\left(\frac{\Delta E_t}{V_{th}}\right)$$

where γ_n and γ_p are the electron and hole degeneracy factors, $N_{c,0}$ and $N_{v,0}$ are the effective densities of states for the conduction and valence band, E_g is the band gap and ΔE_g the band gap narrowing energies (SI unit: V) — scaled by the electron charge, q. $V_{th} = k_B T / q$, where k_B is Boltzmann's constant and T is the temperature. The parameters τ_n and τ_p are carrier lifetimes (SI unit: s) and E_t is the trap energy level (SI unit: V) — scaled by the electron charge.

Enter values for the following:

- The **Electron lifetime, SRH** τ_n (SI unit: s) is taken **From material**. For **User defined** enter a value in the text field. The default is 10 µs.

- The **Hole lifetime, SRH** τ_p (SI unit: s) is taken **From material**. For **User defined** enter a value in the text field. The default is 10 µs.

- Enter a value for **Energy difference between the defect level and the intrinsic level** ΔE_t (SI unit: V) in the text field. The default is 0 V.

TRAPPING

This section is available when **Explicit trap distribution** is selected as the **Domain trapping model**.

By default, **Specify the discrete levels only** is selected. Or select **Specify continuous and/or discrete levels**.

📝	When **Explicit trap distribution** is selected as the **Domain trapping model**, and **Specify continuous and/or discrete levels** is selected above, the Continuous Energy Levels (Domains) subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

For either choice:

- The **Specify trap species** check box is not selected by default. In this case the software does not distinguish between different types of trap and the charge due to the traps is determined by the neutral energy level.

- To set the **Neutral energy level**, select — **Midgap** (the default), **From valence band edge**, **From conduction band edge**, or **Relative**. Then enter the applicable information:

  - **Neutral level for traps** (available when **From valence band edge** or **From conduction band edge** is selected) E_0 (SI unit: V). The default is 0 V.

  - **Neutral level for traps (between 0 and 1, 0.5 is midgap)** (available when **Relative** is selected) E_0 (dimensionless). The default is 0.5.

Discrete Energy Level (Domains)

The **Discrete Energy Level** subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu when **Explicit trap distribution** is selected as the **Domain trapping model** for the Trap-Assisted Recombination node. Use this feature to specify a single discrete energy level for the traps.

TRAP TYPE

This section is available when the **Specify trap species** check box is selected for the parent node. Different trap types have a different charge when they are occupied or unoccupied. Select a **Trap type**:

- **Donor traps**. Neutral when unionized (occupied by electron) and positively charged when ionized (unoccupied by electron).

- **Acceptor traps**. Neutral when unionized (occupied by hole) and negatively charged when ionized (unoccupied by hole, i.e. filled by electron).

- **Neutral electron traps**. Negatively charged when occupied (electron trapped) and neutral when unoccupied (no electron trapped).

- **Neutral hole traps**. Positively charged when occupied (hole trapped) and neutral when unoccupied (no hole trapped).

TRAPS

When there is no **Trap type** defined, enter a **Trap number density** N_t (SI unit: $1/m^3$). The default is 1×10^{12} $1/cm^3$.

When the **Trap type** is defined, enter one of the following:

- **Donor trap density** $N_{t,d}$ (SI unit: $1/m^3$). The default is 1×10^{12} $1/cm^3$.

- **Acceptor trap density** $N_{t,a}$ (SI unit: $1/m^3$). The default is 1×10^{12} $1/cm^3$.
- **Neutral electron trap density** $N_{t,ne}$ (SI unit: $1/m^3$). The default is 1×10^{12} $1/cm^3$.
- **Neutral hole trap density** $N_{t,nh}$ (SI unit: $1/m^3$). The default is 1×10^{12} $1/cm^3$.

For any option, select an **Impurity energy level** — **Midgap** (the default), **From valence band edge**, **From conduction band edge**, or **Relative**. Then enter the applicable information:

- **Impurity energy level** (available when **From valence band edge** or **From conduction band edge** is selected) $E_{t,0}$ (SI unit: V). The default is 0 V.
- **Impurity energy level (between 0 and 1, 0 being the valence band)** (available when **Relative** is selected) $E_{t,0}$ (dimensionless). The default is 0.5.

Enter the **Ground-state degeneracy factor** g_d (dimensionless). The default is 1.

Enter the **Trap occupancy initial value** $f_{t,\text{init}}$ (dimensionless). The default is 0.5.

CARRIER CAPTURE

Choose how to define the **Probability of electron capture** (C_n) — **From cross section** (the default) or **User defined**.

- For **From cross section**, enter an **Averaged cross section for electron capture** $<\sigma_n>$ (SI unit: m^2; the default is 1×10^{18} $1/cm^2$) and **Electron thermal velocity** V^{th}_n (SI unit: m/s; the default is 1.562×10^7 m/s).
- For **User defined**, enter C_n (SI unit: m^3/s). The default is 2.042×10^{-11} cm^3/s.

Define the **Probability of hole capture** (C_p) — **From cross section** (the default) or **User defined**.

- For **From cross section**, enter an **Averaged cross section for hole capture** $<\sigma_p>$ (SI unit: m^2; the default is 1×10^{18} $1/cm^2$) and **Hole thermal velocity** V^{th}_p (SI unit: m/s; the default is 1.562×10^7 m/s).
- For **User defined** enter C_p (SI unit: m^3/s). The default is 1.562×10^{-11} cm^3/s.

Continuous Energy Levels (Domains)

The **Continuous Energy Level** subnode is available from the context menu (right-click the Trap-Assisted Recombination parent node) or from the **Physics** toolbar, **Attributes** menu when **Explicit trap distribution** is selected as the **Domain trapping model**, and **Specify continuous and/or discrete levels** is selected under Trapping. Use this node to define a density of trap states.

This section is available when the **Specify trap species** check box is selected for the parent node. See Discrete Energy Level (Domains).

TRAPS

Select a **Trap density distribution** — **Gaussian** (the default), **Rectangle**, **Exponential**, or **User defined**. Then enter the applicable information:

- **Width** (for Gaussian distribution) σ (SI unit: V). The default is 0.333 V.

- **Width** (for rectangle distribution) E_{width} (SI unit: V). The default is 0 V.

- **Size of transition zone** (for rectangle distribution) ΔE_{tran} (SI unit: V). The default is 0.05 V. This value determines the width of the smoothing employed on the step function for the rectangle distribution.

- **Damping coefficient** (for exponential distribution) d (SI unit: V). The default is 0.1 V.

- **Density of trap states** (for user defined) $g_{t(E)}$ (SI unit: $s^3 \cdot A/(m^5 \cdot kg)$). The default is $0\ s^3 \cdot A/(m^5 \cdot kg)$.

Enter a **Trap number density** N_t (SI unit: $1/m^3$). The default is $1 \times 10^{12}\ 1/cm^3$.

When the **Trap type** is defined, enter one of the following:

- **Donor trap density** $N_{t,d}$ (SI unit: $1/m^3$). The default is $1 \times 10^{12}\ 1/cm^3$.

- **Acceptor trap density** $N_{t,a}$ (SI unit: $1/m^3$). The default is $1 \times 10^{12}\ 1/cm^3$.

- **Neutral electron trap density** $N_{t,ne}$ (SI unit: $1/m^3$). The default is $1 \times 10^{12}\ 1/cm^3$.

- **Neutral hole trap density** $N_{t,nh}$ (SI unit: $1/m^3$). The default is $1 \times 10^{12}\ 1/cm^3$.

This quantity represents the total trap density, or the integrated density of states:

$$N_t = \int_{E_{t,min}}^{E_{t,max}} g_t(E)dE$$

where $g(E)$ is the density of trap states, and $E_{t,\min}$ and $E_{t,\max}$ define the range of the energy (see user inputs below), with the default being the energy levels corresponding to the conduction and valence band edges in the absence of band gap narrowing. The energy range is truncated within the default range so that there is no trap level within the conduction band or the valence band.

Select a **Distribution center point** — **Midgap** (the default), **From valence band edge**, **From conduction band edge**, or **Relative**. Then enter the applicable information:

- **Distribution center point** $E_{t,0}$ (SI unit: V). The default is 0 V.

- **Distribution center point (between 0 and 1, 0 being the valence band)** $E_{t,0}$ (dimensionless). The default is 0.5.

Enter the **Ground-state degeneracy factor** g_d (dimensionless). The default is 1.

Enter the **Trap occupancy initial value** $f_{t,\text{init}}$ (dimensionless). The default is 0.5.

Enter the **Continuous energy discretization, number of mesh points** N^{xd}_{elem} (dimensionless). The default is 25.

Enter the **Continuous energy discretization, min energy** $E_{t,\text{min}}$ (SI unit: V). The default is semi.Ev0, the valence band edge in the absence of band gap narrowing.

Enter the **Continuous energy discretization, max energy** $E_{t,\text{max}}$ (SI unit: V). The default is semi.Ec0, the conduction band edge in the absence of band gap narrowing.

CARRIER CAPTURE

These settings are the same as for Discrete Energy Level (Domains).

Auger Recombination

Use the **Auger Recombination** model to set the electron and hole recombination rates at high nonequilibrium carrier densities in semiconducting materials. Select this option from the **Generation-Recombination** submenu.

   🔍   Recombination and Generation and Theory for Auger Recombination

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The Auger recombination rate is defined as:

$$R_n = R_p = (C_n n + C_p p)(np - n_{i,\text{mod}}^2)$$

with

$$n_{i,\text{mod}} = \gamma_n \gamma_p \sqrt{N_{c0} N_{v0}} \exp\left(-\frac{E_g - \Delta E_g}{2V_{th}}\right)$$

where γ_n and γ_p are the electron and hole degeneracy factors, $N_{c,0}$ and $N_{v,0}$ are the effective densities of states for the conduction and valence band, E_g is the band-gap (SI unit: V), and ΔE_g the band gap narrowing (SI unit: V). The parameters C_n and C_p are material constants (SI unit: m^6/s).

AUGER RECOMBINATION

The electron lifetime **Auger recombination factor, electron**s C_n (SI unit: m^6/s) is taken **From material**. For **User defined**, enter a value in the text field, the default value is for silicon, 2.8e-31 cm^6/s.

The electron lifetime **Auger recombination factor, holes** C_p (SI unit: m^6/s) is taken **From material**. For **User defined**, enter a value in the text field, the default value is for silicon, 9.9e-32 cm^6/s.

Direct Recombination

Use the **Direct Recombination** to set the recombination rate in direct band-gap semiconductor materials such as gallium arsenide. Select this option from the **Generation-Recombination** submenu.

🔍	Recombination and Generation and Theory for the Direct Recombination Feature

The recombination rate for both electrons and holes is set using the following equation:

$$R_n = R_p = C(np - n_{i,mod}^2)$$

with

$$n_{i,mod} = \gamma_n \gamma_p \sqrt{N_{c0} N_{v0}} \exp\left(-\frac{E_g - \Delta E_g}{2V_{th}}\right)$$

where γ_n and γ_p are the electron and hole degeneracy factors, $N_{c,0}$ and $N_{v,0}$ are the effective densities of states for the conduction and valence band, E_g is the band-gap and ΔE_g the band-gap narrowing (SI unit: V).

DIRECT RECOMBINATION

The default **Direct recombination factor** C (SI unit: m^3/s) is taken **From material**. For **User defined** enter a value in the text field. The default value is $0\ m^3/s$.

Impact Ionization Generation

Impact Ionization Generation occurs when, for example, an energetic electron undergoes a collision in which it loses sufficient energy to promote an electron in the valence band to the conduction band, resulting in an additional electron hole pair being produced. It is the mechanism responsible for avalanche breakdown. Select this option from the **Generation-Recombination** submenu.

Recombination and Generation and Theory for Impact Ionization

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The carrier generation rate due to impact ionization is given by:

$$R_n^{II} = R_p^{II} = -\frac{\alpha_n}{q}|\mathbf{J}_n| - \frac{\alpha_p}{q}|\mathbf{J}_p|$$

The values of α_n and α_p can be user-defined or can be related to the material properties in the following manner:

$$\alpha_n = a_n(1 + c_n(T - T_{ref}))E_{||,n}\exp\left(-\left(\frac{b_n(1 + d_n(T - T_{ref}))}{E_{||,n}}\right)^2\right)$$

$$\alpha_p = a_p(1 + c_p(T - T_{ref}))E_{||,p}\exp\left(-\left(\frac{b_p(1 + d_p(T - T_{ref}))}{E_{||,p}}\right)^2\right)$$

where $E_{||,n}$ and $E_{||,p}$ are the components of the electric field parallel to the electron and hole currents respectively and T_{ref}, a_n, a_p, b_n, b_p, d_n, and d_p are material properties.

IMPACT IONIZATION GENERATION

The default **Impact Ionization model** is **Okuto-Crowell model**. For **User defined**, enter a desired value or expression in the input field for the values of α_n and α_p.

For the **Okuto-Crowell model**, the default **Temperature reference** T_{ref} is 300 K.

For the **Okuto-Crowell model**, the defaults for the following are all taken **From material**. For **User defined**, enter a different value or expression in the text field.

- **a factor, electrons, impact ionization** a_n (SI unit: 1/V). The default is 0.426 (1/V).
- **a factor, holes, impact ionization** a_p (SI unit: 1/V). The default is 0.243 (1/V).
- **b factor, electrons, impact ionization** b_n (SI unit: V/m). The default is 4.81×10^5 V/cm.
- **b factor, holes, impact ionization** b_p (SI unit: V/m). The default is 6.53×10^5 V/cm.
- **c factor, electrons, impact ionization** c_n (SI unit: 1/K). The default is 3.05×10^{-4} (1/K).
- **c factor, holes, impact ionization** c_p (SI unit: 1/K). The default is 5.35×10^{-4} (1/K).
- **d factor, electrons, impact ionization** d_n (SI unit: 1/K). The default is 6.86×10^{-4} (1/K).
- **d factor, holes, impact ionization** d_p (SI unit: 1/K). The default is 5.67×10^{-4} (1/K).

User-Defined Recombination

Use the **User-Defined Recombination** feature to manually set a recombination rate for electrons and holes in the semiconducting material. Select this option from the **Generation-Recombination** submenu.

USER DEFINED RECOMBINATION

Enter the following recombination rates:

- **User-defined recombination rate, electrons** $R_{n,0}$ (SI unit: $1/(m^3 s)$).
- **User-defined recombination rate, holes** $R_{p,0}$ (SI unit: $1/(m^3 s)$).

🔍   Recombination and Generation and User-Defined Recombination

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User-Defined Generation

Use the **User-Defined Generation** feature to manually set a generation rate for electrons and holes in the semiconducting material. Select this option from the **Generation-Recombination** submenu.

Enter the following generation rates:

- **User-defined generation rate, electrons** $G_{n,0}$ (SI unit: $1/(m^3s)$).

- **User-defined generation rate, holes** $G_{p,0}$ (SI unit: $1/(m^3s)$).

🔍	Recombination and Generation and User-Defined Generation

Metal Contact

The **Metal Contact** node is used for modeling metal-semiconductor contacts.

The **Harmonic Perturbation** subnode (it is of the exclusive type) is available from the context menu (right-click the parent node) or on the **Physics** toolbar, click the **Attributes** menu and select **Harmonic Perturbation**.

TERMINAL

Specify the terminal properties. To indicate which boundaries belong to the same terminal, enter the same name in the **Terminal name** field. The **Terminal name** should be numeric for sweeps to work properly.

Select a **Terminal type** — **Voltage** (the default), **Current**, or **Circuit**. Select:

- **Voltage** to enter an electric potential V_0 (SI unit: V). The default is 0 V.

- **Current** to enter a current I_0 (SI unit: A). The default is zero current, corresponding to an open circuit.

- **Circuit (current)** to specify a terminal connected to an external circuit, where the external circuit acts as a current source for the semiconductor model.

- **Circuit (voltage)** to specify a terminal connected to an external circuit, where the external circuit acts as a voltage source for the semiconductor model.

- **Power** to enter a current P_0 (SI unit: W). The default is zero power, corresponding to an open circuit.

Select a **Type** — **Ideal ohmic** (the default) or **Ideal Schottky**.

- Use the **Ideal ohmic** option for a nonrectifying metal-semiconductor junction, that is a contact with negligible resistance relative to the total resistance of the modeled semiconductor device.

- Use the **Ideal Schottky** option for a simple rectifying metal-semiconductor junction, that is, when the current-voltage characteristics at the interface depend on the potential barrier formed at the junction. For this option, surface recombination effects and surface charge densities associated with surface traps can be included in the model by adding Trap-Assisted Surface Recombination boundary conditions to the same boundary selection as the Metal Contact boundary condition.

CONTACT PROPERTIES

This section is available if **Ideal Schottky** is selected as the contact **Type**.

Choose between an **Ideal** (the default) and **User defined** definition of the **Barrier height**.

For the **Ideal** barrier height, the default **Metal work function** Φ (SI unit: V) is 4.5 V. The metal work function is the difference in energy between the vacuum level and the conduction band at equilibrium in the metal in contact with the semiconductor. The ideal barrier height is given by the difference between the metal work function and the electron affinity of the semiconductor.

For the **User defined** barrier height, enter a value for the **Barrier height** Φ_B (SI unit: V). In this case, the metal work function is not used.

THERMIONIC CURRENTS

This section is available if **Ideal Schottky** is selected as the contact **Type**.

Select the **Thermionic currents** — **Richardson's coefficients** (the default) or **Surface recombination velocities**.

For **Richardson's coefficients** enter an:

- **Effective Richardson constant for electrons** $A_n{}^\star$ (SI unit: A/(m^2·K^2)). The default constant is 110 A/(K·cm)^2 for silicon.

- **Effective Richardson constant for holes** $A_p{}^\star$ (SI unit: A/(m^2·K^2)). The default constant is 90 A/(K·cm)^2 for silicon.

For **Surface recombination velocities** enter a:

- **Surface recombination velocity, electrons** $V_{s,n}$ (SI unit: m/s). The default is 21605 m/s for silicon.

- **Surface recombination velocity, holes** $V_{s,p}$ (SI unit: m/s). The default is 19006 m/s for silicon.

EXTRA CURRENT CONTRIBUTION

This section is available if **Ideal Schottky** is selected as the contact **Type**.

The settings are the same as described in this section Extra Current Contribution.

CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.

Q	• Boundary Conditions and Metal Contacts
	• Small-Signal Analysis
	• Harmonic Perturbation, Prestressed Analysis, and Small-Signal Analysis in the *COMSOL Multiphysics Reference Manual*.

Thin Insulator Gate

Use the **Thin Insulator Gate** node to model a thin insulating material between the semiconductor and a metal. The layer has the thickness d_{ins} and the relative permittivity ε_{ins}. The indices ins and s refer r to the insulator and semiconductor side of the boundary, respectively.

The **Harmonic Perturbation** subnode (it is of the exclusive type) is available from the context menu (right-click the parent node) or on the **Physics** toolbar, click the **Attributes** menu and select **Harmonic Perturbation**.

Q	• Small-Signal Analysis
	• Harmonic Perturbation — Exclusive and Contributing Nodes in the *COMSOL Multiphysics Reference Manual*.

These settings are the same as for Fletcher Mobility Model (C).

🔍	Solving

TERMINAL

Specify the terminal properties. To indicate which boundaries belong to the same terminal, enter the same name in the **Terminal name** field. The **Terminal name** should be numeric for sweeps to work properly.

Select a **Terminal type** — **Voltage** (the default), **Charge**, or **Circuit**. Select:

- **Voltage** to enter an electric potential V_0 (SI unit: V). The default is 0 V.
- **Charge** to specify a charge Q_0 (SI unit: C). This is the charge on the contact side of the parallel plate capacitor. The default is 0 V.
- **Circuit** to specify a terminal connected to an external circuit.

❗	It is important to realize that the **Charge** setting does not specify an interface charge at the boundary between the semiconductor and the insulator—it specifies the charge on the top conductor of the gate capacitor.

GATE CONTACT

Specify the insulator dimensions and permittivity as well as the metal work function.

- **Oxide relative permittivity** ε_{ins} (dimensionless). The default relative permittivity is 1.
- **Oxide thickness** d_{ins} (SI unit: m). The default thickness is 0.1 μm.
- **Metal work function** Φ (SI unit: V). The default barrier height is 4.1 V. The metal work function is the difference in energy between the vacuum level and the conduction band at equilibrium in the metal in contact with the semiconductor.

📑	The functionality of the **Surface traps** check box in versions prior to 5.4 has been replaced and expanded by the Trap-Assisted Surface Recombination boundary condition.

- Boundary Conditions and Thin Insulating Gates
- Harmonic Perturbation, Prestressed Analysis, and Small-Signal Analysis in the *COMSOL Multiphysics Reference Manual*.

Trap-Assisted Surface Recombination

The **Trap-Assisted Surface Recombination** boundary condition adds contributions to the surface recombination rate or the surface charge density associated with the surface traps for the following boundary conditions: Insulation, Thin Insulator Gate, Insulator Interface, and Metal Contact (**Ideal Schottky** type only). This feature replaces and expands the functionality of the **Surface traps** check box seen in versions prior to 5.4. Both the **Shockley-Read-Hall model** and the **Explicit trap distribution** options are available. All the settings are the same as its domain condition counterpart Trap-Assisted Recombination.

Discrete Energy Level (Boundaries)

The **Discrete Energy Level** subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu when the **Trapping model** drop-down menu is set to the **Explicit trap distribution** option for the Trap-Assisted Surface Recombination boundary condition.

	The settings for this node are the same as for Discrete Energy Level (Domains). The only difference is that the units for **Trap number density** are $1/m^2$ instead of $1/m^3$.

Continuous Energy Levels (Boundaries)

The **Continuous Energy Level** subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu when the **Trapping model**

drop-down menu is set to the **Explicit trap distribution** option for the Trap-Assisted Surface Recombination boundary condition.

📝 The settings for this node are the same as for Continuous Energy Levels (Domains). The only difference is that the units for **Trap number density** are $1/m^2$ instead of $1/m^3$.

Floating Gate

Use the **Floating Gate** feature to model a gate contact to a dielectric domain (not a semiconductor domain), which is unconnected to any voltage source, or which is connected to a circuit with a floating potential.

In combination with the Insulator Interface feature that connects the dielectric domain and an adjacent semiconductor domain, the Floating Gate can model both the charging and discharging of a floating gate by tunneling from the semiconductor domain through the dielectric domain.

Add this feature from the boundary level **Electrostatics** submenu.

FLOATING GATE

Select an **External connection** — **None** (the default) or **Circuit** (to connect the terminal to an electrical circuit).

Select a **Tunnel current** I_{tun} (SI unit: A) from the list — **None**, **User defined**, or choose a tunnel current announced by one of the **Insulator Tunneling** features in the model. Current injected into the gate accumulates as charge.

Enter a **Contact work function** Φ_c (SI unit: V).

Use the **Initial charge** Q_{init} (SI unit: C) setting to determine the initial charge on the gate in a transient simulation, or the charge on the gate in a stationary simulation.

Insulator Interface

The **Insulator Interface** feature is automatically applied to the boundaries at the interface between Semiconductor Material Model domains and **Charge Conservation**

(dielectric) domains. A number of options are available to modify the behavior of the boundary.

> The functionality of the **Surface traps** check box in versions prior to 5.4 has been replaced and expanded by the Trap-Assisted Surface Recombination boundary condition.

TUNNELING

Select a **Tunneling type** — **None** (the default), **Fowler-Nordheim tunneling**, or **User defined**.

FOWLER-NORDHEIM TUNNELING

In combination with the Floating Gate feature, use this option to model both the charging and discharging of a floating gate by Fowler-Nordheim tunneling from the domain.

For **Fowler-Nordheim tunneling**, select an option from the **Fowler-Nordheim tunneling** list — **Electrons** (the default), **Holes**, or **Electrons and holes**. This determines the species for which the tunnel current is computed. Based on this selection, enter:

- **Electron Fowler-Nordheim coefficients** A^n_{FN} (SI unit: A/V^2) and B^n_{FN} (SI unit: V/m).
- **Hole Fowler-Nordheim coefficients** A^p_{FN} (SI unit: A/V^2) and B^p_{FN} (SI unit: V/m).

USER DEFINED TUNNELING

For **User defined**, enter an **Electron tunnel current density** J^n_{UD} (SI unit: A/m^2). Enter a **Hole tunnel current density** J^p_{UD} (SI unit: A/m^2) to define a user defined tunnel current expression.

Theory for the Semiconductor Interface

Detailed introductions to the physics of semiconductors are available in Refs 1 to 5. Ref. 6 is an introduction to semiconductor device modeling using the drift-diffusion method used by COMSOL Multiphysics. A brief summary of the physics of semiconductors is included here, to a level sufficient to derive the drift-diffusion equations and to develop a basic understanding of semiconductor band structures.

To completely describe the dynamics of electrons within a solid, the *many body Schrödinger equation* must be solved in the periodic structure defined by the crystal structure of the solid. In practice this is not possible and approximations must be made. Solid state physicists have devised a number of methods to solve simplified forms of this equation and these methods have been validated through experiment (see, for example, chapters 9 to 11 of Ref. 1 and chapters 4 and 5 of Ref. 2). A starting point for many of these methods is to consider only the motion of the electrons through an essentially stationary lattice of nuclei (known as the *adiabatic approximation*). Then the *many electron wave function* is simplified into a form in which it reduces to a set of *one electron wave functions*. The effect of the nuclei and of electron-electron interactions can be incorporated into these one electron models by modifications to the effective potential. Models within the so-called one-electron approximation have been very successful at predicting the properties of semiconductors and semiconductor transport. Although the one electron model explained in this section seems very simplistic (particularly when considering the complexity of electron-electron and electron-ion interactions), in practice this model can be used to develop a very detailed understanding of transport in semiconductors.

In this section:

🔍 Modeling Guidelines

The Sommerfeld Model and the Density of States

Sommerfeld was the first person to successfully apply quantum mechanics to the physics of transport in solids. The Sommerfeld model considers the physics of independent electrons in a large potential well. The starting point for this model is the time-independent Schrödinger equation for an independent electron:

$$-\frac{\hbar}{2m}\nabla^2\psi = E\psi \tag{3-1}$$

where $\hbar$ is Planck's constant divided by 2π and m is the electron mass. The time-independent Schrödinger equation takes the form of an eigenvalue equation. The modulus squared of the (complex) eigenfunctions (ψ) or wave functions that solve the equation represent the probability that an electron in the corresponding state can be found at a given position $p(\mathbf{r})$ (that is, $p(\mathbf{r}) = |\psi|^2$). The corresponding eigenvalue E

for the state gives the energy associated with the state. For a detailed introduction to quantum mechanics see Ref. 7 and Ref. 8.

Since it is expected that the solid is periodic, the equation is solved on a cube of side L assuming the periodic boundary condition:

$$\psi(x + L, y + L, z + L) \ = \ \psi(x, y, z) \tag{3-2}$$

The solutions of Equation 3-1 and Equation 3-2 are plane waves of the form:

$$\psi(x, y, z) \ = \ \frac{1}{\Omega^{1/2}} \exp(i[k_x x + k_y y + k_z z]) \tag{3-3}$$

where $\Omega = L^3$ is the volume of the solid (which appears in the equation to correctly normalize the wave function) and:

$$k_x \ = \ \frac{2\pi n_x}{L}$$

$$k_y \ = \ \frac{2\pi n_y}{L}$$

$$k_z \ = \ \frac{2\pi n_z}{L}$$

where n_x, n_y, and n_z are integers.

Since these states are all periodic, it is convenient to label them by means of the wave number **k**. Think of a *k-space* populated by these states in a regular cubic grid. As a consequence of the *Pauli exclusion principle* each state can hold two electrons (one spin up and one spin down).

The *density of states* $(g(\mathbf{k}) = dn_s/d\xi_{\mathbf{k}})$, that is, the number of states (n_s) per unit volume of k-space $(\xi_{\mathbf{k}})$ for unit volume of the material, is given by:

$$g(\mathbf{k}) \ = \ \frac{1}{4\pi^3}$$

Substituting Equation 3-3 into Equation 3-1 gives the energy of the particle in a given state:

$$E_{\mathbf{k}} \ = \ \frac{\hbar^2 (k_x^2 + k_y^2 + k_z^2)}{2m} \ = \ \frac{\hbar^2 k^2}{2m} \tag{3-4}$$

At zero temperature electrons fill up the states with the lowest energy first, filling the grid so as to minimize the total energy. The surface dividing the filled states from the empty states — known as the *Fermi surface* — is spherical for large numbers of electrons as a result of Equation 3-4. For an electron number density n at zero temperature the magnitude of the wave vector corresponding to the states at the Fermi surface $(k_{F,0})$ is given by:

$$\frac{4}{3}\pi k_{F,0}^3 = \frac{n}{g(\mathbf{k})} = 4\pi^3 n$$

so that:

$$k_{F,0} = (3\pi^2 n)^{1/3}$$

At finite temperatures and at equilibrium, the principles of statistical mechanics (see for example Ref. 10) give the mean occupancy of the states $(f_0(\mathbf{k}))$ as:

$$f_0(\mathbf{k}) = \frac{1}{1 + \exp[(E_{\mathbf{k}} - E_F)/(k_B T)]} \tag{3-5}$$

where E_F is the Fermi energy or the chemical potential. At finite temperatures E_F is determined by the requirement that the total number of electrons per unit volume is equal to n:

$$n = \int_0^\infty f_0(\mathbf{k})g(E)dE = \int_0^\infty \frac{g(E)}{1 + \exp[(E_{\mathbf{k}} - E_F)/(k_B T)]}dE \tag{3-6}$$

where $g(E) = dn_s/dE$ is the energy density of states, given by:

$$g(E)dE = g(\mathbf{k})d\xi_{\mathbf{k}} = \frac{k^2}{\pi^2}\frac{dk}{dE}dE = \frac{mk}{\pi^2 \hbar^2}dE = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}E^{1/2}dE \tag{3-7}$$

In deriving Equation 3-7, the *E-k* relationship (Equation 3-4) was used to evaluate the derivative and to convert from $\mathbf{k}$ to E.

📝 The density of states varies with the square root of the energy.

These results form the basis of the Sommerfeld model and are useful in this discussion. Using this simple model, you can predict the thermal and electrical properties of some metals with reasonable accuracy (see Ref. 1 and Ref. 2 for details). However, the

model does not explain the existence of *insulators* or semiconductors because it is missing important information about the microscopic periodicity of the material. The Effect of Periodicity section describes how this periodicity can be treated.

The Effect of Periodicity

THE LATTICE AND THE RECIPROCAL LATTICE

The 3D periodicity of crystalline materials is conventionally described by a set of lattice vectors and a basis (a specific pattern of atoms) associated with each lattice point. Consider the case of a "primitive lattice", that is, a crystal made up of a single atom, where the atomic locations are coincident with the lattice points. Such a lattice does not require a basis (or more formally the basis is a single atom located at $(0,0,0)$). The set of lattice vectors $\mathbf{R}$ can be written as:

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \tag{3-8}$$

where n_1, n_2, and n_3 are integers (taking all values between $-\infty$ and ∞) and $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are the lattice vectors. For a primitive lattice, the unit cell is the parallelepiped constructed from the vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$.

A useful way to represent the lattice is by means of an array of delta functions. A physical quantity of interest (for example the electric potential) can then be represented by the convolution of the variation in the potential within a single unit cell of the lattice with the delta function array. This approach is easiest to understand in 1D, when the delta function array is known as a *Dirac comb*. A 1D lattice can be represented as:

$$\sum_{n = -\infty}^{n = \infty} \delta(x - na)$$

where a is the lattice parameter. This periodic function can be represented by a Fourier series of the form:

$$\sum_{n = -\infty}^{n = \infty} \delta(x - na) = \sum_{n = -\infty}^{n = \infty} \frac{1}{a}e^{2\pi inx/a} \tag{3-9}$$

Of particular importance to understand semiconductor transport is the concept of the *reciprocal lattice*. This is the lattice produced by taking the Fourier transform of the real space lattice. For the Dirac comb this is given by:

$$FT\left\{\sum_{n=-\infty}^{n=\infty} \delta(x - na)\right\} = \sum_{n=-\infty}^{n=\infty} \int \delta(x - na)e^{ikx}dx = \sum_{n=-\infty}^{n=\infty} e^{ikna}$$

$$= \sum_{n=-\infty}^{n=\infty} \frac{2\pi}{a}\delta\left(k - \frac{2\pi n}{a}\right)$$

where the final step follows from Equation 3-9. The reciprocal lattice is another Dirac comb with spacing proportional to the reciprocal of the real space lattice.

In 3D the lattice can be represented as $\delta(\mathbf{r}-\mathbf{R})$ where the summation over all combinations of lattice vectors is implied by the use of the set of vectors $\mathbf{R}$. The Fourier transform of the lattice is:

$$FT\left\{\sum_{n=-\infty}^{n=\infty} \delta(\mathbf{r} - \mathbf{R})\right\} = \int \delta(\mathbf{r} - \mathbf{R})e^{i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r} = e^{i\mathbf{k}\cdot\mathbf{R}}$$

$$= \frac{(2\pi)^3}{\Omega}\delta(\mathbf{k} - \mathbf{K}^*)$$

where Ω is the volume of the real space unit cell ($\Omega = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$) and $\mathbf{K}^*$ is the set of reciprocal lattice vectors given by:

$$\mathbf{K}^* = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3$$

where n_1, n_2, and n_3 are integers (taking all values between $-\infty$ and ∞) and $\mathbf{b}_1, \mathbf{b}_2$, and $\mathbf{b}_3$ are the reciprocal lattice vectors given by:

$$\mathbf{b}_1 = \frac{2\pi}{\Omega}\mathbf{a}_2 \times \mathbf{a}_3$$

$$\mathbf{b}_2 = \frac{2\pi}{\Omega}\mathbf{a}_3 \times \mathbf{a}_1 \qquad\qquad (3\text{-}10)$$

$$\mathbf{b}_3 = \frac{2\pi}{\Omega}\mathbf{a}_1 \times \mathbf{a}_2$$

Understanding the reciprocal lattice in terms of Fourier transforms as described above is useful. The Heisenberg uncertainty principle can be seen to be related to the properties of the Fourier transform (in the time domain: $\Delta f \Delta t \approx 1$). Also the effect of a lattice basis can be straightforwardly introduced by taking the convolution of the basis with the lattice in real space. The convolution theorem then tells us that the result in reciprocal space (or k-space) is the product of the reciprocal lattice and the Fourier transform of the basis. The main effect of the basis is to modulate the amplitude (and phase) of the reciprocal lattice points. When zeros in the Fourier transform of the basis coincide with reciprocal lattice points, the basis leads to the elimination of these points in the reciprocal lattice. In X-ray imaging experiments, which sample the reciprocal lattice by crystal diffraction, this is referred to as *extinction*.

Importantly, any physical quantity with a periodicity that matches that of the lattice can straightforwardly be represented as the convolution of some function with the reciprocal lattice in real space, or as a modulating function for the reciprocal lattice in k-space, changing the amplitudes of each of the lattice points in k-space. Since each of these points represents a single harmonic component of the quantity of interest this construction can be thought of as a representation of a three dimensional Fourier series. For example, consider a periodic potential $V(\mathbf{r}) = V(\mathbf{r} + \mathbf{R})$. $V(\mathbf{r})$, which can be written in the form:

$$V(\mathbf{r}) = \sum_{\mathbf{K}^*} V_{\mathbf{K}^*} e^{-i\mathbf{K}^* \cdot \mathbf{r}} \tag{3-11}$$

where the summation occurs over all the reciprocal lattice vectors $\mathbf{K}^*$. The reciprocal lattice is therefore a representation of the Fourier components required in 3D to represent a function with the periodicity of the lattice.

BLOCH FUNCTIONS

The Sommerfeld model did not attempt to include the effective electric potential of the crystal or the other electrons. It is clear that the effective potential must be periodic with the same periodicity as the crystal lattice. The periodicity of the lattice has important consequences for the electrons. First, since the problem has periodic symmetry, observable physical quantities must also have periodic symmetry. As a consequence $|\psi|$ must be periodic, so that, using the notation developed previously:

$$|\psi(\mathbf{r} + \mathbf{R})| = |\psi(\mathbf{r})|$$

equivalently:

$$\psi(\mathbf{r} + \mathbf{R}) = \psi(\mathbf{r})e^{i\theta(\mathbf{R})} \tag{3-12}$$

The translational symmetry of the lattice imposes additional restrictions on the form of $\theta(\mathbf{R})$. For two lattice vectors, $\mathbf{R}_A$ and $\mathbf{R}_A + \mathbf{R}_B$, translational symmetry implies:

$$\theta(\mathbf{R}_A + \mathbf{R}_B) - \theta(\mathbf{R}_A) = \theta(\mathbf{R}_B)$$

which leads to the requirement that θ depends linearly on the three integers, n_1, n_2, and n_3, which specify $\mathbf{R}$ (see Equation 3-8):

$$\theta(\mathbf{R}_A + \mathbf{R}_B) = \theta(\mathbf{R}_A) + \theta(\mathbf{R}_B)$$

θ can therefore be written in the form:

$$\theta = n_1 c_1 + n_2 c_2 + n_3 c_3$$

for constants c_1, c_2, and c_3. Writing $\mathbf{k} = c_1 \mathbf{b}_1 + c_2 \mathbf{b}_1 + c_3 \mathbf{b}_1$ leads to the requirement $\theta = \mathbf{k} \cdot \mathbf{R}$ and Equation 3-12 then becomes:

$$\psi(\mathbf{r} + \mathbf{R}) = \psi(\mathbf{r})e^{i\mathbf{k} \cdot \mathbf{R}} \tag{3-13}$$

If $\psi(\mathbf{r})$ is written in the form:

$$\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k} \cdot \mathbf{r}} \tag{3-14}$$

substituting into Equation 3-13 shows that $u_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{\mathbf{k}}(\mathbf{r})$. Equation 3-14, along with the periodicity requirement on $u_{\mathbf{k}}(\mathbf{r})$, is known as *Bloch's theorem*. It is extremely useful as it allows the wave function corresponding to a particular $\mathbf{k}$ vector to be expanded in a Fourier series of the same form as that of the potential (Equation 3-11):

$$u_{\mathbf{k}} = \sum_{\mathbf{K}} C_{\mathbf{K}} e^{-i\mathbf{K} \cdot \mathbf{r}}$$

Wave functions which satisfy Bloch's theorem are frequently referred to as *Bloch functions*.

INDEPENDENT ELECTRONS IN A PERIODIC POTENTIAL

The time-independent Schrödinger equation can now be written using the periodic expansion for both the potential and the *Bloch wave function*:

$$\frac{\hbar^2}{2m}\nabla^2\sum_{\mathbf{K}}C_{\mathbf{K}}e^{i(\mathbf{k}-\mathbf{K})\cdot\mathbf{r}} + \left(\sum_{\mathbf{G}}V_{\mathbf{G}}e^{-i\mathbf{G}\cdot\mathbf{r}}\right)\left(\sum_{\mathbf{K}}C_{\mathbf{K}}e^{i(\mathbf{k}-\mathbf{K})\cdot\mathbf{r}}\right)$$

$$= E\sum_{\mathbf{K}}C_{\mathbf{K}}e^{i(\mathbf{k}-\mathbf{K})\cdot\mathbf{r}}$$

where $\mathbf{G}$ is used for the potential reciprocal lattice vector to distinguish it from $\mathbf{K}$. Simplifying this equation gives:

$$\frac{\hbar^2}{2m}\sum_{\mathbf{K}}C_{\mathbf{K}}(\mathbf{k}-\mathbf{K})^2 e^{-i\mathbf{K}\cdot\mathbf{r}} + \sum_{\mathbf{G},\mathbf{K}}V_{\mathbf{G}}C_{\mathbf{K}}e^{-i(\mathbf{G}+\mathbf{K})\cdot\mathbf{r}}$$

$$= E\sum_{\mathbf{K}}C_{\mathbf{K}}e^{-i\mathbf{K}\cdot\mathbf{r}}$$

To obtain the equation for the coefficients of the sum, premultiply the sum by

$$e^{i\mathbf{K}'\cdot\mathbf{r}}$$

and integrate over all space. This gives:

$$\frac{\hbar^2}{2m}C_{\mathbf{K}'}(\mathbf{k}-\mathbf{K}')^2 + \sum_{\mathbf{G}}V_{\mathbf{G}}C_{\mathbf{K}'-\mathbf{G}} = EC_{\mathbf{K}'} \qquad (3\text{-}15)$$

Equation 3-15 is valid for any periodic potential, small or large.

THE NEARLY FREE ELECTRON MODEL

To obtain the small potential limit of Equation 3-15, consider the case of a single sinusoidal potential component with a small amplitude:

$$V(\mathbf{r}) = 2V_1\cos(\mathbf{K}_1\cdot\mathbf{R}) = V_1(e^{i\mathbf{K}_1\cdot\mathbf{R}} + e^{-i\mathbf{K}_1\cdot\mathbf{R}})$$

Since the periodicity of the potential is one dimensional, it is only necessary to consider Fourier components in the direction of $\mathbf{K}_1$ in the expansion of $u_{\mathbf{k}}(\mathbf{r})$, which can therefore be written in the form:

$$u_{\mathbf{k}} = \sum_{p}C_p e^{-ip\mathbf{K}_1\cdot\mathbf{r}}$$

and Equation 3-15 takes the form:

$$\frac{\hbar^2}{2m}C_p(\mathbf{k}-p\mathbf{K}_1)^2 + V_1(C_{p-1}+C_{p+1}) = EC_p \qquad (3\text{-}16)$$

In the limit $V_1 = 0$, $p = 0$, and Equation 3-16 recovers the form of the Sommerfeld E-k relationship, Equation 3-4. However, for $V_1 = 0$, additional solutions now also exist for nonzero values of p, which take the form of a set of parabolas with origins shifted by p times the reciprocal lattice vector $\mathbf{K}_1$. As a result of the periodicity of the lattice, E has become multivalued for a given $\mathbf{k}$ as shown in Figure 3-1. The E-k relationship is periodic, with a single repeating unit contained within the dashed lines (shown at $\pm\mathbf{K}_1/2$). Since the parts of the plot outside the dashed lines consist of repeated information, $E_\mathbf{k}$ plots are conventionally drawn showing only the region between the dashed lines. This region is called the Brillouin zone and in 3D it consists of all the points in k-space closer to one particular reciprocal lattice point $\mathbf{K}$ than to any other point.
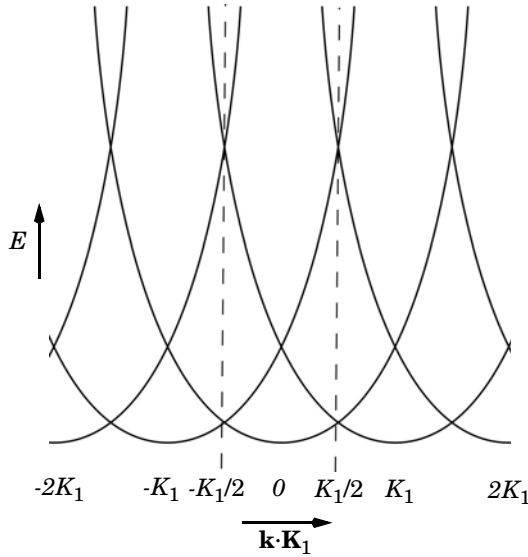
Figure 3-1: Diagram illustrating how the energy becomes multivalued for the case of a periodic potential.

Writing Equation 3-16 explicitly for the case $V_1 = 0$ gives:

$$E = \frac{\hbar^2}{2m}(\mathbf{k} - p\mathbf{K}_1)^2 \qquad\qquad (3\text{-}17)$$

Figure 3-1 shows that on the planes half between the lattice vectors (defined by the equations $\mathbf{k}\cdot\mathbf{K}_1 = q\mathbf{K}_1/2$, for integers q, and indicated by the dashed line), the energy associated with two different values of p, for example p_1 and p_2, can be equal. Note that p_1 and p_2 are associated with two (different) periodic components of the wave function or with two different $E_\mathbf{k}$ curves in the figure. Away from these planes, the energy associated with each periodic component of the wave function differs from all the other components.

Next consider the energy on the plane $\mathbf{k}\cdot\mathbf{K}_1 = q\mathbf{K}_1/2$, at the point corresponding to $p_1 = 0$ and $p_2 = 1$ as Equation 3-17 changes into Equation 3-16 by a slow increase of V_1 from zero. Close to the plane it is expected that initially, as V_1 is increased, a solution exists in which C_0 and C_1 are significant but all other coefficients are extremely small; that is, a solution in which only the $p_1 = 0$ and $p_2 = 1$ components of the wave function play a significant role. Making the assumption that the other coefficients are zero reduces the set of Equation 3-16 to just two equations:

$$C_0\left(E - \frac{\hbar^2}{2m}(\mathbf{k}_\perp^2 - \mathbf{k}_\parallel^2)\right) = V_1 C_1$$

$$C_1\left(E - \frac{\hbar^2}{2m}(\mathbf{k}_\perp^2 + (\mathbf{k}_\parallel - \mathbf{K}_1)^2)\right) = V_1 C_0$$

where the vector $\mathbf{k}$ has been decomposed into components parallel ($\mathbf{k}_\parallel$) and perpendicular ($\mathbf{k}_\perp$) to $\mathbf{K}_1$. Taking the product of these two equations leads to a quadratic equation that can be solved to obtain the value of E. It is most convenient to use the following nondimensional variables when solving the equation:

$$\varepsilon = \frac{8mE}{\hbar^2|\mathbf{K}_1|^2} - \left(\frac{2|\mathbf{k}_\perp|}{|\mathbf{K}_1|}\right)^2$$

$$U = \frac{8mV_1}{\hbar^2|\mathbf{K}_1|^2}$$

$$\delta = 1 - 2\frac{|\mathbf{k}_\parallel|}{|\mathbf{K}_1|}$$

A little algebra then leads to the equation:

$$\varepsilon^2 - 2(1 - \delta^2)\varepsilon + (1 + \delta)^2(1 - \delta)^2 - U^2 = 0$$

that has solutions:

$$\varepsilon = 1 + \delta^2 \pm \sqrt{U^2 + 4\delta^2} \qquad (3\text{-}18)$$

In the case $U = 0$, $\mathbf{k}_\perp = 0$, this equation reproduces the two parabolas centered on 0 and $\mathbf{K_1}$ (Figure 3-1). A nonzero value of $\mathbf{k}_\perp$ simply shifts the parabolas to greater energies. At the edge of the *Brillouin zone* (indicated by the dashed line), where the two parabolas cross, δ is zero, and as $\mathbf{k}_\parallel$ decreases, δ increases, reaching a maximum of 1 at the origin. When a small but finite value of U is introduced (for example $U < 0.1$) there is little effect on the curve away from the Brillouin zone edge, but as δ becomes comparable to, or less than, U its effect becomes significant. At the edge of the Brillouin zone the two $E_\mathbf{k}$ curves (corresponding to two different Fourier components of the wave function) no longer cross but are separated by a small gap such that $\varepsilon = 1 \pm U$. This corresponds to a gap between the lowest two $E_\mathbf{k}$ curves of magnitude $2V_1$.

The form of Equation 3-16 makes it clear what the effect of other harmonics in the periodic potential would be. For a potential of the form:

$$V(\mathbf{r}) = \sum_h V_h e^{-ih\mathbf{K_1} \cdot \mathbf{r}}$$

Equation 3-16 becomes:

$$\frac{\hbar^2}{2m} C_p (\mathbf{k} - p\mathbf{K_1})^2 + V_h(C_{p-h} + C_{p+h}) = EC_p$$

The effect of V_h is to couple the equations involving C_p and $C_{p\pm h}$, and it therefore perturbs apart the parabolas centered on $p\mathbf{K_1}$ and on $(p \pm h)\mathbf{K_1}$. Provided V_h is small, its effect is only significant near the edge of the Brillouin zone. Thus, for a more general periodic potential with higher harmonics, the $E_\mathbf{k}$ relationship takes the form shown in Figure 3-2.
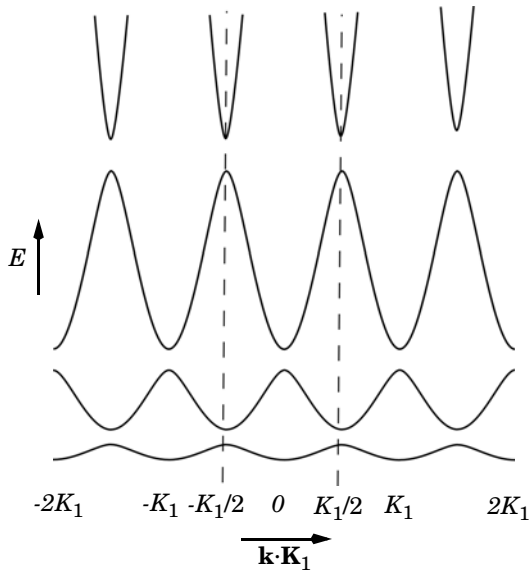
Figure 3-2: Diagram showing the effect of a periodic potential on the E-k relationship. The repeated zone scheme is used.

The E_k diagram has now changed so that certain energies are forbidden. The allowed states exist within bands of permitted energies, with *band gaps* separating them. Figure 3-2 can be redrawn in various ways. In the figure the repeated zone scheme is shown. This scheme highlights the periodicity of the lattice and makes clear the concept of energy bands and band gaps. An alternative is to show only the nth band in the nth Brillouin zone (known as the extended band scheme). This approach produces results that look similar to the equivalent (parabolic) plot for the Sommerfeld model, with gaps appearing in the curve at the edges of the Brillouin zones. Practically, the more compact reduced zone scheme is usually employed, which shows only the information in the first Brillouin zone (between the dashed lines). When the band structure information of real materials is displayed in this form, it is typical to show the

bands along several connected lines within the first Brillouin zone and to use the reduced zone scheme.

> There are now several states corresponding to a given wave number $\mathbf{k}$ with several associated energies. It is conventional to label the individual states with a band number, n, to distinguish between them. Thus the wave function $\Psi_{n\mathbf{k}}$ with energy $E_{n\mathbf{k}}$ corresponds to the state in the nth band with wave vector $\mathbf{k}$ (note that in the above argument, the band index n corresponds to the harmonic p, which dominates in the Bloch function away from the Brillouin zone edges).

Before considering the effect of a potential varying in three dimensions, it is useful to visualize Equation 3-18 in a different way. Figure 3-3 shows two surfaces of constant energy for the solution to this equation (the nondimensionalized form of the equation is not used for the plot). In the free electron model the constant energy surfaces are spheres, centered on the origin. The periodicity of the structure means that there are now spheres centered on each of the reciprocal lattice points. The effect of the periodic potential is to split apart the spherical surfaces at the points where they would have overlapped, to form a set of nonintersecting surfaces.
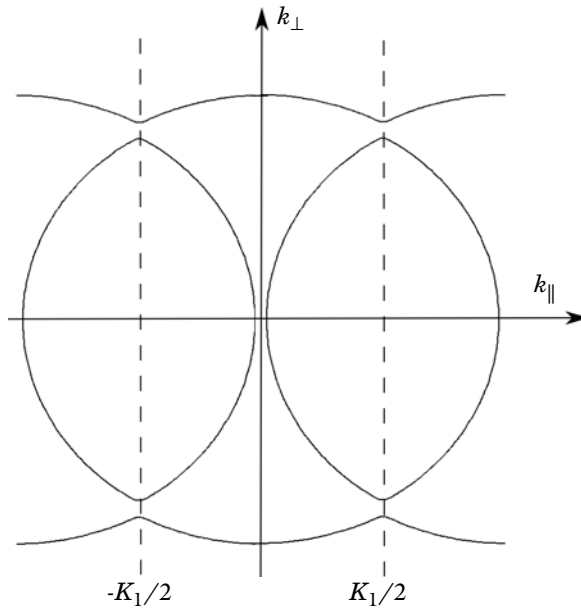
Figure 3-3: Constant energy contours produced by a one-dimensional periodic potential. Two contours are shown with slightly different energy levels.

In the more general case where the potential varies periodically in all three dimensions, exactly the same arguments apply, provided that the potential coefficients are small, (that is $V_G << h^2 |G^2|/8m$). Where the spheres centered on the different lattice points $\mathbf{K}$ and $\mathbf{K}- \mathbf{G}$ intersect, the effect of the potential is to cause the kind of remapping shown in Figure 3-2 and Figure 3-3—where the two surfaces intersect it splits apart instead. The nearly free electron energy surfaces can therefore be constructed by drawing spheres of equal radius centered on each lattice point $\mathbf{K}$ and rejoining them in this manner where they intersect, to form a set of nonintersecting surfaces. Although this procedure sounds simple, in practice rather complicated energy surfaces result from the procedure. Ref. 2 considers the example of a simple cubic material in detail and Ref. 1 shows several examples of constant energy surfaces for different lattices.

Considering the approximations made in deriving the *nearly free electron model*, it is quite remarkable that the model agrees so well with the measured $E_\mathbf{k}$ surfaces of many real materials, particularly considering that the true potential is expected to vary rapidly in the vicinity of the atomic cores. The reason for the success of the nearly free electron

theory is related to many-body effects. In materials where it is possible to divide the electrons into tightly bound core electrons and weakly bound valence electrons, the core electrons and the ions can be replaced by a pseudo-ion with a weakly varying pseudopotential, surrounded by the outermost valence electrons. The wave function for the valence states must be orthogonal to that of the core states and the pseudopotential is constructed to ensure that this is the case. The resulting potential varies much more slowly than the true potential as a result of the *Pauli repulsion effect*. This effect repels the valence electrons away from the core states in order to ensure that the corresponding wave functions are orthogonal. The nearly free electron model can then be applied to real materials if the pseudopotential, rather than the true potential, is used.

THE DENSITY OF STATES IN A PERIODIC POTENTIAL

To compute the density of states in k-space the periodic boundary condition is applied, in this case on a crystal made up of $N_c = N_1 \times N_2 \times N_3$ unit cells in the $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ directions, respectively. Using the periodic boundary condition for the wave function gives the equation:

$$\left| \psi(\mathbf{r} + N_i \mathbf{a}_i) \right| = \left| \psi(\mathbf{r}) \right|$$

Equation 3-13 adds the additional requirements:

$$\psi(\mathbf{r} + N_i \mathbf{a}_i) = \psi(\mathbf{r}) e^{i N_i (\mathbf{k} \cdot \mathbf{a}_i)}$$

Thus:

$$e^{i N_i (\mathbf{k} \cdot \mathbf{a}_i)} = 1$$

and the allowed values of $\mathbf{k}$ are:

$$\mathbf{k} = \frac{n_1}{N_1} \mathbf{b}_1 + \frac{n_2}{N_2} \mathbf{b}_2 + \frac{n_3}{N_3} \mathbf{b}_3$$

where n_1, n_2, and n_3 are integers. The reciprocal space volume per allowed $\mathbf{k}$-vector is given by:

$$\delta\xi = \frac{b_1 \cdot b_2 \times b_3}{N_1 N_2 N_3} = \frac{\xi_{BZ}}{N_c}$$

where ξ_{BZ} is the volume of the Brillouin zone in $\mathbf{k}$-space. Consequently the number of allowed wave vectors in a single Brillouin zone is equal to the number of unit cells

in the crystal. Since each state can accommodate two electrons of opposite spin, filling one band over the entire Brillouin zone corresponds to a crystal with two valence electrons per unit cell. The density of states in **k**-space is given by:

$$g(\mathbf{k}) \ = \ \frac{2N_c}{\Omega\xi_{BZ}} \ = \ \frac{1}{4\pi^3} \tag{3-19}$$

where the volume of the Brillouin zone (ξ_{BZ}=$8\pi^3/\Omega_u$ where Ω_u is the unit cell volume) has been calculated explicitly using Equation 3-10 and vector algebra (note also that $\Omega = N_c\Omega_u$ is the volume of the crystal itself). This result is identical to that obtained by the Sommerfeld model.

The available states in the crystal are filled up in the same way as in the Sommerfeld model. The occupancy of the states is still given by Equation 3-5 and the *Fermi level* is defined by Equation 3-6. For a metal, the Fermi surface geometry in a periodic potential reflects the equipotential surfaces of the band structure at the Fermi energy (for example in the previous section surfaces like those shown in Figure 3-3). In semiconductors and insulators the Fermi energy lies within the band gap so there is no clear Fermi surface. However, in semiconductors the Fermi function slightly overlaps the band above (below) the Fermi level, known as the *conduction band* (or the *valence band*), and the states near the bottom (top) of the band have a low but significant probability of being occupied (unoccupied). Since it is these states that lead to the conductivity of semiconductors (see The Semiclassical Model), it is worth considering what form the density of states takes at the very edge of a band.

Consider first the minimum of a conduction band. Choose a new coordinate system such that the Taylor series for the *E-k* relationship expanded about the band minimum up to second order takes the form:

$$E(\mathbf{k'}) \ = \ E_c + \frac{\hbar^2}{2m_x^*}k'^2_x + \frac{\hbar^2}{2m_y^*}k'^2_y + \frac{\hbar^2}{2m_z^*}k'^2_z \tag{3-20}$$

Here the constants m^*_x, m^*_y, and m^*_z are associated with the k'_x, k'_y, and k'_z terms in the series, respectively. The reason for choosing this form of the (arbitrary) constant becomes apparent below. The coordinate system for the vectors $\mathbf{k'}$ has its origin at the minimum of the band in k-space and is aligned so that Equation 3-20 applies in the form given. There are no first-order terms in the expansion since it is at a minimum in the $E(k')$ relationship (that is, it is at the bottom of a band), which represents the equation of an ellipsoidal surface. Close to the band edge the constant energy surfaces are therefore ellipsoids, with a semi-axis in the k'_x direction given by

$$k'_{E,x} = \frac{1}{\hbar}(2m_x{}^*(E - E_c))^{1/2}$$

and similarly for the k'_y and k'_z directions. A given constant energy surface contains a volume given by

$$V_E = \frac{4}{3}\pi k_{E,x}k_{E,x}k_{E,x} = \frac{4\pi}{3\,\hbar^3}(8m_x{}^*m_y{}^*m_z{}^*)^{1/2}(E - E_c)^{3/2}$$

The number of states enclosed by the constant energy surfaces is therefore

$$N_c(E) = \frac{V_E}{4\pi^3} = \frac{1}{3\pi^2\,\hbar^3}(8m_x{}^*m_y{}^*m_z{}^*)^{1/2}(E - E_c)^{3/2}$$

and the density of states $g_c\,(E)$ is given by:

$$g_c(E) = \frac{dN_c(E)}{dE} = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}(E - E_c)^{1/2} \tag{3-21}$$

This result is identical in form to Equation 3-7, except that the mass has been replaced by an effective mass, $m^* = (m^*_x\, m^*_y\, m^*_z)^{1/3}$ (the constants in Equation 3-20 are named in a manner consistent with this result).

The same argument can be applied to the top of the valence band (using a new axis system, $\mathbf{k}''$) leading to the similar result:

$$g_v(E) = \frac{1}{2\pi^2}\left(\frac{2m_h{}^*}{\hbar^2}\right)^{3/2}(E_v - E)^{1/2} \tag{3-22}$$

ALTERNATIVE REPRESENTATIONS OF THE WAVE FUNCTION: WANNIER FUNCTIONS

At this point it is useful to consider an alternative representation of the wave function, known as the *Wannier function*. Wannier functions, $W_n(\mathbf{r} - \mathbf{R})$, are wave packets of Bloch functions ($\Psi_{n\mathbf{k}}(\mathbf{r})$) that are localized at a particular lattice vector $\mathbf{R}$. These are defined in the following way:

$$W_n(\mathbf{r} - \mathbf{R}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\psi_{n\mathbf{k}}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{R}} \tag{3-23}$$

where N is the number of unit cells in the crystal. The Wannier functions are orthogonal since:

$$\int\limits_{crystal} W_n(\mathbf{r} - \mathbf{R})^* W_n(\mathbf{r} - \mathbf{R}')d^3\mathbf{r}$$

$$= \frac{1}{N}\sum_{\mathbf{k},\mathbf{k}'}\int\limits_{crystal} e^{i(\mathbf{k}\cdot\mathbf{R} - \mathbf{k}'\cdot\mathbf{R}')}\psi_{n\mathbf{k}}(\mathbf{r})^*\psi_{n\mathbf{k}'}(\mathbf{r})d^3\mathbf{r}$$

$$= \frac{1}{N}\sum_{\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}\cdot\mathbf{R} - \mathbf{k}'\cdot\mathbf{R}')}\delta(\mathbf{k} - \mathbf{k}') = \frac{1}{N}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R} - \mathbf{R}')} = \delta(\mathbf{R} - \mathbf{R}')$$

A single Bloch state can be represented in the form:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{R}} W_n(\mathbf{r} - \mathbf{R})e^{i\mathbf{k}\cdot\mathbf{R}} \qquad (3\text{-}24)$$

Wannier functions are useful to represent tightly bound, localized states, since the spatial extent is limited. The functions themselves are not unique, since the phase of the Bloch states $\Psi_{n\mathbf{k}}(\mathbf{r})$ is arbitrary. However, it is possible to define a maximally localized Wannier function, which gives an intuitive picture of the bonding in the solid.

Wannier functions are important because these form the basis of alternative approaches to computing the band structures of solids. For example, in the tight binding approximation (TBA) it is assumed that the Wannier function is an atomic orbital, enabling the wave function to be constructed directly from Equation 3-24. Instead of using a single atomic wave function, one can employ a linear combination of them, resulting in the linear combination of atomic orbitals (LCAO) approach.

SILICON BAND STRUCTURE AND DENSITY OF STATES

The band structure of silicon is illustrated in Figure 3-4. Although the three-dimensional band structure is considerably more complex than the simple picture described, many of the principles described are appropriate. Silicon is an indirect band-gap semiconductor, which means that the bottom of the conduction bands occur at a different point in k-space to the top of the valence bands. The valence band maxima occur at the center of the Brillouin zone. The conduction band minima occur at approximately $4/5$ of the distance from the zone center to its edge along the k_x, k_y, and k_z axes.

Considering first the conduction bands, there are six symmetry equivalent minima in the locations shown in Figure 3-4. Physically the form of the energy density of states is important to determine the transport properties of the semiconductor. All six of the conduction band minima are equivalent and consequently the contributions to the density of states can be added. The constant energy surfaces near the band minima are

close to being ellipsoidal; Equation 3-21 gives a good description of the energy density of states. The transport properties of the band can be characterized by a single effective mass without any loss of accuracy in the model.
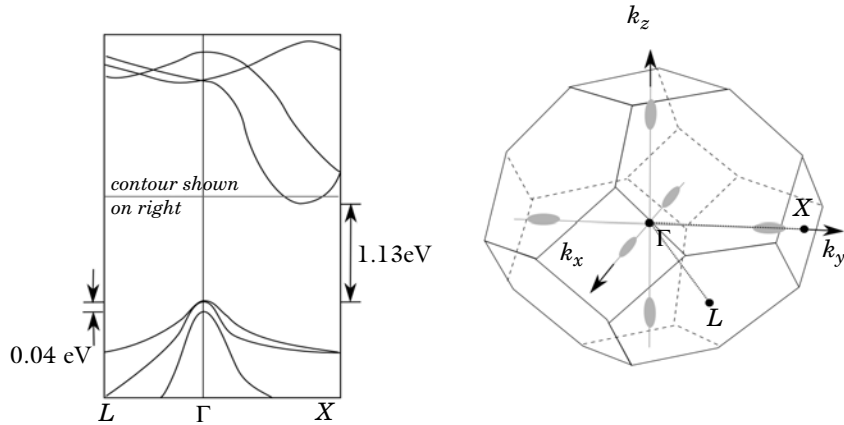
Figure 3-4: Band structure of silicon. Left: Schematic E-k diagram showing energy along the directions indicated by the dotted lines in the figure to the right. This part of the figure is equivalent to Figure 3-2. Right: Constant energy surfaces (shown in gray) corresponding to the contour indicated in the figure on the left. The first Brillouin zone is also shown. This part of the figure is equivalent to a 3D version of Figure 3-3.

There are two coincident valence band maxima located at point Γ. An additional valence band, with a slightly lower maximum energy (produced by spin-orbit coupling, see Ref. 1) is also located at this point. Each of these bands has a different effective mass associated with it. It is common to represent the effect of the three valence bands with an average density of states so that Equation 3-22 is assumed. Strictly speaking this assumption is less accurate for holes than it is for electrons, as a result of the different energies associated with the band minima.

This discussion motivates the adoption of the so-called one-band model, in which a single valence and conduction band is considered in the transport model. The one-band model can be applied to many practical semiconducting materials.

Electrons in a Perturbed Periodic Potential

Semiconductor devices are almost never homogeneous, and consequently it is necessary to consider the effect of perturbations to the periodic potential. First

consider solutions of the Schrödinger equation for the unperturbed problem, with a Hamiltonian, H_0:

$$H_0\psi_{\mathbf{k}}^0(\mathbf{r}) = E_0(\mathbf{k})\psi_{\mathbf{k}}^0(\mathbf{r})$$

	For simplicity, the band number n is dropped from the wave function in the above equation.

The perturbed problem has a set of solutions in the form:

$$H\psi_m(\mathbf{r}) = E_m\psi_m(\mathbf{r}) \tag{3-25}$$

where $H=H_0+H_1$.

	The perturbed wave functions do not necessarily have a constant wave vector, so the subscript $\mathbf{k}$ is dropped and a different quantum number, m replaces it. In many practical applications H_1 varies slowly on the length scale of the lattice and this assumption is subsequently made.

The approach taken in Ref. 9 (and originally derived by Wannier) is inspired by Equation 3-24. The unperturbed wave function can be written in the form:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{R}} W(\mathbf{r}-\mathbf{R})e^{i\mathbf{k}\cdot\mathbf{R}}$$

where $W(\mathbf{r}\text{-}\mathbf{R})$ is the Wannier function. Solutions of the form:

$$\psi_m(\mathbf{r}) = \sum_{\mathbf{R}} \Psi_m(\mathbf{R})W(\mathbf{r}-\mathbf{R}) \tag{3-26}$$

are sought. Here $\Psi_m(\mathbf{R})$ is a function that is employed to weight the Wannier functions in an expansion of the perturbed wave function. In the limit $H_1\to 0$, $\Psi_m(\mathbf{R})\to\exp(i\mathbf{k}\cdot\mathbf{R})/\sqrt{N}$.

Substituting Equation 3-26 into Equation 3-25 gives:

$$(H_0 + H_1)\sum_{\mathbf{R}}\Psi_m(\mathbf{R})W(\mathbf{r}-\mathbf{R}) = E_m\sum_{\mathbf{R}}\Psi_m(\mathbf{R})W(\mathbf{r}-\mathbf{R}) \tag{3-27}$$

This equation is premultiplied by $W^*(\mathbf{r}\text{-}\mathbf{R}')$ and integrated over the crystal:

$$\int\limits_{crystal} W^*(\mathbf{r} - \mathbf{R}') H_0 \left(\sum_{\mathbf{R}} \Psi_m(\mathbf{R}) W(\mathbf{r} - \mathbf{R}) \right) d^3\mathbf{r}$$

$$+ \int\limits_{crystal} W^*(\mathbf{r} - \mathbf{R}') H_1 \sum_{\mathbf{R}} \Psi_m(\mathbf{R}) W(\mathbf{r} - \mathbf{R}) d^3\mathbf{r} \qquad (3\text{-}28)$$

$$= \int\limits_{crystal} W^*(\mathbf{r} - \mathbf{R}') E_m \left(\sum_{\mathbf{R}} \Psi_m(\mathbf{R}) W(\mathbf{r} - \mathbf{R}) \right) d^3\mathbf{r}$$

Consider first the right-hand side of Equation 3-28:

$$\int\limits_{crystal} W^*(\mathbf{r} - \mathbf{R}') E_m \left(\sum_{\mathbf{R}} \Psi_m(\mathbf{R}) W(\mathbf{r} - \mathbf{R}) \right) d^3\mathbf{r} = E_m \Psi_m(\mathbf{R}) \sum_{\mathbf{R}} \delta(\mathbf{R} - \mathbf{R}')$$

$$= E_m \Psi_m(\mathbf{R})$$

where both the orthogonality of the Wannier functions is employed.

The term in H_1 on the left-hand side of Equation 3-28 gives:

$$\int\limits_{crystal} W^*(\mathbf{r} - \mathbf{R}') H_1 \left(\sum_{\mathbf{R}} \Psi_m(\mathbf{R}) W(\mathbf{r} - \mathbf{R}) \right) d^3\mathbf{r}$$

$$= H_1 \sum_{\mathbf{R}} \Psi_m(\mathbf{R}) \delta(\mathbf{R} - \mathbf{R}') = H_1 \Psi_m(\mathbf{R}')$$

where the fact that the Wannier function is localized around $\mathbf{R}$ or $\mathbf{R}'$ and the assumption that H_1 is a constant on this length scale is employed.

Finally the H_0 term is considered. Using the definition of the Wannier function given in Equation 3-23, this term is written as:

$$\frac{1}{N} \int_{crystal} \left(\sum_{\mathbf{k'}} \psi_{\mathbf{k'}}^{0\,*}(\mathbf{r}) e^{\mathbf{k'} \cdot \mathbf{R'}} \right) H_0 \left(\sum_{\mathbf{R}} \Psi_m(\mathbf{R}) \sum_{\mathbf{k}} \psi_{\mathbf{k}}^{0}(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{R}} \right) d^3\mathbf{r}$$

$$= \frac{1}{N} \int_{crystal} \left(\sum_{\mathbf{k'}} \psi_{\mathbf{k'}}^{0\,*}(\mathbf{r}) e^{\mathbf{k'} \cdot \mathbf{R'}} \right) \left(\sum_{\mathbf{R}} \Psi_m(\mathbf{R}) \sum_{\mathbf{k}} H_0 \psi_{\mathbf{k}}^{0}(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{R}} \right) d^3\mathbf{r}$$

$$= \frac{1}{N} \int_{crystal} \left(\sum_{\mathbf{k'}} \psi_{\mathbf{k'}}^{0\,*}(\mathbf{r}) e^{\mathbf{k'} \cdot \mathbf{R'}} \right) \left(\sum_{\mathbf{R}} \Psi_m(\mathbf{R}) \sum_{\mathbf{k}} E_0(\mathbf{k}) \psi_{\mathbf{k}}^{0}(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{R}} \right) d^3\mathbf{r} \quad (3\text{-}29)$$

$$= \frac{1}{N} \sum_{\mathbf{R}} \Psi_m(\mathbf{R}) \sum_{\mathbf{k'}} E_0(\mathbf{k}) e^{-i\mathbf{k'} \cdot (\mathbf{R} - \mathbf{R'})}$$

$$= \sum_{\mathbf{R''}} \Psi_m(\mathbf{R'} - \mathbf{R''}) \sum_{\mathbf{k'}} \frac{1}{N} E_0(\mathbf{k}) e^{i\mathbf{k'} \cdot \mathbf{R''}}$$

where the orthogonality of the unperturbed wave functions is used and the dummy variable, $\mathbf{R''} = \mathbf{R'} - \mathbf{R}$ is defined. Next we note that ground state energy, $E_0(\mathbf{k})$, is periodic in k-space (see for example Figure 3-2), and can be written as a Fourier series in the form:

$$E_0(\mathbf{k}) = \sum_{\mathbf{R}} E_{\mathbf{R}} e^{-i\mathbf{R} \cdot \mathbf{k}} \quad (3\text{-}30)$$

where $\mathbf{R}$ is the set of real space lattice vectors (real space forms a reciprocal space for k-space). The coefficients of the series $E_{\mathbf{R}}$ are given by:

$$E_{\mathbf{R}} = \frac{1}{\Omega} \int_{BZ} E_0(\mathbf{k}) e^{-i\mathbf{R} \cdot \mathbf{k}} d^3\mathbf{k} = \sum_{\mathbf{k}} \frac{1}{N} E_0(\mathbf{k}) e^{i\mathbf{R} \cdot \mathbf{k}} \quad (3\text{-}31)$$

where the integral over the Brillouin zone (with volume Ω) is replaced with a summation over the individual k-states in the zone for consistency with the notation employed in this section. Note that there are N states in the Brillouin zone, as shown in The Density of States in a Periodic Potential. Recognizing that the final term in Equation 3-29 takes the same form as the definition of $E_{\mathbf{K}^*}$ given in Equation 3-31, it is possible to write Equation 3-29 in the form:

$$\frac{1}{N}\left(\int\limits_{crystal} \left(\sum_{\mathbf{k'}} \psi_{\mathbf{k'}}^{0\;*}(\mathbf{r})e^{\mathbf{k'}\cdot\mathbf{R'}} \right) H_0 \left(\sum_{\mathbf{R}} \Psi_m(\mathbf{R}) \sum_{\mathbf{k}} \psi_{\mathbf{k}}^0(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{R}} \right) d^3\mathbf{r} \right)$$

$$= \sum_{\mathbf{R''}} \Psi_m(\mathbf{R'} - \mathbf{R''})E_{\mathbf{R''}}$$

Finally, expanding $\Psi_m(\mathbf{R'} - \mathbf{R''})$ in a Taylor series about the point $\mathbf{R''}$ gives:

$$\Psi_m(\mathbf{R'} - \mathbf{R''}) = \Psi_m(\mathbf{R'}) - \mathbf{R''}\cdot\nabla\Psi_m(\mathbf{R'}) + \frac{1}{2!}(\mathbf{R''}\cdot\nabla)(\mathbf{R''}\cdot\nabla)\Psi_m(\mathbf{R'}) + \ldots$$

$$= \exp(-\mathbf{R''}\cdot\nabla)\Psi_m(\mathbf{R'})$$

where the final step introduces an operator based on the Taylor series expansion of the exponential function. Equation 3-29 can be written as:

$$\frac{1}{N}\left(\int\limits_{crystal} \left(\sum_{\mathbf{k'}} \psi_{\mathbf{k'}}^{0\;*}(\mathbf{r})e^{\mathbf{k'}\cdot\mathbf{R'}} \right) H_0 \left(\sum_{\mathbf{R}} \Psi_m(\mathbf{R}) \sum_{\mathbf{k}} \psi_{\mathbf{k}}^0(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{R}} \right) d^3\mathbf{r} \right)$$

$$= \sum_{\mathbf{R''}} E_{\mathbf{R''}} \exp(-\mathbf{R''}\cdot\nabla)\Psi_m(\mathbf{R'})$$

(3-32)

Next an operator $E_0(-i\nabla)$ is introduced that results from replacing every instance of $\mathbf{k}$ in the function $E_0(\mathbf{k})$ with $-i\nabla$. Comparing Equation 3-32 with equation Equation 3-30 shows that:

$$\frac{1}{N}\left(\int\limits_{crystal} \left(\sum_{\mathbf{k'}} \psi_{\mathbf{k'}}^{0\;*}(\mathbf{r})e^{\mathbf{k'}\cdot\mathbf{R'}} \right) H_0 \left(\sum_{\mathbf{R}} \Psi_m(\mathbf{R}) \sum_{\mathbf{k}} \psi_{\mathbf{k}}^0(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{R}} \right) d^3\mathbf{r} \right)$$

$$= E_0\left(\frac{1}{i}\nabla\right)\Psi_m(\mathbf{R'})$$

Assembling the terms derived above into Equation 3-28 (with $\mathbf{R'}\rightarrow\mathbf{r}$) gives the following equation for $\Psi_m(\mathbf{r})$:

$$(E_0(-i\nabla) + H_1)\Psi_m(\mathbf{r}) = E_m\Psi_m(\mathbf{r})$$

(3-33)

Equation 3-33 is an equation for $\Psi_m(\mathbf{r})$, similar in form to the Schrödinger equation, with the perturbing potential H_1 appearing as the potential energy and the operator $E_0(-i\nabla)$ replacing the kinetic energy operator. This equation can be used to derive the semiclassical model, which in turn determines the transport properties of electrons.

The Semiclassical Model

Consider the motion of a wave packet, constructed using the functions $\Psi_m(\mathbf{r})$ which modulate the Wannier functions. The wave function evolves according to Equation 3-33. Note that the perturbing potential, H_1, is a function of position $\mathbf{r}$ and $E_0(-i\nabla)$ can be straightforwardly written as a function of the quantum mechanical momentum operator $\mathbf{p} = -i\hbar\nabla$. The equivalent classical Hamiltonian is $H = E_0(p) + H_1(\mathbf{r})$ (where E_0 is written as a function of $\mathbf{p} = \hbar\mathbf{k}$). The quantity $\hbar\mathbf{k}$, which is analogous to the classical momentum in the Hamiltonian, is often referred to as the crystal momentum of the wave packet. The classical Hamiltonian results in classical particles that move according to the equations:

$$\frac{d\mathbf{r}}{dt} = \frac{\partial H}{\partial \mathbf{p}} = \frac{\partial E_0}{\partial \mathbf{p}}$$

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{r}} = -\frac{\partial H_1}{\partial \mathbf{r}}$$

According to Ehrenfest's theory (see Ref. 7 for a detailed discussion), the center of gravity of the wave packet moves in the same way as the corresponding classical Hamiltonian. Consequently the motion of a wave packet with associated charge -q, in a perturbing Hamiltonian of the form $H_1 = -qV$ moves according to the equations:

$$\mathbf{v}(\mathbf{k}) = \frac{\partial \mathbf{r}}{\partial t} = \frac{1}{\hbar}\frac{\partial E(\mathbf{k})}{\partial \mathbf{k}} \tag{3-34}$$

$$\hbar\frac{\partial \mathbf{k}}{\partial t} = q\frac{\partial V}{\partial \mathbf{r}} = -q\mathbf{E} = \mathbf{F} \tag{3-35}$$

Here $\mathbf{v}(\mathbf{k})$ is the velocity of the wave packet, and $\mathbf{F}$ is the Lorentz force acting on it.

These equations are referred to as the *semiclassical model* (in the absence of magnetic fields). When magnetic fields are present Equation 3-35 takes the form:

$$\hbar\frac{\partial \mathbf{k}}{\partial t} = -q(\mathbf{E} + \mathbf{v}(\mathbf{k}) \times \mathbf{B})$$

(Ref. 1 provides references that derive this equation in full. Note also that Equation 3-34 is also modified in modern solid state theory to include an additional term due to the Berry curvature of the band. This term is usually zero for

semiconducting materials of interest). The model is extremely successful to describe a range of practical transport phenomena.

📄   The instantaneous velocity and momentum of a single electron fluctuates rapidly as it passes through the periodic potential of the crystal, so the crystal momentum is not directly related to the actual electron momentum and the wave packet velocity should be interpreted as an average drift velocity.

The semiclassical model is valid for wave packets that are localized to within greater than approximately ten lattice spacings. This restriction is apparent from the previous analysis but is also implied by the *Heisenberg uncertainty principle* $\Delta x \approx \hbar / \Delta p \approx 1/k_f$ where k_f is the approximate magnitude of wave vectors at the Fermi surface. It would be unreasonable to use more than approximately 10% of the available states in a single wave packet. The wave packet is therefore large compared to the lattice size, and so sees only the average effect of the lattice.

Additionally, the physical size of the wave packets must be small compared to the length scale of electric or magnetic field variation. This is why the model is called semiclassical; the external fields are treated classically, but the periodic potential of the lattice is not. There is a further restriction on the local validity of the semiclassical model, which results from the fact that in the limit of zero periodic potential the classical limit should be recovered. In the classical limit the electron momentum and the crystal momentum become identical. At a given point in k-space the semiclassical equations are valid provided:

$$ea|\mathbf{E}| \ll \frac{E_g(\mathbf{k})^2}{E_f}$$

$$\frac{e|\mathbf{B}|}{m} \ll \frac{E_g(\mathbf{k})^2}{E_f}$$

where a is of the order of the lattice constant, E_f is the Fermi energy, and $E_g(\mathbf{k})$ is the energy difference to the nearest energy in a different band at the specified k-space point. In semiconductors the first condition is violated during electric breakdown, when electrons can make an interband transition driven by a large electric field. A similar phenomenon known as magnetic breakdown can occur in high magnetic fields. Although the semiclassical model really describes the transport of wave packets,

conventionally the transport of electrons is discussed in the literature. This convention is therefore adopted from here onwards.

The semiclassical model has important consequences for charge transport in materials. One of the more surprising consequences is that a filled band is completely inert. Since the semiclassical model does not allow intraband transitions, the electrons can only move between states within a band. Each state has a particular velocity associated with it (given by Equation 3-34) and electrons move between states according to Equation 3-35. In the reduced zone scheme, electrons that pass out of the Brillouin zone immediately reappear unchanged (except for a relabeling of the k-vector) at the opposite face. Summing the drift velocity over all the states in the band produces exactly the same result in the presence of applied fields as without them, since the band structure remains unchanged and since all the states are still occupied (see Ref. 1 for a formal derivation that integrates over all the states in a band). This result explains the existence of metals, insulators, and semiconductors. Metals are materials without a full band, in which an applied electric field can produce a large current. Insulators have a set of full bands and the Fermi energy lies within the band gap. The band gap is sufficiently large that the occupancy of the bands below the Fermi level is essentially one for all states at temperatures of interest. Similarly the band above the gap is essentially unoccupied in an insulator. Semiconductors are materials in which the Fermi level lies within the band gap, but in which the variation in the Fermi function overlaps the edges of adjacent bands at temperatures of interest, so that not all the states in the bands above (or below) the Fermi level are unoccupied (or occupied). This is why semiconductors usually have a higher resistance than metals since only a relatively small number of states in the band are unoccupied. The physics of semiconductor transport is determined by the band structure close to the top or the bottom of the bands adjacent to the Fermi level.

In 3D the band gap must extend across all directions in k-space to produce a semiconductor or insulator.

Before considering how to compute the transport properties of bands that are not full, it is worth considering the implications of Equation 3-34 and Equation 3-35 for the relationship between force and electron velocity. In order to do so, the velocity must be related to the wave vector **k**. Therefore:

$$\frac{\partial \mathbf{v}}{\partial t} = \frac{\partial \mathbf{v}}{\partial \mathbf{k}}\frac{\partial \mathbf{k}}{\partial t} = \frac{1}{\hbar^2}\frac{\partial^2 E(\mathbf{k})}{\partial \mathbf{k}^2}\mathbf{F} \tag{3-36}$$

Note that both $\partial\mathbf{v}/\partial\mathbf{k}$ and $\hbar^{-2}\partial^2 E(\mathbf{k})/\partial\mathbf{k}^2$ are rank 2 tensors (matrices). Equation 3-36 defines the effective masses introduced in Equation 3-20.

In general, the effective mass matrix is defined as:

$$
m^{*-1} = \frac{1}{\hbar^2}
\begin{vmatrix}
\dfrac{\partial^2 E(\mathbf{k})}{\partial k_x^{\,2}} & \dfrac{\partial^2 E(\mathbf{k})}{\partial k_x \partial k_y} & \dfrac{\partial^2 E(\mathbf{k})}{\partial k_x \partial k_z} \\[2ex]
\dfrac{\partial^2 E(\mathbf{k})}{\partial k_y \partial k_x} & \dfrac{\partial^2 E(\mathbf{k})}{\partial k_y^{\,2}} & \dfrac{\partial^2 E(\mathbf{k})}{\partial k_y \partial k_z} \\[2ex]
\dfrac{\partial^2 E(\mathbf{k})}{\partial k_z \partial k_x} & \dfrac{\partial^2 E(\mathbf{k})}{\partial k_z \partial k_y} & \dfrac{\partial^2 E(\mathbf{k})}{\partial k_z^{\,2}}
\end{vmatrix}
$$

such that $\mathbf{F} = \mathbf{m}^* \, \mathbf{v}$. In Equation 3-20 the coordinate system for $\mathbf{k}'$ was chosen such that the $\mathbf{m}^*$ matrix has zero for the off-diagonal terms. For an isotropic band $\mathbf{m}^*$ is proportional to the identity matrix. In this instance, near the top of a band, it is easy to see that its value could be negative. Instead of thinking in terms of negative mass, it is more conventional to reverse the sign on the force and to consider a wave packet corresponding to a particle with positive charge and mass (this is known as a hole).

Finally consider the form of Equation 3-33 in the case where the band structure takes the form given by Equation 3-20. For simplicity consider the case of an isotropic effective mass so that:

$$
E(\mathbf{k}) = E_0 + \frac{\hbar^2}{2m^*}\mathbf{k}^2
$$

Equation 3-33 now takes the form:

$$
\left(-\frac{\hbar^2}{2m^*}\nabla^2 + E_0 + H_1\right)\Psi_m(\mathbf{r}) = E_m\Psi_m(\mathbf{r}) \tag{3-37}
$$

which is identical in form to the Schrödinger equation, except that the effective mass rather than the electron mass appears in the equation system. It is important to remember that for Equation 3-37 to apply the E–k relationship must be defined in an appropriate coordinate system. Note, however, that for the case of an anisotropic effective mass there are different coefficients for the derivatives in different directions in the Laplacian operator. Equation 3-37 also applies near the top of a band, so it is relevant for holes.

The Boltzmann Equation

TRANSPORT PROPERTIES AND HOLES

To compute the transport properties of a material without full bands it is necessary to know the occupancy of the states within each of the partially filled bands. Under the influence of an applied force the distribution becomes distorted from that obtained at thermal equilibrium (Equation 3-5) and additionally can vary in space (for example in the presence of nonuniform electric fields, temperatures, or material properties) and time. The distribution function ($f(\mathbf{m}, \mathbf{r}, t)$) is related to the number of electrons ($\delta n(\mathbf{k}, \mathbf{r})$) in a volume element $\delta^3\mathbf{k}$ of k-space and $\delta^3\mathbf{r}$ of real space at point $\mathbf{k}, \mathbf{r}$ in the following way:

$$\delta n(\mathbf{k,r}) = \frac{1}{4\pi^3}f(\mathbf{k,r},t)\delta^3\mathbf{k}\delta^3\mathbf{r}$$

Transport properties can be derived directly from the distribution function, for example the current density is given by:

$$\mathbf{J}_n(\mathbf{r},t) = -\frac{q}{4\pi^3}\int \mathbf{v}(\mathbf{k})f(\mathbf{k,r},t)d^3\mathbf{k} = -\frac{q}{4\pi^3}\int \frac{1}{\hbar}\frac{\partial E(\mathbf{k})}{\partial \mathbf{k}}f(\mathbf{k,r},t)d^3\mathbf{k} \qquad (3\text{-}38)$$

Here the integral is performed over the first Brillouin zone in k-space. Since $f(\mathbf{k}, \mathbf{r}, t)$ gives information about the electron occupancy of states, at a given instant in time Equation 3-38 can be rewritten in the following form:

$$\mathbf{J}(\mathbf{r},t) = -\frac{q}{4\pi^3}\int_{\text{occupied}} \mathbf{v}(\mathbf{k})d^3\mathbf{k}$$

Noting that:

$$\int_{\text{band}} \mathbf{v}(\mathbf{k})d^3\mathbf{k} = \int_{\text{occupied}} \mathbf{v}(\mathbf{k})d^3\mathbf{k} + \int_{\text{unoccupied}} \mathbf{v}(\mathbf{k})d^3\mathbf{k} = 0$$

it is clear that the current density can be written in the form:

$$\mathbf{J}_p(\mathbf{r},t) = \frac{q}{4\pi^3}\int_{\text{unoccupied}} \mathbf{v}(\mathbf{k})d^3\mathbf{k} = \frac{q}{4\pi^3}\int \mathbf{v}(\mathbf{k})(1-f(\mathbf{k,r},t))d^3\mathbf{k} \qquad (3\text{-}39)$$

Equation 3-39 is useful when computing the current contribution from a band that is nearly full, as only a small fraction of the band needs to be considered in the integral. The current is exactly the same as that which would be produced if the unoccupied

electron states were occupied by positively charged particles (referred to as holes) and the occupied electron states were empty. The hole occupancy factor, $f_h(\mathbf{k}, \mathbf{r}, t)$, is simply given by:

$$f_h(\mathbf{k},\mathbf{r},t) \ = \ 1 - f(\mathbf{k},\mathbf{r},t)$$

and holes respond within the semiclassical equations as if they had a charge opposite to that of electrons.

THE BOLTZMANN EQUATION

Equation 3-38 shows that the time- and space-dependence of electric currents in a semiconductor is determined by the distribution function $f(\mathbf{k}, \mathbf{r}, t)$. Within a volume element $\delta^3\mathbf{k}\delta^3\mathbf{r}$ there are $f(\mathbf{k}, \mathbf{r}, t)\delta^3\mathbf{k}\delta^3\mathbf{r}/4\pi^3$ electrons. In the presence of an external force the electrons move through real space at a velocity $\mathbf{v}(\mathbf{k})$ (given by Equation 3-34) and through k-space at a velocity $\partial\mathbf{k}/\partial t$ (from Equation 3-35). At a time $f(\mathbf{k}, \mathbf{r})$ the electrons that occupy the volume element are those which were at $\mathbf{k} - \delta\mathbf{k}, \mathbf{r} - \delta\mathbf{r}$, at time $t - \delta t$. Therefore:

$$f(\mathbf{k},\mathbf{r},t) \ = \ f(\mathbf{k} - \delta\mathbf{k},\mathbf{r} - \delta\mathbf{r},t - \delta t)$$

$$f(\mathbf{k},\mathbf{r},t) \ = \ f(\mathbf{k},\mathbf{r},t) - \left(\frac{\partial\mathbf{k}}{\partial t} \cdot \nabla_k f + \frac{\partial\mathbf{r}}{\partial t} \cdot \nabla_r f + \frac{\partial f}{\partial t}\right)\delta t$$

Here the subscript to the gradient term indicates that derivatives are taken with respect to the coordinates indicated. Therefore, in the absence of collisions:

$$\frac{\partial f}{\partial t} \ = \ -\frac{\partial\mathbf{k}}{\partial t} \cdot \nabla_k f - \frac{\partial\mathbf{r}}{\partial t} \cdot \nabla_r f$$

Note that the assumption has been made that the size of the volume element ($\delta^3\mathbf{k}\delta^3\mathbf{r}$) remains unchanged in time — *Liouville's theorem* asserts that it is (see Ref. 1). In practice electrons collide with defects in the lattice (impurities) and with lattice distortions caused by mechanical waves in the lattice (phonons). The electrons do not collide with the lattice itself as the effect of the lattice is already incorporated into the Bloch functions. However, any deviation from perfect periodicity produce collisions. The effect of collisions is to add additional time dependence to the equation system, so the full *Boltzmann equation* is given by:

$$\frac{\partial f}{\partial t} \ = \ -\frac{\partial\mathbf{k}}{\partial t} \cdot \nabla_k f - \frac{\partial\mathbf{r}}{\partial t} \cdot \nabla_r f + \left[\frac{\partial f}{\partial t}\right]_{coll}$$

Using Equation 3-35 and substituting $\partial\mathbf{r}/\partial t = \mathbf{v}$ gives the final form of the Boltzmann equation for electrons:

$$\frac{\partial f}{\partial t} = -\frac{1}{\hbar}\mathbf{F} \cdot \nabla_k f - \mathbf{v} \cdot \nabla_r f + \left[\frac{\partial f}{\partial t}\right]_{\text{coll}} \tag{3-40}$$

The *hole distribution function* can be shown to obey a similar Boltzmann equation:

$$\frac{\partial f_h}{\partial t} = -\frac{1}{\hbar}\mathbf{F}_h \cdot \nabla_k f_h - \mathbf{v}_h \cdot \nabla_r f_h + \left[\frac{\partial f_h}{\partial t}\right]_{\text{coll}}$$

These equations are difficult to solve and consequently approximations are usually made to simplify them significantly.

Doped Semiconductors

In practical applications it is common to modify the properties of the semiconductor to add impurity atoms or dopants in a controlled manner. Using silicon as an example (with a chemical valency of 4), impurity atoms such as phosphorous or arsenic (with a valency of 5), have the effect of adding extra electrons to the conduction band. Such impurities are called *donors*. Similarly impurities such as boron and gallium (with a valency of 3) can capture an electron from the valence band, creating holes. These impurities are called *acceptors*.

Consider the case of a donor atom. If the atom loses its additional electron, it has enough remaining electrons to fit into the lattice of the crystal. However the atom is now positively charged, and consequently a perturbing coulomb potential exists around it. Equation 3-37 can be used to compute the states that the additional electron can occupy within this potential. The problem becomes that of the hydrogen atom, except that the medium typically has a large relative dielectric permittivity ($\varepsilon_r \approx 12$ for silicon) and the electron has an effective mass m^* that is typically less than the electron mass. The solutions to the corresponding Schrödinger equation are swollen orbits (typically 2.5–5.0 nm in radius) similar to that of a hydrogen atom. The reduced mass and larger dielectric constant cause a reduction in the effective ionization energy of the electron so that it is significantly less than that of a hydrogen atom — donor ionization levels are typically 10s of meV. The energy of the donor states is consequently just below that of the conduction band as shown in Figure 3-5. Similarly, the energy of the acceptor states lies just above the valence band (also in the figure). Figure 3-5 shows an n-type semiconductor. This is a material with significantly more donors than acceptors so that the majority carriers are electrons.
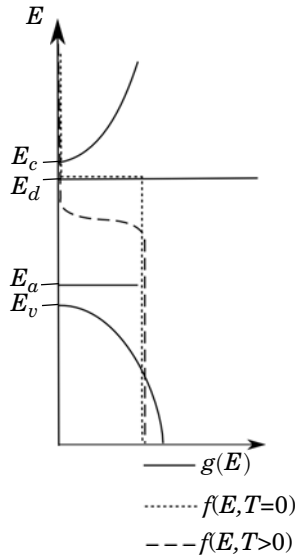
Figure 3-5: Density of states and Fermi function for an n-type semiconductor. The Fermi function is shown at zero temperature and at a finite temperature.

Since donor and acceptor states cannot hold two electrons (unlike states within the band), the carrier statistics are modified slightly. The occupancy of the states in equilibrium is determined from statistical mechanics as:

$$\frac{N_d^+}{N_d} = \frac{1}{1 + g_d \exp\left(\dfrac{E_f - E_d}{k_B T}\right)} \tag{3-41}$$

where g_d is the donor degeneracy factor, which is 2 if the conduction band minimum is nondegenerate but which varies when the degeneracy of the donor levels is altered by the band structure having degenerate conduction bands. Similarly, the occupancy of the acceptor states is given by:

$$\frac{N_a^-}{N_a} = \frac{1}{1 + g_a \exp\left(\dfrac{E_a - E_f}{k_B T}\right)} \tag{3-42}$$

where g_a is the acceptor degeneracy factor.

In equilibrium the value of the Fermi level is determined self-consistently from the charge neutrality condition, along with the requirement that the number of holes and electrons is determined from the Fermi function:

$$N_d^+ - N_a^- + p - n = 0$$

$$n = \int g_c(E)f(E)dE$$

$$p = \int g_v(E)f_h(E)dE$$

Here $g_c(E)$ is the density of states in the conduction band, $g_v(E)$ is the density of states in the valence band, and $f(E)$ is the (equilibrium) Fermi function.

Specifying the Dopant Distribution

The distribution of dopants within the semiconductor can be specified using the Analytic Doping Model and Geometric Doping Model features. The Analytic Doping Model enables distributions to be defined in terms of the coordinate system; the Geometric Doping Model enables definitions in terms of the distance from selected boundaries in the geometry.

ℚ	Doping

THEORY FOR THE ANALYTIC DOPING MODEL

The Analytic Doping Model has two options to specify the doping concentration in terms of the coordinate system — User defined or Box. It supports the use of a local coordinate system that is rotated relative to the global coordinates.

User Defined Profiles

For user defined profiles any arbitrary dopant concentration can be created with user-defined functions or imported data (which can be specified using an interpolation function). Any expression written in terms of the local coordinate system can be used to define the distribution. Use of the COMSOL Multiphysics built-in functions enables the creation of intricate distributions.

Box Profiles

The Box profile enables a box-shaped region of uniform doping to be defined away from which the dopant concentration decays with one of three preset functions. The

location of the region of constant doping is defined by specifying either the corner or center coordinate using the global coordinate system. The size of the region is defined by specifying its extent in each of the directions parallel to the local coordinate axis. In 3D the height, width, and depth are supplied to create a block; in 2D the width and depth are supplied to create a rectangle; and in 1D the width is supplied to create a line. It is possible to set the constant region to have zero extend in a given direction to, for example, create a plane of constant doping in a 3D geometry. The orientation of the constant region is aligned with the local coordinate axes. If a rotated local coordinate system is used the constant region rotates around its specified corner or center coordinate, which is expressed using the global coordinate system.

The distribution outside of the constant region decays with one of three preset functions: Gaussian, Linear, or Error Function. These functions are defined using Ramp functions with unity gradient that begin at the edges of the constant region and which continue throughout the remainder of the domain. Thus there are two Ramp functions for each geometry axis. Figure 3-6 shows the four Ramp functions used to create a 2D Box profile. Note how each Ramp function is zero inside the constant region, and that the unity gradient outside the region creates and effective coordinate axis for each direction that is zeroed at the region boundary.

In 3D, the Gaussian distribution is given by

$$N_{d,a} = N_0 \exp\left(-\left[\left(\frac{r_x^-}{l_x}\right)^2 + \left(\frac{r_x^+}{l_x}\right)^2 + \left(\frac{r_y^-}{l_y}\right)^2 + \left(\frac{r_y^+}{l_y}\right)^2 + \left(\frac{r_z^-}{l_z}\right)^2 + \left(\frac{r_z^+}{l_z}\right)^2\right]\right) \quad (3\text{-}43)$$

where $N_{d,a}$ is the donor or acceptor concentration, N_0 is the concentration inside the uniformly doped region, l_i is the Decay length in the i-direction, and $r_x^-, r_x^+, r_y^-, r_y^+,$ $r_z^-,$ and r_z^+ are the Ramp functions.

	In models with less than three dimensions the unused Ramp functions are omitted from this expression. Also, 2D-axisymmetric profiles are obtained in the same manner but using ramp functions $r_r^-, r_r^+, r_z^-,$ and r_z^+.

	Functions and Ramp in the *COMSOL Multiphysics Reference Manual*.

The decay length can be specified directly or calculated from a specified junction depth via:

$$l_i = \frac{d_{j,i}}{\sqrt{\ln\left(\left|\frac{N_0}{N_b}\right|\right)}}$$

where $d_{j,i}$ is the junction depth in the i-direction, and N_b is the background doping concentration that can be entered directly or taken from the output of another doping feature in the model. By default $d_{j,x}=d_{j,y}=d_{j,z}=d_j$, such that $l_x=l_y=l_z$. To use different decay lengths in different directions select the **Specify different length scales for each direction** check box under the Profile section.

The linear distribution is given by

$$N_{a,d} = N_0 + g_x(r_x^- + r_x^+) + g_y(r_y^- + r_y^+) + g_z(r_z^- + r_z^+) \qquad (3\text{-}44)$$

where g_i is the gradient in i-direction. The gradient can be supplied directly or calculated from a specified junction depth via:

$$g_i = \frac{N_b - N_0}{d_{j,i}}$$

By default the gradient is the same in all directions, however it can be set to be direction dependent using the **Specify different length scales for each direction** check box. Note that a negative dopant distribution is not physical, so the concentration is set to zero in regions where Equation 3-44 gives $N_{a,d}<0$.

The Error Function distribution is given by

$$N_{a,d} = N_0[1 - \text{erf}(m_x(r_x^- + r_x^+) + m_y(r_y^- + r_y^+) + m_z(r_z^- + r_z^+))]$$

where m_x is an argument factor which controls the length scale of the profile. The argument factor can be entered directly or calculated from a specified junction depth via:

$$m_i = \frac{1}{d_{j,i}}\text{erfinv}\left(1 - \frac{N_b}{N_0}\right)$$

By default the argument factor is the same in all directions, however it can be set to be direction dependent using the **Specify different length scales for each direction** check box.
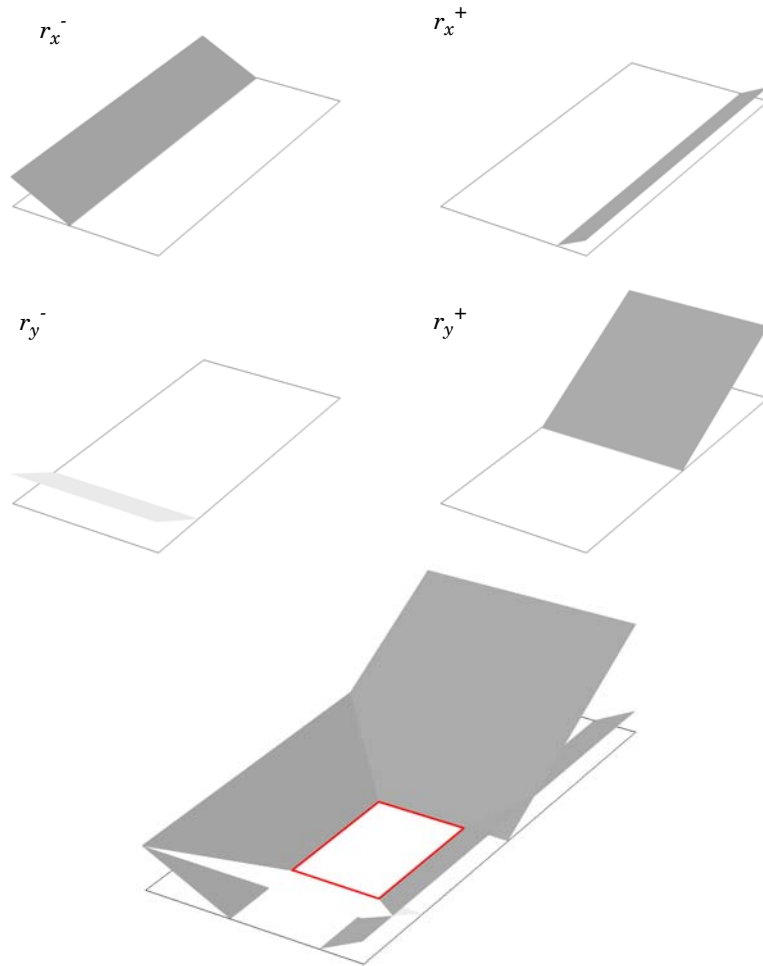
Figure 3-6: Ramp functions used to specify box doping profiles on a rectangular domain in 2D. The height out of the plane shows the magnitude of the ramp function (not to scale). Top: Individual ramp functions for the x-direction. Middle: Individual ramp functions for the y-direction. Bottom: Composite of all the ramp functions, showing the region of constant doping (highlighted in red).

THEORY FOR THE GEOMETRIC DOPING MODEL

The Geometric Doping Model feature enables doping distributions to be defined in terms of the distance from selected boundaries in the geometry. This is convenient when working with geometries with intricate shapes that would be challenging to

describe analytically using the coordinate system. The boundaries from which the distance is calculated are selected using the Boundary Selection for Doping Profile node. Any boundary that bounds, or is within, the domains to which the corresponding Geometric Doping Model feature is applied can be selected. The form of the distribution can be selected from a range of preset functions or a user defined expression can be supplied.

User Defined Profiles

When a user defined profile is selected any arbitrary distribution that can be written in terms of the distance from the selected boundaries can be defined. This distance is available as the variable `semi.gdm#.D`, where # corresponds to the number of the Geometric Doping Model feature.

Preset Profiles

The other selections in the **Dopant profile away from the boundary** list allow either Gaussian, Linear, or Error Function profiles to be generated. These profiles are defined in terms of the distance, $D,$ from the selected boundaries as described below.

The Gaussian profile is given by

$$N_{a,d} = N_0 \exp\left(-\left(\frac{D}{l}\right)^2\right)$$

where $N_{a,d}$ are the concentration of the acceptors or donors, N_0 is the concentration of dopants at the selected boundaries, and l is the decay length of the Gaussian function. The decay length can be entered directly or can be calculated from a specified junction depth, d_j, via:

$$l = \frac{d_j}{\sqrt{\ln\left(\left|\frac{N_0}{N_b}\right|\right)}}$$

where N_b is a specified *background doping concentration* that can either be directly defined or taken from the output of another doping model feature.

The Linear profile is given by

$$N_{a,d} = N_0 + gD \tag{3-45}$$

where g is the gradient, which can be entered directly or calculated from a specified junction depth via

$$g = \frac{N_b - N_0}{d_j}$$

Note that, as a negative concentration is not physical, the dopant concentration is set to zero in regions where Equation 3-45 gives $N_{a,d}<0$.

The Error Function profile is given by

$$N_{a,d} = N_0(1 - \mathrm{erf}(mD))$$

where m is an argument factor which controls the length scale of the profile. The argument factor can be defined directly or calculated from a specified junction depth via:

$$m = \frac{1}{d_j}\mathrm{erfinv}\left(1 - \frac{N_b}{N_0}\right)$$

USING ANALYTIC AND GEOMETRIC DOPING FEATURES TOGETHER

A doping distribution can be created by combining the functionality of the two doping model features. Often it is desirable to specify a domain of constant doping using a user defined profile in the Analytic Doping Model feature, and then to set the profile away from this region using the Geometric Doping Model feature. This approach has the advantage that the constant user defined profile can be assigned to a domain of any shape, thus removing the requirement for the uniformly doped region to be block-shaped that is imposed by a Box profile. The use of the Geometric Doping Model to specify the profile away from the constant domain has the advantage that it can accommodate a constant region that has curved boundaries. This is because the Geometric Doping Model profile only depends on the distance from the selected boundaries, rather than on the coordinate system.

Equilibrium Carrier Concentrations

The carrier concentrations at equilibrium are given by the equations:

$$n = \int \frac{g_c(E)}{1 + \exp[(E - E_f)/(k_B T)]}dE$$

$$p = \int \frac{g_v(E)}{1 + \exp[(E_f - E_h)/(k_B T)]}dE$$

The variables W and W_h are defined such that $E = E_c + W$ and $E_h = E_v - W_h$. The density of states for electrons and holes then becomes (from Equation 3-21 and Equation 3-22):

$$g_c(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2} W^{1/2}$$

$$g_v(E) = \frac{1}{2\pi^2}\left(\frac{2m_h^*}{\hbar^2}\right)^{3/2} W_h^{1/2}$$

So the electron and hole densities are written in the form:

$$n = \frac{1}{4}\left(\frac{2m^*}{\pi\,\hbar^2}\right)^{3/2}\frac{2}{\pi^{1/2}}\int_0^\infty \frac{W^{1/2}}{1 + \exp[(W + E_c - E_f)/(k_B T)]}dW$$

$$p = \frac{1}{4}\left(\frac{2m_h^*}{\pi\,\hbar^2}\right)^{3/2}\frac{2}{\pi^{1/2}}\int_0^\infty \frac{W_h^{1/2}}{1 + \exp[(W_h + E_f - E_c)/(k_B T)]}dW_h$$

The following equations are obtained with the substitutions $\varepsilon = W/(k_B T)$:

$$n = 2\left(\frac{m^* k_B T}{2\pi\,\hbar^2}\right)^{3/2}\frac{2}{\pi^{1/2}}\int_0^\infty \frac{\varepsilon^{1/2}}{1 + \exp[\varepsilon - (E_f - E_c)/(k_B T)]}d\varepsilon$$

$$p = 2\left(\frac{m_h^* k_B T}{2\pi\,\hbar^2}\right)^{3/2}\frac{2}{\pi^{1/2}}\int_0^\infty \frac{\varepsilon_h^{1/2}}{1 + \exp[\varepsilon_h - (E_v - E_f)/(k_B T)]}d\varepsilon_h$$

The jth order *Fermi-Dirac integral* $(F_j(\eta))$ is defined in the following manner:

$$F_j(\eta) = \frac{1}{\Gamma(j+1)}\int_0^\infty \frac{\varepsilon^j}{1 + \exp[\varepsilon - \eta]}d\varepsilon = -\mathrm{Li}_{j+1}(-e^\eta) \qquad (3\text{-}46)$$

where Γ is the gamma function and Li the polylogarithm (see Ref. 15 for a brief review on the properties of the Fermi-Dirac integral). Note that $\Gamma(3/2) = \pi^{(1/2)}/2$. The electron and hole densities can be written in the compact forms:

$$n = N_c F_{1/2}\left(-\frac{E_c - E_f}{k_B T}\right)$$

$$p = N_v F_{1/2}\left(-\frac{E_f - E_v}{k_B T}\right) \qquad (3\text{-}47)$$

where:

$$N_c = 2\left(\frac{m^* k_B T}{2\pi \, \hbar^2}\right)^{3/2}$$

$$N_v = 2\left(\frac{m_h^* k_B T}{2\pi \, \hbar^2}\right)^{3/2}$$

(3-48)

One of the properties of the Fermi-Dirac integral is that $F_j(\eta) \to e^\eta$ as $\eta \to -\infty$ (this result applies for all j). In semiconductors this limit is known as the *nondegenerate limit* and is often applicable in the active region of semiconductor devices. In order to emphasize the nondegenerate limit, Equation 3-47 is rewritten in the form:

$$n = N_c \gamma_n \exp\left(-\frac{E_c - E_f}{k_B T}\right)$$

$$p = N_v \gamma_p \exp\left(-\frac{E_f - E_v}{k_B T}\right)$$

(3-49)

where:

$$\gamma_n = \frac{F_{1/2}\left(-\dfrac{E_c - E_f}{k_B T}\right)}{\exp\left(-\dfrac{E_c - E_f}{k_B T}\right)}$$

$$\gamma_p = \frac{F_{1/2}\left(-\dfrac{E_f - E_v}{k_B T}\right)}{\exp\left(-\dfrac{E_f - E_v}{k_B T}\right)}$$

(3-50)

In the nondegenerate limit, the *Fermi-Dirac distribution* reverts to the Maxwell-Boltzmann distribution and γ_n and γ_p are 1. By default, COMSOL Multiphysics uses Maxwell-Boltzmann statistics for the carriers, with γ_n and γ_p set to 1 in Equation 3-49, irrespective of the Fermi level. When Fermi-Dirac statistics are selected Equation 3-50 is used to define γ_n and γ_p.

In the **Semiconductor Equilibrium** study step, the above equations are used to express the carrier concentrations as functions of the electric potential, and the electric potential is solved via the resulting partial differential equations.

Away from equilibrium the above equations can still be applied but instead of using the Fermi level, the *quasi-Fermi level* is employed in Equation 3-41 and

Equation 3-42 (Ref. 11). For a detailed description of the origin of the quasi-Fermi levels for electrons and holes see The Semiconductor Equations. The final results are:

$$n = N_c F_{1/2}\left(\frac{E_{fn} - E_c}{k_B T}\right) = N_c \gamma_n \exp\left(-\frac{E_c - E_{fn}}{k_B T}\right)$$

$$p = N_v F_{1/2}\left(\frac{E_v - E_{fp}}{k_B T}\right) = N_v \gamma_p \exp\left(-\frac{E_{fp} - E_v}{k_B T}\right)$$

(3-51)

and:

$$\gamma_n = \frac{F_{1/2}\left(-\dfrac{E_c - E_{fn}}{k_B T}\right)}{\exp\left(-\dfrac{E_c - E_{fn}}{k_B T}\right)}$$

$$\gamma_p = \frac{F_{1/2}\left(-\dfrac{E_{fp} - E_v}{k_B T}\right)}{\exp\left(-\dfrac{E_{fp} - E_v}{k_B T}\right)}$$

(3-52)

The formulas above are used to compute the carrier concentrations as functions of the quasi-Fermi levels, when the quasi-Fermi level formulation is used. In other formulations where the carrier concentrations are solved for, the formulas above are used to compute the quasi-Fermi levels as functions of the carrier concentrations.

The Semiconductor Equations

NONUNIFORM BAND STRUCTURE AND THE REFERENCE ENERGY

Most practical simulations deal with a band structure that varies in space—it is therefore necessary to define quantities such as the band energies with respect to a reference energy. In order to make the definition of boundary conditions simpler, the reference energy chosen is the Fermi energy in an equilibrium state when no potentials are applied to any of the boundaries in the system and when there are no thermal gradients in the system (note that in COMSOL Multiphysics, the reference temperature used to define the equilibrium Fermi energy can be changed in the Semiconductor interface's Settings window under Reference Temperature). This is illustrated in Figure 3-7 for an isothermal, abrupt *p-n junction* (that is a boundary between a p- and n-doped region of a semiconductor with a constant doping level on the two sides of the device). In equilibrium the Fermi energy is well-defined and is

constant throughout space (since there are no gradients in the Fermi level/chemical potential). As a result in the immediate vicinity of the junction, the bands bend to accommodate a constant Fermi energy. In this region of *band bending* the Fermi level lies close to the center of the gap and consequently the carriers are depleted — this is known as the *depletion region*. A space charge layer is associated with the depletion region since the charges of the ionized donors and acceptors are no longer compensated by free carriers. It is the space charge layer that generates an electric field and the corresponding potential gradient that results in the bending of the vacuum level, E_0, and the conduction band and valence band edges (E_c and E_v, respectively). This results in a self-consistent picture of the band structure in the vicinity of the junction. As a result of the bending of the vacuum level and bands, a built-in potential, V_{bi}, develops across the junction. When an additional potential difference is applied to the p-side of the junction, V_p, the junction is in a condition known as reverse bias. The Fermi energy is no longer well-defined in the vicinity of the depletion region, but the equilibrium Fermi level, E_{f0} is still used as a reference potential. Away from the depletion region the semiconductor is close to equilibrium and the concept of the Fermi level can still be applied. On the p-side of the junction, the Fermi energy shifts up to a value E_{f1}, which differs from E_{f0} by qV_p where q is the electron charge.

In the most general case the electron affinity, $q\chi = E_0 - E_c$, and the band gap, $E_g = E_c - E_v$, can vary with position. However, the values can be considered to be material properties. This means that the conduction band edge cannot be parallel to the valence band edge or to the vacuum level (this is not shown in Figure 3-7).
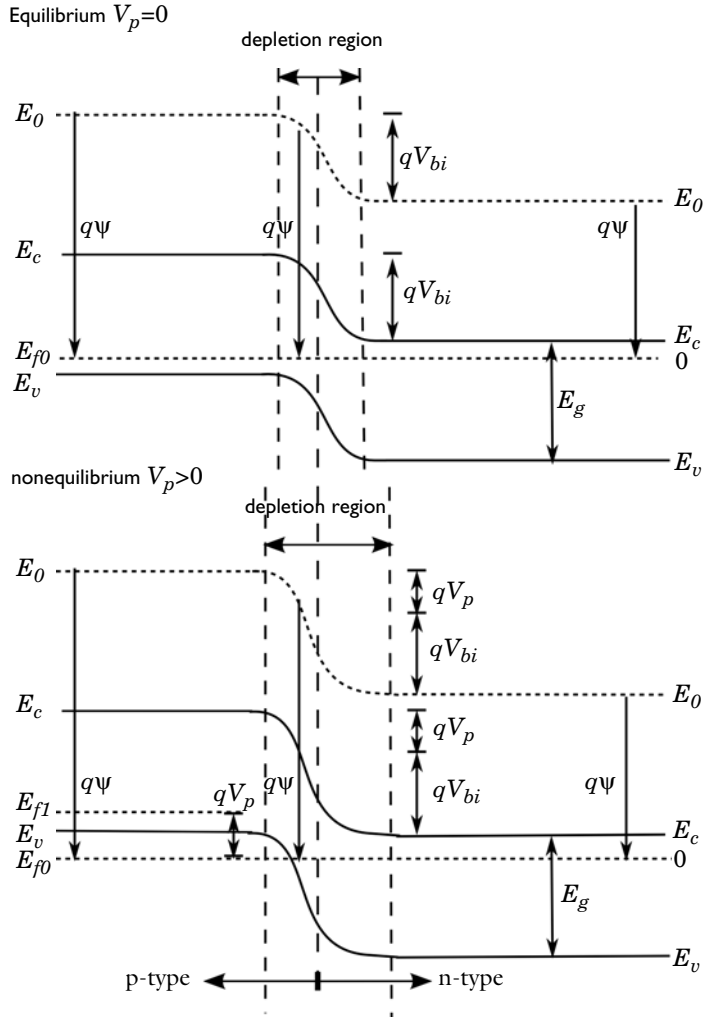
Figure 3-7: Diagram showing the variation in the band structure in a p-n diode. The horizontal axis represents position in the device and the vertical axis indicates energy. The vacuum level E_0, the bottom of the conduction band E_c, and the top of the valence band E_v, are shown. Top: The band structure when there is no applied potential. A built-in potential, V_{bi}, develops across the junction as a result of the space charge layers associated with the depletion region. The Fermi energy E_{f0}, is constant throughout the device. Bottom: A potential V_p is applied to the p-type side of the junction, resulting in a reverse bias. Away from the junction, where the material is close to equilibrium, a second Fermi level, E_{f1}, can be defined in the p-type region–shifted by the applied potential.

QUASI-FERMI LEVELS

Consider the motion of an individual electron moving in the curved conduction band (see Figure 3-8). In between collisions the energy of the electron remains approximately constant (although the force accelerates the electron, its velocity only increases slightly in between collisions). The energy of the electron measured with respect to the band edge, W, increases as a result of band bending. The total energy associated with an electron is given by:

$$E(\mathbf{k},\mathbf{r}) = E_c(\mathbf{r}) + W(\mathbf{k},\mathbf{r})$$

Similarly the energy of a hole is defined with respect to the band edge in the following manner:

$$E_h(\mathbf{k},\mathbf{r}) = E_v(\mathbf{r}) + W_h(\mathbf{k},\mathbf{r})$$
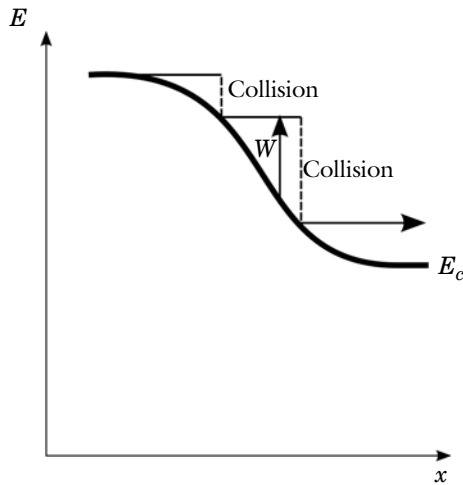
Figure 3-8: Motion of an individual electron within a curved band.

It is assumed that scattering processes within the band cause the electrons (or holes) to reach a collective equilibrium on timescales small compared to the simulation timescales (if highly nonequilibrium/hot electron effects are important within the band then it is necessary to account for the deviation of the Fermi function from a Fermi-Dirac distribution by solving an additional energy equation — currently this is not possible in the Semiconductor interface). Since the relaxation time for electrons within the conduction band is much less than the corresponding relaxation time for

transitions across the band gap, the electron and hole distributions can have different associated Fermi levels (E_{fn} for electrons and E_{fp} for holes). In nonequilibrium circumstances (for example in the presence of an electric field or a thermal gradient) these *quasi-Fermi levels* are not coincident. The electron and hole quasi-Fermi levels typically lie within the band gap and consequently the electrons are scattered to states close to the band edge as they travel through space, as shown in Figure 3-8.

SIMPLIFYING THE BOLTZMANN EQUATION

As discussed in The Semiclassical Model, the evolution of the distribution function for electrons and holes is governed by the Boltzmann equation (see Equation 3-40). Since this equation is difficult to solve, it is common to make simplifying approximations in its solution. Ultimately these approximations produce the drift-diffusion equations. The analysis presented here is based on Ref. 12 and Ref. 13.

The first step taken when simplifying the Boltzmann equation is usually to make the relaxation-time approximation, which assumes that the collision terms in the Boltzmann equations take the form:

$$\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} = -\frac{f - f_0(E, E_{fn}, T)}{\tau(W)}$$

$$\left[\frac{\partial f_h}{\partial t}\right]_{\text{coll}} = -\frac{f_h - f_0^h(E_h, E_{fn}, T)}{\tau_h(W_h)}$$

Where $f_0(E, E_{fn}, T)$ is the Fermi function for electrons and $f_0^h(E, E_{fp}, T)$ is the Fermi function for holes. This is essentially the simplest form of the collision term that returns the electrons to the Fermi-Dirac distribution desired. In practice this assumption is a significant simplification; Ref. 1 and Ref. 2 provide more detailed discussions of collision mechanisms in real solids.

From Hamilton's equations the spatial gradient of the electron total energy is equal to the rate of change of crystal momentum, which in turn is related to the applied force (Equation 3-35 in The Semiclassical Model), so that:

$$F = -\nabla E = -\nabla E_c - \nabla W$$

$$F_h = -\nabla E_h = \nabla E_v - \nabla W_h$$

Using these results the Boltzmann equations become

$$\frac{\partial f}{\partial t} - \frac{1}{\hbar}(\nabla E_c + \nabla W) \cdot \nabla_k f + \mathbf{v} \cdot \nabla_r f = -\frac{f - f_0}{\tau}$$

$$\frac{\partial f_h}{\partial t} + \frac{1}{\hbar}(\nabla E_v - \nabla W_h) \cdot \nabla_k f_h + \mathbf{v}_h \cdot \nabla_r f_h = -\frac{f_h - f_0^h}{\tau_h}$$

For compactness, the explicit dependence of f_0 and τ is dropped. Considering first the electron density, the assumption that the *electron distribution function* is close to its quasi-equilibrium state allows the distribution function to be written in the form:

$$f = f_0 + f_1$$

where $f_1 \ll f_0$. The spatial gradient terms are dominated by terms involving the gradient of f_0, so the f_1 terms are neglected in comparison to these. Likewise the term df/dt is also small since the deviation from the quasi-equilibrium is small and the f_0 term varies on timescales much slower than the collision time if the temperature is a function of time. The Boltzmann equation can be expressed in the approximate form:

$$\mathbf{v} \cdot \nabla_r f_0 - \frac{1}{\hbar}(\nabla E_c + \nabla W) \cdot \nabla_k f_0 = -\frac{f_1}{\tau} \tag{3-53}$$

Next the gradients in $f_0 = 1/(1 + \exp[(E\text{-}E_{fn})/(k_b T)])$ are expressed in terms of parameters related to the band structure, using the chain rule:

$$\nabla_k f_0 = \frac{\partial f_0}{\partial E} \nabla_k E = \hbar \, \mathbf{v} \frac{\partial f_0}{\partial E} \tag{3-54}$$

where the last step follows from the semiclassical definition of velocity (Equation 3-34 in The Semiclassical Model). From the chain rule the spatial gradient of f_0 is given by:

$$\nabla f_0 = \frac{\partial f_0}{\partial E} \nabla E + \frac{\partial f_0}{\partial E_{fn}} \nabla E_{fn} + \frac{\partial f_0}{\partial T} \nabla T$$

Since $f_0 = f_0([E\text{-}E_{fn}]/T)$:

$$\frac{1}{T}\frac{\partial f_0}{\partial E} = -\frac{1}{T}\frac{\partial f_0}{\partial E_{fn}} = -\frac{E - E_{fn}}{T^2}\frac{\partial f_0}{\partial E}$$

therefore:

$$\nabla f_0 = \frac{\partial f_0}{\partial E}\left(\nabla E - \nabla E_{fn} - \frac{E - E_{fn}}{T^2}\nabla T\right) \tag{3-55}$$

Substituting Equation 3-55 and Equation 3-54 into Equation 3-53, using the definition $E = E_c + W$ and rearranging gives:

$$f_1 = -\tau\frac{\partial f_0}{\partial E}\left(\mathbf{v}\cdot\nabla E_{fn} + \frac{E - E_{fn}}{T^2}\mathbf{v}\cdot\nabla T\right)$$

By definition the number of electrons is given by:

$$n = \frac{1}{4\pi^3}\int fg(\mathbf{k})d^3\mathbf{k} = \frac{1}{4\pi^3}\int f_0 g(\mathbf{k})d^3\mathbf{k}$$

The final equality holds because f_1 is an odd function when integrated over the region of k-space in the vicinity of a band edge and f_0 is an even function (assuming, without loss of generality, that the origin of k-space at the band minimum). To see why this is the case, consider Equation 3-38 in The Semiclassical Model (shown below for convenience).

$$\mathbf{J}_n(\mathbf{r},t) = -\frac{q}{4\pi^3}\int \mathbf{v}(\mathbf{k})f(\mathbf{k},\mathbf{r},t)d^3\mathbf{k} = -\frac{q}{4\pi^3}\int \frac{1}{\hbar}\frac{\partial E(\mathbf{k})}{\partial \mathbf{k}}f(\mathbf{k},\mathbf{r},t)d^3\mathbf{k}$$

In equilibrium ($f = f_0$) no current flows so the integrand must be an odd function (since it is not zero over all k-space). Since the origin is at a band minimum, $\partial E(\mathbf{k})/\partial\mathbf{k}$ is odd so f_0 must be even. Deviations from equilibrium produce a current without changing the total number of electrons, so f_1 must be an odd function. The electron current density can be written in the form:

$$\mathbf{J}_n(\mathbf{r},t) = -\frac{q}{4\pi^3}\int \mathbf{v}(\mathbf{k})f_1 d^3\mathbf{k} = \frac{q}{4\pi^3}\left(\int \tau\frac{\partial f_0}{\partial E}\mathbf{v}\mathbf{v}^T d^3\mathbf{k}\cdot\nabla E_{fn}\right.$$
$$\left. + \frac{E_c - E_{fn}}{T^2}\int \tau\frac{\partial f_0}{\partial E}\mathbf{v}\mathbf{v}^T d^3\mathbf{k}\cdot\nabla T + \frac{1}{T}\int \tau\frac{\partial f_0}{\partial E}W\mathbf{v}\mathbf{v}^T d^3\mathbf{k}\cdot\nabla T\right)$$

Note that the definition $E = E_c + W$ is used to split the energy terms.

The rigid band assumption is made next. This asserts that even when the bands bend, the functional form of W in k-space (measured with respect to the band edge) is unchanged. Thus $W = W(\mathbf{k})$. Given this assumption the quantities inside the integrals are dependent only on the local band structure, except for the df_0/dE term.

Next define the quantities:

$$\mu_n = -\frac{q}{4\pi^3 n} \int \tau \frac{\partial f_0}{\partial E} \mathbf{v} \mathbf{v}^T d^3 \mathbf{k} \tag{3-56}$$

$$Q_n = -\frac{q}{4\pi^3 n} \int \tau \frac{\partial f_0}{\partial E} W \mathbf{v} \mathbf{v}^T d^3 \mathbf{k} \tag{3-57}$$

To obtain:

$$\mathbf{J}_n(\mathbf{r},t) = n\mu_n \nabla E_{fn} + \frac{n}{T}((E_c - E_{fn})\mu_n + qQ_n)\nabla T \tag{3-58}$$

Q_n and μ_n are tensor quantities (although most semiconducting materials are cubic) so that the corresponding tensors are diagonal with identical elements and consequently can be represented by means of a scalar (cubic materials are assumed in the Semiconductor interface). Careful examination of Equation 3-56 and Equation 3-57 shows that these cannot straightforwardly be considered material constants because both depend on the quasi-Fermi level through the quantities df_0/dE and $1/n$. In the nondegenerate limit, the quasi-Fermi level dependence of these two quantities cancels out, since:

$$1/n \propto \exp[-E_{fn}/(k_B T)] \text{ and } \partial f_0/\partial E \propto \exp[-E_{fn}/(k_B T)]$$

These quantities can therefore only strictly be considered material constants in the nondegenerate limit. In the degenerate limit it is, however, possible to relate Q_n to the mobility for specific models for the relaxation time (see below). In principle a mobility model could be used, which is dependent on the electron quasi-Fermi level (or the electron density) in the degenerate limit.

Exactly the same arguments are applied for holes, leading to the equation for the hole current:

$$\mathbf{J}_p(\mathbf{r},t) = -p\mu_p \nabla E_{fp} - \frac{p}{T}((E_v - E_{fp})\mu_p + qQ_p)\nabla T \tag{3-59}$$

Here, the symbols introduced with the subscript change $n \rightarrow p$ have the same definitions as the electron quantities except that the relevant integrals are over the hole band.

Equation 3-58 and Equation 3-59 describe the evolution of the quasi-Fermi levels within a semiconductor. It is possible to formulate the whole equation system so that the hole and electron quasi-Fermi levels are the dependent variables, which is one of

the discretization options available in the Semiconductor Module (the quasi-Fermi level formulation). Before deriving the more familiar drift-diffusion equations it is useful to derive the relationship between Q_n and μ_n, and Q_p and μ_p.

RELATING Q_n TO μ_n

For isotropic materials within the rigid band approximation, Equation 3-20 can be written as:

$$W(\mathbf{k}) = E(\mathbf{k},\mathbf{r}) - E_c(\mathbf{r}) = \frac{\hbar^2}{m^*}(k_x^2 + k_y^2 + k_z^2) \qquad (3\text{-}60)$$

Since $E_c(\mathbf{r})$ is independent of $\mathbf{k}$ the derivatives with respect to E can be replaced by derivatives with respect to W, enabling the (scalar) mobility to be written as:

$$\mu_n = -\frac{q}{4\hbar^2\pi^3 n}\int \tau \frac{\partial f_0}{\partial W}\left(\frac{\partial W(\mathbf{k})}{\partial k_x}\right)^2 d^3\mathbf{k}$$

where the semiclassical result $\mathbf{v}=(1/\hbar)(\partial E(\mathbf{k})/\partial \mathrm{k})$ is used and the xx element of the mobility tensor is evaluated to compute the scalar (the yy and zz elements produce the same result). From Equation 3-60:

$$\frac{\partial W(\mathbf{k})}{\partial k_x} = \frac{2\hbar^2 k_x}{m^*}$$

The integral in the mobility expression can be transformed to spherical polar coordinates using the definitions:

$$k_x = k\sin(\theta)\cos(\phi)$$
$$k_y = k\sin(\theta)\sin(\phi)$$
$$k_x = k\cos(\theta)$$

and a functional form can be assumed for the relaxation time:

$$\tau(W) = \tau_0 W^r \qquad (3\text{-}61)$$

In Equation 3-61 $r = -1/2$ corresponds to acoustic phonon scattering and $r = 3/2$ is appropriate for ionized impurity scattering (Ref. 14). In general r can be considered a function of temperature. In COMSOL Multiphysics, r is assumed to be $-1/2$.

The mobility integral can now be written as:

$$\mu_n = -\frac{q\tau_0}{4\,\hbar^2\pi^3 n}\int W^r\frac{\partial f_0}{\partial W}\left(\frac{k\sin(\theta)\cos(\phi)}{m^*}\right)^2 k^2\sin(\theta)dkd\theta d\phi$$

To transform the integral over k to an integral over W note that $W = h^2 k^2/(2m^*)$ so that $dk = (m^*/2\,\hbar^2)^{1/2}W^{-1/2}dW$. Writing each quantity in the integral as a function of W and rearranging gives:

$$\mu_n = -\frac{q\tau_0\sqrt{m^*}}{\sqrt{2}\,\hbar^3\pi^3 n}\int_0^\infty W^{r+3/2}\frac{\partial f_0}{\partial W}dW\int_0^\pi \sin^3(\theta)d\theta\int_0^{2\pi}\cos^2(\phi)d\phi$$

Evaluating the angular integrals and integrating the energy integral by parts gives:

$$\mu_n = \frac{q\tau_0\sqrt{8m^*}}{3\,\hbar^3\pi^2 n}\left(r+\frac{3}{2}\right)\int_0^\infty W^{r+1/2}f_0 dW \qquad (3\text{-}62)$$

Where the result:

$$[W^{r+3/2}f_0]_{W=0}^\infty = 0$$

is used. Equation 3-62 can be rewritten in the form:

$$\mu_n = \frac{q\tau_0\sqrt{8m^*}}{3\,\hbar^3\pi^2 n}\left(r+\frac{3}{2}\right)(k_B T)^{r+3/2}\Gamma(r+3/2)F_{r+1/2}\left(-\frac{E_c - E_{fn}}{k_B T}\right) \qquad (3\text{-}63)$$

where the definition of the Fermi-Dirac function (Equation 3-46) and of f_0 (Equation 3-5) is used.

Following the same procedure for Q_n gives:

$$Q_n = \frac{\tau_0\sqrt{8m^*}}{3\,\hbar^3\pi^2 n}\left(r+\frac{5}{2}\right)(k_B T)^{r+5/2}\Gamma(r+5/2)F_{r+3/2}\left(-\frac{E_c - E_{fn}}{k_B T}\right) \qquad (3\text{-}64)$$

Equation 3-63 and Equation 3-64 show that Q_n can be related to μ_n:

$$Q_n = \frac{k_B T}{q}\left(r+\frac{5}{2}\right)\frac{F_{r+3/2}\left(-\dfrac{E_c - E_{fn}}{k_B T}\right)}{F_{r+1/2}\left(-\dfrac{E_c - E_{fn}}{k_B T}\right)}\mu_n \qquad (3\text{-}65)$$

where the result $\Gamma(j+1) = j\Gamma(j)$ is used.

Similarly Q_p is related to μ_p in exactly the same manner:

$$Q_p = \frac{k_B T}{q}\left(r + \frac{5}{2}\right)\frac{F_{r+3/2}\left(-\dfrac{E_{fp} - E_v}{k_B T}\right)}{F_{r+1/2}\left(-\dfrac{E_{fp} - E_v}{k_B T}\right)}\mu_p \tag{3-66}$$

In COMSOL Q_n and Q_p are computed from μ_n and μ_p using Equation 3-65 and Equation 3-66 with $r=-1/2$. Note that in the nondegenerate limit:

$$Q_n = \frac{k_B T}{q}\left(r + \frac{5}{2}\right)\mu_n$$

$$Q_p = \frac{k_B T}{q}\left(r + \frac{5}{2}\right)\mu_p$$

THE DRIFT-DIFFUSION EQUATIONS

Having related Q_n and Q_p to the corresponding mobilities the next task is to derive equations relating the current to the carrier concentrations from Equation 3-58 and Equation 3-59. Once again the case of electrons is considered in detail and the results for holes are similar.

Inverting Equation 3-51 gives the following equation for the electron quasi-Fermi level:

$$E_{fn} = E_c + k_B T F_{1/2}^{-1}\left(\frac{n}{N_c}\right) \tag{3-67}$$

where we have defined the inverse Fermi-Dirac integral ($F_{1/2}^{-1}(\alpha)=\eta$ implies that $\alpha=F_{1/2}(\eta)$). Let $\alpha=n/N_c$ and $\eta=F_{1/2}^{-1}(\alpha)$. To obtain the drift-diffusion equations Equation 3-67 is substituted into Equation 3-58. Note that $N_c=N_c(T)$ so that $\eta=F_{1/2}^{-1}(n/N_c)=\eta(n,T)$. To compute the current the gradient of the quasi-Fermi level is required:

$$\nabla E_{fn} = \nabla E_c + \nabla(k_B T\eta) = \nabla E_c + \eta k_B \nabla T + k_B T\frac{\partial\eta}{\partial T}\nabla T + k_B T\frac{\partial\eta}{\partial n}\nabla n$$

Since $\alpha=n/N_c$ and $N_c\propto T^{3/2}$ (Equation 3-48):

$$\frac{\partial\eta}{\partial n} = \frac{\partial\alpha}{\partial n}\frac{d\eta}{d\alpha} = \frac{\alpha}{n}\frac{d\eta}{d\alpha}$$

$$\frac{\partial\eta}{\partial T} = \frac{\partial\alpha}{\partial T}\frac{d\eta}{d\alpha} = -\frac{3}{2}\frac{\alpha}{T}\frac{d\eta}{d\alpha} \tag{3-68}$$

In order to evaluate $\partial\eta/\partial\alpha$ the result $dF_n(\eta)/d\eta=F_{n-1}(\eta)$ is required (see Ref. 15 for details). Given this result:

$$\frac{dF_{1/2}(\eta)}{d\eta} = F_{-1/2}(\eta) = \frac{d\alpha}{d\eta}$$

so that:

$$\frac{d\eta}{d\alpha} = \frac{1}{F_{-1/2}(\eta)} \tag{3-69}$$

Substituting Equation 3-68 and Equation 3-69 into Equation 3-46 and then using $\alpha = F_{1/2}(\eta)$ gives:

$$\nabla E_{fn} = \nabla E_c + \eta k_B \nabla T - \frac{3}{2}\frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)} k_B \nabla T + \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)}\frac{k_B T}{n}\nabla n \tag{3-70}$$

Substituting Equation 3-70 into Equation 3-58 gives:

$$\mathbf{J}_n(\mathbf{r},t) = n\mu_n \nabla E_c + \mu_n k_B T \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)}\nabla n + \frac{n}{T}\left(qQ_n - \frac{3}{2}\mu_n k_B T \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)}\right)\nabla T$$

where the result $\eta = (E_{fn} - E_c)/(k_B T)$ is used and follows from Equation 3-67.

Defining the function:

$$G(\alpha) = \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)} = \frac{\alpha}{F_{-1/2}(F_{1/2}^{-1}(\alpha))} \qquad \eta = F_{1/2}^{-1}(\alpha)$$

This result can be written in the form:

$$\mathbf{J}_n(\mathbf{r},t) = n\mu_n \nabla E_c + \mu_n k_B T G(n/N_c)\nabla n + \frac{nq}{T}D_{n,th}\nabla T \tag{3-71}$$

Following the same argument for the hole current gives:

$$\mathbf{J}_p(\mathbf{r},t) = p\mu_p \nabla E_v - \mu_p k_B T G(p/N_v)\nabla p - \frac{pq}{T}D_{p,th}\nabla T \tag{3-72}$$

The thermal diffusion coefficients $D_{n,th}$ and $D_{p,th}$ are defined as:

$$D_{n,th} = Q_n - \frac{3}{2}\frac{k_B T}{q}G(n/N_c)\mu_n$$

$$D_{p,th} = Q_p - \frac{3}{2}\frac{k_B T}{q}G(p/N_v)\mu_p$$

In the nondegenerate limit $G(\alpha)\rightarrow 1$ and the following equations are obtained:

$$\mathbf{J}_n(\mathbf{r},t) = n\mu_n\nabla E_c + \mu_n k_B T\nabla n + (r+1)n\mu_n k_B\nabla T$$

$$\mathbf{J}_p(\mathbf{r},t) = p\mu_p\nabla E_v - \mu_p k_B T\nabla p - (r+1)p\mu_p k_B\nabla T$$

For a relaxation time dominated by phonon scattering (currently assumed by the COMSOL software) $r = -1/2$.

POISSON'S EQUATION AND THE CONTINUITY EQUATIONS

Equation 3-71 and Equation 3-72 define the hole and electron currents used by COMSOL Multiphysics in the Semiconductor interface. To solve a model the Semiconductor interface uses these definitions in combination with Poisson's equation and the current continuity equations.

Poisson's equation takes the form:

$$\nabla \cdot (-\varepsilon_r\nabla V) = q(p - n + N_d^+ - N_a^-) \qquad (3\text{-}73)$$

and the current continuity equations are given by:

$$\frac{\partial n}{\partial t} = \frac{1}{q}(\nabla \cdot \mathbf{J}_n) - U_n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}(\nabla \cdot \mathbf{J}_p) - U_p \qquad (3\text{-}74)$$

where $U_n = \Sigma R_{n,i} - \Sigma G_{n,i}$ is the net electron *recombination* rate from all *generation* $(G_{n,i})$ and recombination mechanisms $(R_{n,i})$. Similarly, U_p is the net hole recombination rate from all generation $(G_{p,i})$ and recombination mechanisms $(R_{p,i})$. Note that in most circumstances $U_n = U_p$. Both of these equations follow directly from Maxwell's equations (see Ref. 6).

The **Semiconductor** interface solves Equations 3-73 and 3-74. The current densities $\mathbf{J}_n$ and $\mathbf{J}_p$ are given by Equation 3-71 and Equation 3-72, if the dependent variables are the carrier concentrations or the log of the concentrations. For the quasi-Fermi level formulation, Equation 3-58 and Equation 3-59 are used for the current densities.

Mobility Models

In The Semiconductor Equations section, a closed-form expression was computed for the electron and hole mobilities by making the relaxation-time approximation and by assuming a particular form for the scattering time as a function of energy. Any mechanism that disturbs the perfect periodicity of the lattice can produce scattering of the carriers. Such mechanisms include:

- Phonons (L): Thermally generated acoustic waves traveling through the crystal (scattering by phonons is frequently referred to as lattice scattering, which is somewhat confusing as the lattice itself never scatters the carriers unless perturbed from perfect periodicity).

- Ionized impurities (I): These begin to have an effect at doping levels above approximately 10^{15} cm^{-3} at room temperature.

- Carrier-carrier scattering (C).

- Neutral impurity scattering (N): This is important at low temperatures only, typically below 77K.

- High field velocity saturation (E).

- Surface scattering (S): This includes effects such as interface charges, scattering by surface phonons, and so on. It is important in field effect devices, such as field effect transistors.

In the Semiconductor interface, the letters in brackets in the list above are used to label the effects included in a specific mobility model (the convention used in Ref. 6 is adopted).

In practice the mobility is typically computed using analytic functions with or without a rigorous physical motivation and designed to fit the experimental data to a good degree of accuracy. Often, mobility models are designed to address one particular effect (for example high field velocity saturation) and require other mobility models as a basis (for example a model incorporating scattering due to phonons and impurities). As an example, high field effects are often incorporated into a model by defining the high field mobility as a function of the mobility due to phonon and impurity scattering. In other cases the scattering due to different mechanisms is combined using *Matthiessen's rule* — an approximate method for combining mobilities that, while not rigorously correct, is frequently employed to produce empirical fits to experimental data in the context of mobility models. Matthiessen's rule combines mobilities in the following manner:

$$\frac{1}{\mu_{tot}} = \frac{1}{\mu_1} + \frac{1}{\mu_2}$$

An example of the manner in which mobility models are often combined is:

$$\mu_{tot} = \mu_E(\mu_S(\mu_{LI})) \qquad (3\text{-}75)$$

where μ_E, the mobility including high field effects, is a function of μ_s (the surface mobility), which in turn is a function of the mobility model for phonon (or lattice) and impurity scattering (μ_{LI}).

COMSOL Multiphysics uses a general mechanism to combine both user-defined and predefined mobility models that accommodate combinations of the form given in Equation 3-75. Mobility models are added as subnodes to the Semiconductor Material Model node. If the mobility model requires an input mobility, this is selected from the available mobilities appropriate for this model (individual selections are required for both the electron and hole mobility inputs). Multiple user-defined mobility models can be added and these can be used as inputs to predefined or other user-defined mobility models. The user-defined mobility models are always available as inputs in predefined mobility models (if the model requires an input). Within this system it is possible to mix user-defined mobility models with models predefined by COMSOL Multiphysics in a very general manner. The model used within the simulation is selected for electrons and holes by changing the electron mobility and the hole mobility settings in the Mobility Model section of the Semiconductor Material Model node, which by default uses a constant mobility obtained from the material properties.

| ! | It is important to understand that each type of mobility model subnode only defines mobility variables for electrons and holes that can be used by other models, or by the Semiconductor Material Model node. The mobility models for electrons and holes actually used in the simulation are determined by the selections or settings in the Semiconductor Material Model node (the parent node) which do not change when additional mobility models are added. In order to add a mobility model to a simulation it is therefore necessary to both add the sequence of mobility model subnodes to the model tree and then to *select the desired final mobility for both electrons and holes in the Semiconductor Material Model node*. |

The following sections describe the predefined mobility models currently available in the Semiconductor interface.

THEORY FOR THE POWER LAW MOBILITY MODEL (L)

The Power Law Mobility Model (L) is a simple mobility model and requires no input as it includes scattering due to phonons. The electron ($\mu_{n,pl}$) and hole ($\mu_{p,pl}$) mobilities are determined by the equations:

$$\mu_{n,pl} = \mu_{0,n}\left(\frac{T}{T_{ref}}\right)^{-\alpha_n} \qquad \mu_{p,pl} = \mu_{0,p}\left(\frac{T}{T_{ref}}\right)^{-\alpha_p}$$

where T is the lattice temperature and $\mu_{p,pl}$, $\mu_{p,pl}$, α_n, α_p, and T_{ref} are material properties. For silicon the values of the material properties are taken from Ref. 16.

THEORY FOR THE ARORA MOBILITY MODEL (LI)

The empirical Arora Mobility Model (LI) includes both phonon and impurity scattering. The electron ($\mu_{n,ar}$) and hole ($\mu_{p,ar}$) mobilities are determined by the equations:

$$\mu_{n,ar} = \mu_{min,n} + \frac{\mu_{0,n}}{1 + \left(\frac{N}{N_{0,n}}\right)^{\alpha}} \qquad \mu_{p,ar} = \mu_{min,p} + \frac{\mu_{0,p}}{1 + \left(\frac{N}{N_{0,p}}\right)^{\alpha}}$$

$$\mu_{min,n} = \mu_{min,n}^{ref}\left(\frac{T}{T_{ref}}\right)^{\beta_1} \qquad \mu_{min,p} = \mu_{min,p}^{ref}\left(\frac{T}{T_{ref}}\right)^{\beta_1}$$

$$\mu_{0,n} = \mu_{0,n}^{ref}\left(\frac{T}{T_{ref}}\right)^{\beta_2} \qquad \mu_{0,p} = \mu_{0,p}^{ref}\left(\frac{T}{T_{ref}}\right)^{\beta_2}$$

$$N_{0,n} = N_{0,n}^{ref}\left(\frac{T}{T_{ref}}\right)^{\beta_3} \qquad N_{0,p} = N_{0,p}^{ref}\left(\frac{T}{T_{ref}}\right)^{\beta_3}$$

$$\alpha = \alpha_{0,n}^{ref}\left(\frac{T}{T_{ref}}\right)^{\beta_4} \qquad N = N_a^- + N_d^+$$

where T is the lattice temperature, N_a^- is the ionized acceptor concentration, and N_d^+ is the ionized donor concentration. All the other parameters are material properties. For silicon the values of the material properties are taken from Ref. 16.

THEORY FOR THE FLETCHER MOBILITY MODEL (C)

The Fletcher Mobility Model (C) adds carrier-carrier scattering to an existing mobility model (or to a constant input mobility). It accepts input mobilities of type L or LI, as well as user-defined input mobilities.

The model uses Matthiessen's rule to combine the input mobility with a carrier-carrier scattering mobility term that is identical for electrons and holes. The model is based on Ref. 17. The electron ($\mu_{n,ar}$) and hole ($\mu_{p,ar}$) mobilities are determined by the equations:

$$\frac{1}{\mu_{n,fl}} = \frac{1}{\mu_{in,n}} + \frac{1}{\mu_{cc}} \qquad \frac{1}{\mu_{p,fl}} = \frac{1}{\mu_{in,p}} + \frac{1}{\mu_{cc}}$$

$$\mu_{cc} = \frac{\left(\dfrac{T}{T_{ref}}\right)^{3/2} F_1}{(np)^{1/2} \ln\left(1 + \left(\dfrac{T}{T_{ref}}\right)^2 (np)^{-1/3} F_2\right)}$$

where T is the lattice temperature, $\mu_{in,n}$ and $\mu_{in,p}$ are the electron and hole input mobilities, n is the electron concentration, and p is the hole concentration. F_1 (SI unit: $s^2 A/(m^3 kg)$), F_2 (SI unit: $1/m^2$), and T_{ref} are material properties. For silicon the values of the material properties are taken from Ref. 18.

THEORY FOR THE LOMBARDI SURFACE MOBILITY MODEL (S)

The Lombardi Surface Mobility Model (S) adds surface scattering resulting from surface acoustic phonons and from surface roughness. Mobility contributions corresponding to these effects are combined with the input mobility using Matthiessen's rule. The model accepts input mobilities of type L, LI, or C as well as user defined input mobilities. The model is based on Ref. 19. The electron ($\mu_{n,lo}$) and hole ($\mu_{p,lo}$) mobilities are determined by the following equations:

$$\frac{1}{\mu_{n,lo}} = \frac{1}{\mu_{in,n}} + \frac{1}{\mu_{ac,n}} + \frac{1}{\mu_{sr,n}} \qquad \frac{1}{\mu_{p,lo}} = \frac{1}{\mu_{in,p}} + \frac{1}{\mu_{ac,p}} + \frac{1}{\mu_{sr,p}}$$

$$\mu_{ac,n} = \frac{\mu_{1,n}}{\left(\dfrac{E_{\perp,n}}{E_{ref}}\right)} + \frac{\mu_{2,n}\left(\dfrac{N}{N_{ref}}\right)^{\alpha_n}}{\left(\dfrac{E_{\perp,n}}{E_{ref}}\right)^{1/3}\left(\dfrac{T}{T_{ref}}\right)} \qquad \mu_{ac,p} = \frac{\mu_{1,p}}{\left(\dfrac{E_{\perp,p}}{E_{ref}}\right)} + \frac{\mu_{2,p}\left(\dfrac{N}{N_{ref}}\right)^{\alpha_p}}{\left(\dfrac{E_{\perp,p}}{E_{ref}}\right)^{1/3}\left(\dfrac{T}{T_{ref}}\right)}$$

$$\mu_{sr,n} = \frac{\delta_n}{E_{\perp,n}^2} \qquad\qquad \mu_{sr,p} = \frac{\delta_p}{E_{\perp,p}^2}$$

$$N = N_a^- + N_d^+$$

where T is the lattice temperature, $\mu_{in,n}$ and $\mu_{in,p}$ are the electron and hole input mobilities, N_a^- is the ionized acceptor concentration, N_d^+ is the ionized donor concentration, $E_{\perp,n}$ is the component of the electric field perpendicular to the

electron current and $E_{\perp,p}$ is the component of the electric field perpendicular to the hole current. All other parameters in the model are material properties (note that δ_n and δ_p have units of V/s). The material properties for silicon are also obtained from this reference Ref. 19.

THEORY FOR THE CAUGHEY-THOMAS MOBILITY MODEL (E)

The Caughey-Thomas Mobility Model (E) adds high field velocity scattering to an existing mobility model (or to a constant input mobility). It accepts input mobilities of type L, LI, C, or S as well as user defined input mobilities. The model is based on Ref. 20. The electron ($\mu_{n,lo}$) and hole ($\mu_{p,lo}$) mobilities are determined by the following equations:

$$\mu_{n,ct} = \frac{\mu_{in,n}}{\left(1 + \left(\frac{\mu_{in,n}F_n}{v_{sat,n}}\right)^{\alpha_n}\right)^{1/\alpha_n}} \qquad \mu_{p,ct} = \frac{\mu_{in,p}}{\left(1 + \left(\frac{\mu_{in,p}F_p}{v_{sat,p}}\right)^{\alpha_p}\right)^{1/\alpha_p}}$$

$$\alpha_n = \alpha_{n,0}\left(\frac{T}{T_{ref}}\right)^{\beta_{n,1}} \qquad \alpha_p = \alpha_{p,0}\left(\frac{T}{T_{ref}}\right)^{\beta_{p,1}}$$

$$v_{sat,n} = v_{n,0}\left(\frac{T}{T_{ref}}\right)^{\beta_{n,2}} \qquad v_{sat,p} = v_{p,0}\left(\frac{T}{T_{ref}}\right)^{\beta_{p,2}}$$

where T is the lattice temperature, $\mu_{in,n}$ and $\mu_{in,p}$ are the electron and hole input mobilities and F_n and F_p are the driving forces for electrons and holes (currently $F_n = E_{||,n}$ and $F_p = E_{||,p}$ where $E_{||,n}$ is the component of the electric field parallel to the electron current and $E_{||,p}$ is the component of the electric field parallel to the electron current). All other parameters in the model are material properties (note that $v_{n,0}$ and $v_{p,0}$ are the saturation velocities for electrons and holes and have units of m/s). The material properties for silicon are also obtained from Ref. 20.

THEORY FOR THE USER-DEFINED MOBILITY MODEL

The User-Defined Mobility Model can be used to create electron and hole mobilities with user-defined expressions for the electron and hole mobilities. These mobility models can be combined with other user-defined or predefined mobility models in arbitrary combinations. These mobility models can take other defined mobilities as inputs. By default the output mobility is set to the input mobility for both electrons and holes. However, it is possible to change the expression for the output mobility so that it is any function of the input mobility (or indeed a function that does not depend

on the input mobility). The default value is set in this way to make it straightforward to access the variable in which the input mobility is stored.

	In the finite volume method, the dependent variables are constant within each mesh element and the gradients cannot be defined using the differentiation operator in COMSOL. A detailed understanding of the finite volume method is required in order to set up mobility models that depend on the gradients of the dependent variables in COMSOL (∇n, ∇p, and ∇V). These variables include the currents $\mathbf{j}_n$ and $\mathbf{j}_p$, the electric field $\mathbf{E}$, and the electric displacement field $\mathbf{D}$, as well as the gradients of the quasi-Fermi levels ∇E_{fn} and ∇E_{fp}. In the finite element method these limitations do not apply and the gradients of the dependent variables (and quantities which depend on them) can be used in expressions.

	Defining the Carrier Mobility

Traps

Many semiconductor devices contain a distribution of traps within the band gap. These traps are associated with donor and acceptor atoms, with other impurity atoms in the bulk of the semiconductor, or with "dangling bonds" that occur at defects or exterior surfaces and grain boundaries. It is useful to consider the processes that can occur when trap states at a given energy, E_t, exchange electrons or holes with states in the valence or conduction bands at energy E. This situation is depicted in Figure 3-9. There are four processes that occur, corresponding to the emission and capture of both electrons and holes between states in the bands
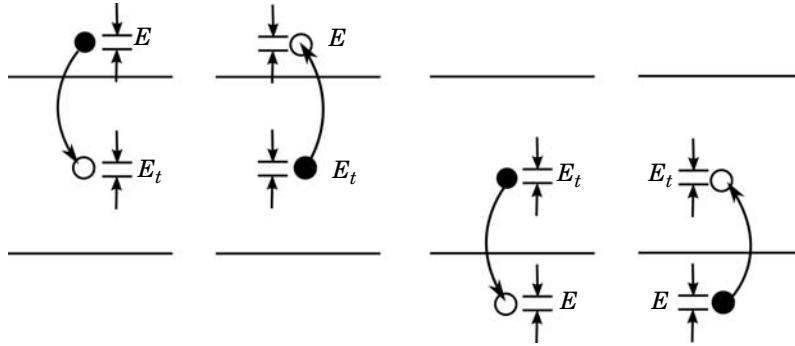
Figure 3-9: The four processes that contribute to SRH recombination. Left: An electron in the conduction band with energy E is captured by a trap with energy E_t (ec). Center left: An electron in a trap at energy E_t is emitted to an empty state with energy E in the conduction band (ee). Center right: An electron in a trap at energy E_t moves to an empty state in the valence band at energy E. Equivalently a hole in the valence band is trapped (hc). Right: An electron from an occupied state in the valence band at energy E is excited into a trap with energy E_t. Equivalently a hole in the trap is emitted (he).

In practice you may want to consider a set of discrete trap levels or a continuum of trap states (with a density of states $g_t(E_t)$). Both of these approaches can be accommodated by defining N_t, the density of traps per unit volume at a particular trap energy, E_t. For a continuum of trap states, N_t is given by:

$$N_t = g_t(E_t)dE_t$$

For the trap energy E_t, carriers in the conduction band or valence band with energy E make the following contributions to the total recombination or generation rate per unit volume for each process:

$$
\begin{aligned}
dr_{ec} &= f(E)g_c(E)(1-f_t)N_tc_{ec}(E)dE \\
dg_{ee} &= (1-f(E))g_c(E)f_tN_tc_{ee}(E)dE \\
dr_{hc} &= (1-f(E))g_v(E)f_tN_tc_{hc}(E)dE \\
dg_{he} &= f(E)g_v(E)(1-f_t)N_tc_{he}(E)dE
\end{aligned}
\tag{3-76}
$$

where N_t is the number of traps per unit volume, f_t is the trap electron occupancy (between 0 and 1), $g_c(E)$ is the conduction band density of states, $g_v(E)$ is the valence band density of states, and $c_{ec}(E)$, $c_{ee}(E)$, $c_{hc}(E)$, and $c_{he}(E)$ are rate constants. The net rate of capture for electrons and holes in the energy interval dE can be written as:

$$dr_e = [f(E)(1-f_t)c_{ec}(E) - (1-f(E))f_t c_{ee}(E)]g_c(E)N_t dE$$

$$dr_h = [(1-f(E))c_{hc}(E)f_t - f(E)(1-f_t)c_{he}(E)]g_v(E)N_t dE$$

(3-77)

In thermal equilibrium the principle of detailed balance implies the reversibility of each microscopic process that leads to equilibrium. Consequently, at equilibrium, the expressions in the square brackets must be equal to zero. This leads to the following relationships between the rate constants:

$$c_{ee}(E) = \frac{f(E)}{1-f(E)}\frac{1-f_t}{f_t}c_{ec}(E)$$

$$c_{he}(E) = \frac{1-f(E)}{f(E)}\frac{f_t}{1-f_t}c_{hc}(E)$$

In thermal equilibrium the occupancy of the electron traps f_t is determined by Fermi-Dirac statistics, $f_{te}=1/(1+\exp[(E_t-E_f)/(k_BT)]/g_D)$ (where g_D is the degeneracy factor). The above equations can be simplified to yield:

$$c_{ee}(E) = \frac{1}{g_D}\exp\left(-\frac{E-E_t}{k_BT}\right)c_{ec}(E)$$

$$c_{he}(E) = g_D\exp\left(-\frac{E_t-E}{k_BT}\right)c_{hc}(E)$$

(3-78)

Equation 3-78 applies even away from equilibrium. Substituting this equation back into Equation 3-77, rearranging and integrating, gives the total rate of electron (r_e) or hole (r_h) capture to traps at the specified energy, E_t:

$$r_e = N_t\left[1 - f_t\left(1 + \frac{1}{g_D}\exp\left(-\frac{E_{fn}-E_t}{k_BT}\right)\right)\right]\int_{E_c}^{\infty} f(E)c_{ec}(E)g_c(E)dE$$

$$r_h = N_t\left[f_t - (1-f_t)g_D\exp\left(-\frac{E_t-E_{fp}}{k_BT}\right)\right]\int_{-\infty}^{E_v} (1-f(E))c_{hc}(E)g_v(E)dE$$

where the quasi-Fermi levels have been introduced.

Introducing the constants C_n and C_p, which represent the average capture probability of an electron over the band:

$$C_n = \frac{\int_{E_c}^{\infty} f(E) c_{ec}(E) g_c(E) dE}{\int_{E_c}^{\infty} f(E) g_c(E) dE}$$

$$C_p = \frac{\int_{-\infty}^{E_v} (1 - f(E)) c_{hc}(E) g_v(E) dE}{\int_{-\infty}^{E_v} (1 - f(E)) g_v(E) dE}$$

and noting that:

$$n = \int_{E_c}^{\infty} f(E) g_c(E) dE = N_c \gamma_n \exp\left(-\frac{E_c - E_{fn}}{k_B T}\right) = \gamma_n n_{i,\text{eff}} \exp\left(\frac{E_{fn} - E_i}{k_b T}\right)$$

$$p = \int_{-\infty}^{E_v} (1 - f(E)) g_v(E) dE = N_v \gamma_p \exp\left(-\frac{E_{fp} - E_v}{k_B T}\right) = \gamma_p n_{i,\text{eff}} \exp\left(\frac{E_i - E_{fp}}{k_b T}\right)$$

the following equations are obtained:

$$r_e = n C_n N_t \left[1 - f_t \left(1 + \frac{1}{g_D} \exp\left(-\frac{E_{fn} - E_t}{k_B T}\right) \right) \right] = C_n N_t \left[n - n f_t - \frac{n_1}{g_D} f_t \right]$$

$$r_h = p C_p N_t \left[f_t - (1 - f_t) g_D \exp\left(-\frac{E_t - E_{fp}}{k_B T}\right) \right] = C_p N_t [p f_t + g_D (p_1 f_t - p_1)]$$

(3-79)

where:

$$n_1 = \gamma_n n_{i,\text{eff}} e^{\Delta E_t / (k_B T)} \qquad p_1 = \gamma_p n_{i,\text{eff}} e^{-\Delta E_t / (k_B T)}$$

$$\Delta E_t = -E_i + E_t$$

(3-80)

Equation 3-79 and Equation 3-80 define the electron and hole recombination rates associated with the trap energy level. The total rate of change of the number of trapped electrons is given by:

$$N_t \frac{\partial f_t}{\partial t} = r_e - r_h = C_n N_t \left[n - n f_t - \frac{n_1}{g_D} f_t \right] - C_p N_t [p f_t + g_D (p_1 f_t - p_1)] \quad (3-81)$$

Equation 3-81 determines the occupancy of the traps at the level E_t. For a continuous distribution of traps the equivalent expression is:

$$g_t(E_t)\frac{\partial f_t}{\partial t} = g_t(E_t)C_n\left[n - nf_t - \frac{n_1}{g_D}f_t\right] - g_t(E_t)C_p[pf_t + g_D(p_1f_t - p_1)]$$

The total recombination rate for electrons and holes is given by integrating Equation 3-79 over all the distributed traps and summing over the distinct discrete traps (denoted by the superscript i), giving the following result:

$$R_e = \sum_j \int_{E_v}^{E_c} g_t^j(E_t)C_n^j\left[n - nf_t^j - \frac{n_1^j}{g_D^j}f_t^j\right]dE_t + \sum_i C_n^i N_t^i\left[n - nf_t^i - \frac{n_1^i}{g_D^i}f_t^i\right]$$
(3-82)

$$R_h = \sum_j \int_{E_v}^{E_c} g_t^j(E_t)C_p^j[pf_t^j + g_D^j(p_1^jf_t^j - p_1^j)]dE_t + \sum_i C_p^i N_t^i[pf_t^i + g_D^i(p_1^if_t^i - p_1^i)]$$

Finally, the charge resulting from the occupied traps must also be computed. In general the charge on a trap site depends on the nature of the trap. Table 3-1 summarizes the different trap types currently included in the Semiconductor Module.

TABLE 3-1: CHARGE DUE TO DIFFERENT TYPES OF TRAP

TRAP TYPE	SPECIES TRAPPED	CHARGE OCCUPIED	CHARGE UNOCCUPIED	DENSITY OF STATES	NUMBER DENSITY
Donor trap	Electron	0	+	$g_t^D(E_t)$	N_t^D
Acceptor trap	Hole	0	-	$g_t^A(E_t)$	N_t^A
Neutral electron trap	Electron	-	0	$g_t^e(E_t)$	N_t^e
Neutral hole trap	Hole	+	0	$g_t^h(E_t)$	N_t^h

The total density of traps is given by:

$$g_t(E_t) = g_t^D(E_t) + g_t^A(E_t) + g_t^e(E_t) + g_t^h(E_t)$$

For the discrete states the total number of traps at the discrete level E_i is:

$$N_t^i = N_t^{D,i} + N_t^{A,i} + N_t^{e,i} + N_t^{h,i}$$

The total charge density, Q, that results from the traps is given by:

$$Q = q\int_{E_c}^{E_v}\left[\sum_j(1 - f_t^j)g_t^{D,j} - \left(\sum_k f_t^k g_t^{A,k} + \sum_l f_t^l g_t^{e,l}\right) + \sum_m(1 - f_t^m)g_t^{h,m}\right]dE_t$$
(3-83)
$$+ q\sum_i(1 - f_t^i)N_t^{D,i} - q\sum_n f_t^n N_t^{A,n} - q\sum_o f_t^o N_t^{e,o} + q\sum_p(1 - f_t^p)N_t^{h,p}$$

Equation 3-83 can be rewritten in the form:

$$Q = q\int_{E_v}^{E_c}[g_t^D + g_t^h]dE_t - q\int_{E_v}^{E_c}f_tg_tdE_t + q\sum_i[N_t^{D,i} + N_t^{h,i}] - q\sum_i f_t^i N_t^i$$

$$Q = q\int_{E_v}^{E_c}[g_t^D + g_t^h]dE_t - q\int_{E_0}^{E_c}f_tg_tdE_t + q\int_{E_v}^{E_0}(1-f_t)g_tdE_t - q\int_{E_v}^{E_0}g_tdE_t$$

$$+ q\sum_i[N_t^{D,i} + N_t^{h,i}] - q\sum_{E_i \geq E_0}f_t^i N_t^i + q\sum_{E_i < E_0}(1-f_t^i)N_t^i - q\sum_{E_i < E_0}N_t^i$$

where E_0 is an energy within the band gap referred to as the neutral level. E_0 is chosen such that:

$$\int_{E_v}^{E_c}[g_t^D + g_t^h]dE_t + \sum_i[N_t^{D,i} + N_t^{h,i}] = \int_{E_v}^{E_0}g_tdE_t + \sum_{E_i < E_0}N_t^i$$

So if a neutral energy is employed the following equation applies for the charge on the traps:

$$Q = -q\int_{E_0}^{E_c}f_tg_tdE_t + q\int_{E_v}^{E_0}(1-f_t)g_tdE_t - q\sum_{E_i \geq E_0}f_t^i N_t^i + q\sum_{E_i < E_0}(1-f_t^i)N_t^i \quad (3\text{-}84)$$

A neutral level is often a convenient way to characterize a set of traps at a boundary—since the details of the types of trapping sites are frequently not known, but it is possible to assign a neutral level to the boundary using experimental techniques such as capacitance measurements.

Recombination and Generation

Generation and recombination processes produce a source or a sink for electrons or holes in the current continuity equations (Equation 3-74). These terms usually serve to restore the device to equilibrium.

From Equation 3-49 the np product at equilibrium is given by:

$$np = N_cN_v\gamma_n\gamma_p\exp\left(-\frac{E_c - E_v}{k_BT}\right) = \gamma_n\gamma_p n_{i,eff}^2 \equiv n_{i,mod}^2 \quad (3\text{-}85)$$

where the effective intrinsic concentration is introduced:

$$n_{i,eff} = (N_c N_v)^{1/2} \exp\left(-\frac{E_g}{2k_B T}\right) = n_i \exp\left(\frac{\Delta E_g}{2k_B T}\right)$$

$$n_i = (N_c N_v)^{1/2} \exp\left(-\frac{E_{g0}}{2k_B T}\right)$$

Here $E_g=E_{g0}-\Delta E_g=E_c-E_v$ is the effective band gap that includes the material band gap E_{g0} and changes in the band gap (ΔE_g), which result from effects such as *band gap narrowing*. Equation 3-85 is known as the *mass action law*. Note that in an undoped semiconductor, where charge conservation at equilibrium implies $n = p$, the carrier concentrations are equal to the intrinsic concentration, n_i, since band gap narrowing only occurs in heavily doped semiconductors. Equation 3-85 is frequently used in recombination models to define the equilibrium carrier concentration.

In considering recombination processes, it is useful to note that photon momentum is usually negligible in comparison to the carrier momentum, and that the energy of phonons (lattice vibrations) is typically small compared to the band gap. Thus photon mediated transitions are typically vertical in an *E-k* diagram and phonon mediated transitions are frequently horizontal. Direct transitions involving both a photon and a phonon are usually so unlikely that they do not contribute significantly to recombination — in indirect semiconductors recombination is usually mediated by traps (impurities with energies close to the midgap). The following mechanisms are common in practical materials:

- *Direct recombination*: Important for direct band gap semiconductors such as gallium arsenide. An electron-hole pair recombines with the emission of a photon (of energy close to the band gap).

- *Trap-assisted, or Shockley-Read-Hall recombination*: Important in indirect band gap semiconductors, such as silicon and germanium. A defect (usually with an energy close to the midgap) is involved in the recombination process. An electron or hole is first trapped by the defect and then emitted into the valence/conduction band, resulting in a reduction in the number of available carriers. The carrier energy is typically converted to heat.

- *Auger recombination*: In Auger recombination three carriers are involved. A collision between two like carriers (for example, electrons) results in the recombination of one of the electrons with a hole. The energy released by the transition is transferred to the surviving electron. The resulting highly energetic electron subsequently loses energy as it undergoes collisions.

- *Impact ionization*: Impact ionization occurs when, for example, an energetic electron undergoes a collision in which it loses sufficient energy to promote an

electron in the valence band to the conduction band, resulting in an additional electron-hole pair being produced. It is the mechanism responsible for avalanche breakdown.

The Semiconductor interface has features to add Auger Recombination, Direct Recombination, and Trap-Assisted Recombination to a semiconducting domain. Impact Ionization Generation is also available. User-Defined Recombination or User-Defined Generation (use a negative recombination rate for generation) can also be added. Note that the recombination and generation features are additive, so it is possible to model several processes simultaneously.

THEORY FOR THE DIRECT RECOMBINATION FEATURE

Direct recombination is usually the dominant recombination mechanism in direct band gap semiconductors. The recombination rate can be derived phenomenologically from the two process that contribute to the net recombination rate: recombination of a conduction band electron with a hole in the valence band (caused by the emission of a photon by the electron) and generation of an electron hole pair by a valence band electron adsorbing a photon and moving into the conduction band. The corresponding capture (c) and emission (e) processes, are shown in Figure 3-10.
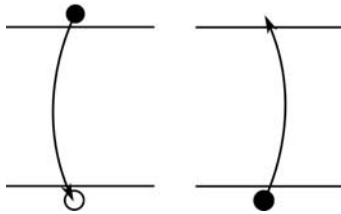
Figure 3-10: The two processes involved in direct recombination. Left: A conduction band electron is captured by an empty state (a hole) in the valence band. A photon is emitted. Right: A valence band electron is emitted into the conduction band. A photon is absorbed.

The recombination process is easiest to treat phenomenologically. Consider electrons in the conduction with energy E. A certain fraction of these electrons decay to states in the valence band with energy E'. This process contributes an amount dr_c to the total recombination process:

$$dr_c = f(E)g_c(E)(1-f(E'))g_v(E')c_c(E,E')dEdE'$$

where $f(E)$ is the Fermi-Dirac function, $g_c(E)$ is the density of states in the valence band, $g_v(E)$ is the density of states in the conduction band and $c_c(E,E')$ is the rate

constant for decay between states E and E'. If it is assumed that the rate constant does not vary significantly in the vicinity of the band edges then $c_c(E,E') \sim C_c$ and the expression can be directly integrated to yield:

$$R_c = C_c \int_{E_c}^{\infty} f(E)g_c(E)dE \int_{-\infty}^{E_v} (1-f(E'))g_v(E')dE' = C_c np$$

The generation process is more difficult to treat phenomenologically since it involves photon mediated transitions that must occur vertically in the band structure with a fixed energy difference (corresponding to the wavelength of the photons). However for a given band structure and frequency, provided that the semiconductor is nondegenerate, the photon transitions occur at a rate approximately independent of the carrier concentrations for a given illumination intensity. Thus a constant generation rate is a reasonable approximation under these circumstances:

$$G_e = C_e$$

Where C_e is a rate constant (dependent on the wavelength and the intensity of the incident light). These approximations do not always apply, and in circumstances where a more detailed model is appropriate, the Semiconductor interface includes the Optical Transitions feature.

In thermal equilibrium these rates must be equal so:

$$R_c^{eq} = G_e^{eq} = C_c \gamma_n \gamma_p n_{i,eff}^2 = C_e$$

So

$$C_e = C_c \gamma_n \gamma_p n_{i,eff}^2$$

The net rate of direct recombination is therefore given by:

$$R_n^d = R_p^d = R_c^d - G_e^d = C(np - \gamma_n \gamma_p n_{i,eff}^2)$$

where $C = C_c$ is a material constant (SI unit: m^3/s). For indirect band gap semiconductors such as silicon and germanium, C is effectively zero. In GaAs (a widely used direct band gap semiconductor) C is approximately 1×10^{-10} cm^3/s.

THEORY FOR TRAP-ASSISTED RECOMBINATION: SHOCKLEY-READ-HALL RECOMBINATION

In an indirect band gap semiconductor at low fields, trap-assisted recombination is usually the dominant contributor to U_n and U_p. This recombination mechanism involves the trapping of an electron or hole followed by re-emission into the valence or conduction band (see Ref. 21 and Ref. 22). The details of this process are described in the Traps section, and COMSOL Multiphysics provides features to model the traps explicitly, solving for the occupancy of the traps. For less detailed modeling it is common to use the original model of Shockley, Read, and Hall, in which steady-state conditions are assumed for traps located at a single energy level. Equation 3-81 determines the occupancy factor for the state, f_t. In the steady state the time derivative is zero and the following occupancy factor is obtained by solving the equation:

$$f_t = \frac{C_n n + C_p p_1}{C_n \left(n + \frac{n_1}{g_D}\right) + C_p(p + g_D p_1)}$$

Consequently:

$$R_e = R_h = N_t \frac{np - \gamma_n \gamma_p n_{i,eff}^2}{\frac{\left(n + \frac{n_1}{g_D}\right)}{C_p} + \frac{(p + g_D p_1)}{C_n}} = \frac{np - \gamma_n \gamma_p n_{i,eff}^2}{\tau_p \left(n + \frac{n_1}{g_D}\right) + \tau_n(p + g_D p_1)}$$

where:

$$\tau_n = \frac{1}{N_t C_n}$$

$$\tau_p = \frac{1}{N_t C_p}$$

Finally note that C_n and C_p can be written in terms of the thermal velocity of the electrons and holes, respectively ($v_{n,th}/v_{p,th}$), as well as their average capture cross sections ($<\sigma_n>/<\sigma_p>$):

$$C_n = v_{n,th} \langle \sigma_n \rangle$$
$$C_p = v_{p,th} \langle \sigma_p \rangle$$

THEORY FOR AUGER RECOMBINATION

Auger recombination becomes important at high nonequilibrium carrier densities, since the process requires three carriers. For example, when two electrons collide the collision can result in the recombination of one of the electrons with a hole. The energy released by the transition is transferred to the surviving electron, which subsequently returns to equilibrium as it undergoes collisions with the lattice. The recombination rate is given by:

$$R_n^{Au} = R_p^{Au} = (C_n n + C_p p)(np - \gamma_n \gamma_p n_{i,eff}^2)$$

where C_n and C_p are material constants (SI unit: m^6/s). For silicon $C_p \approx 2.8 \times 10^{-31}$ cm^6/s and $C_p \approx 9.9 \times 10^{-32}$ cm^6/s. In practice these coefficients are weakly dependent on temperature and doping level.

THEORY FOR IMPACT IONIZATION

Impact ionization becomes important at high electric fields. When the carriers are accelerated by the electric field in between collisions to velocities where their energies are greater than the gap energy, they can dissipate enough energy during collisions that additional electron hole pairs can be generated. Impact ionization is responsible for the phenomenon of avalanche breakdown. The carrier generation rate due to impact ionization is given by:

$$R_n^{II} = R_p^{II} = -\frac{\alpha_n}{q}|\mathbf{J}_n| - \frac{\alpha_p}{q}|\mathbf{J}_p|$$

For the values of α_n and α_p, the Semiconductor interface allows user-defined expressions or using the model of Okuto and Crowell (Ref. 23):

$$\alpha_n = a_n(1 + c_n(T - T_{ref}))E_{||,n} \exp\left(-\left(\frac{b_n(1 + d_n(T - T_{ref}))}{E_{||,n}}\right)^2\right)$$

$$\alpha_p = a_p(1 + c_p(T - T_{ref}))E_{||,p} \exp\left(-\left(\frac{b_p(1 + d_p(T - T_{ref}))}{E_{||,p}}\right)^2\right)$$

Where $E_{||,n}$ and $E_{||,p}$ are the components of the electric field parallel to the electron and hole currents, respectively, and T_{ref}, a_n, a_p, b_n, b_p, d_n, and d_p are material properties (see Ref. 23 for values of these properties for silicon, germanium, gallium arsenide, and gallium phosphide).

USER-DEFINED RECOMBINATION

The user-defined recombination feature allows the recombination rate to be specified by the user for both electrons and holes.

USER-DEFINED GENERATION

The User-Defined Generation feature allows the carrier generation rate to be defined for both the electrons and the holes.

> In the finite volume method, the dependent variables are constant within each mesh element and their gradients cannot be computed using the differentiation operator in COMSOL Multiphysics. However, COMSOL Multiphysics provides special variables that can be differentiated — see Finite Element and Finite Volume Discretization in the Modeling Guidelines chapter.
>
> Recombination and generation terms that are dependent on the gradients of the dependent variables frequently introduce significant nonlinearity into the equation system (whether the finite element or finite volume methods are used). Consequently, it is often necessary to add additional dependent variables to the equation system to assist the solver. Such generation models are only recommended for advanced users.

Incomplete Ionization

Away from equilibrium the ionization of donors and acceptors is still given by Equation 3-41 and Equation 3-42, except that the relevant quasi-Fermi level should be used in the equation system:

$$\frac{N_d^+}{N_d} = \frac{1}{1 + g_d \exp\left(\frac{E_{fn} - E_d}{k_B T}\right)}$$

$$\frac{N_a^-}{N_a} = \frac{1}{1 + g_a \exp\left(\frac{E_a - E_{fp}}{k_B T}\right)}$$

(3-86)

It is often more convenient to express Equation 3-86 in terms of the carrier concentrations rather than the relevant quasi-Fermi levels. From Equation 3-49:

$$E_{fn} = k_B T \ln\left(\frac{n}{\gamma_n N_c}\right) + E_c$$

$$E_{fp} = -k_B T \ln\left(\frac{n}{\gamma_p N_v}\right) + E_v$$

(3-87)

Substituting Equation 3-86 into Equation 3-87 gives:

$$\frac{N_d^+}{N_d} = \frac{1}{1 + \dfrac{g_d n}{\gamma_n N_c} \exp\left(\dfrac{\Delta E_d}{k_B T}\right)}$$

$$\frac{N_a^-}{N_a} = \frac{1}{1 + \dfrac{g_a p}{\gamma_p N_v} \exp\left(\dfrac{\Delta E_a}{k_B T}\right)}$$

(3-88)

where $\Delta E_d = E_c - E_d$ and $\Delta E_a = E_a - E_v$. Equation 3-88 is used in COMSOL Multiphysics when incomplete ionization with the standard ionization model is chosen in the Dopant Ionization section of the Semiconductor Material Model node. It is also possible to select a user defined ionization model, in which case the ionization ratios are specified directly by user-defined expressions. If complete ionization is chosen (the default) then $N_d^+ = N_d$ and $N_a^- = N_a$.

Band Gap Narrowing

In heavily doped materials the swollen orbitals associated with the impurity atoms begin to overlap and as a result the discrete energy level associated with the impurities broadens to form a band of finite width. Potential fluctuations due to the random distribution of the impurities also lead to a broadening of the impurity band. The ionization level of the impurities is consequently reduced. Eventually the impurity band overlaps the conduction band or valence band, effectively narrowing the band gap. In this situation the density of states no longer have the same form as that derived in Equation 3-21 or Equation 3-22. Nonetheless it is common to model band gap narrowing using these equations, but assuming a band gap that varies as a function of doping level.

Several options are available to specify the band gap narrowing.

USER DEFINED

The Semiconductor interface allows for models of band gap narrowing to be defined using an arbitrary expression. To add band gap narrowing to a material, select **User**

defined in the **Band Gap Narrowing** section of the Semiconductor Material Model. Then enter user-defined expressions for ΔE_g (the amount of band gap narrowing) and for α (the fraction of the band gap narrowing taken up by the conduction band). For convenience the energy level is entered in units of volts and is converted to an energy behind the scenes by multiplying by the electron charge, q. When band gap narrowing is active the following equations apply:

$$E_g = E_{g0} - \Delta E_g$$
$$E_c = E_{ci} - \alpha \Delta E_g$$
$$E_v = E_{vi} + (1 - \alpha)\Delta E_g$$

where E_g is the band gap with band gap narrowing, E_{g0} is the material band gap, E_c is the conduction band edge with band gap narrowing, E_{ci} is the conduction band edge in the absence of band gap narrowing, E_v is the valence band edge with band gap narrowing, and E_{vi} is the valence band edge in the absence of band gap narrowing.

SLOTBOOM MODEL

The Slotboom model is frequently used to model band gap narrowing in silicon. It is an empirical model that calculates the narrowing as a function of the total doping concentration (Ref. 27). This empirical model combines all of the physical effects (random potential fluctuations, electron-electron, carrier-impurity, and electron-hole interactions) into one energy narrowing, and consequently the calculated narrowing is the same in neutral and depleted parts of the device. The Slotboom model computes the band gap narrowing according to the equation:

$$\Delta E_g = E_{ref}\left(\ln\left(\frac{N_I}{N_{ref}}\right) + \sqrt{\left[\ln\left(\frac{N_I}{N_{ref}}\right)\right]^2 + \frac{1}{2}} \right) \tag{3-89}$$

where $N_I = N_d + N_a$ and the other parameters are material properties (E_{ref} has the same units as the band gap itself and N_{ref} has SI units of $1/m^3$). For silicon the Semiconductor Module material library uses the updated material properties due to Klassen et. al. (Ref. 28) rather than the original properties given in Ref. 27. Note that the fraction of the band gap narrowing taken up by the conduction band is also treated as a material property (0.5 for silicon).

JAIN-ROULSTON MODEL

The model developed by Jain and Roulston (Ref. 29) is a physics-based model in which the only empirical parameter is the fraction of the band gap narrowing taken up by the conduction band (once again this is defined as a material property, and a default

of 0.5 is usually employed). The model can be rewritten in a simple form with three coefficients. Coefficients for the model are available for a wide range of III-V materials, as well as for silicon and germanium.

$$\Delta E_g = \begin{cases} A_n\left(\dfrac{N_d}{N_{\text{ref}}}\right)^{\frac{1}{3}} + B_n\left(\dfrac{N_d}{N_{\text{ref}}}\right)^{\frac{1}{4}} + C_n\left(\dfrac{N_d}{N_{\text{ref}}}\right)^{\frac{1}{2}} & N_d \geq N_a \\ \\ A_p\left(\dfrac{N_a}{N_{\text{ref}}}\right)^{\frac{1}{3}} + B_p\left(\dfrac{N_a}{N_{\text{ref}}}\right)^{\frac{1}{4}} + C_p\left(\dfrac{N_a}{N_{\text{ref}}}\right)^{\frac{1}{2}} & N_d < N_a \end{cases} \tag{3-90}$$

where A_n, A_p, B_n, B_p, C_n, and C_p are material properties (with the same units as the band gap), and N_{ref} is a reference doping level (with SI units of $1/m^3$). The fraction of the band gap narrowing taken up by the conduction band is also treated as a material property (0.5 for silicon). Material properties for a number of materials are available in the material library, including the original materials described in Ref. 29 and several materials whose properties were obtained from Ref. 30.

Optical Transitions

The Optical Transitions feature is designed to model optical absorption and stimulated and spontaneous emission within the semiconductor. Stimulated emission or absorption occurs when a transition takes place between two quantum states in the presence of an oscillating electric field, typically produced by a propagating electromagnetic wave. For a semiconductor the process of stimulated absorption occurs when an electron in the valence band adsorbs a photon and transitions into the conduction band (resulting in coherent absorption of light). Stimulated emission occurs when an electron in the conduction band is stimulated by the field to transition down to the valence band (resulting in coherent emission of light). Spontaneous emission occurs when transitions from a high energy to a lower energy quantum state occur, with the emission of light. It can be regarded as a process by which a system returns to equilibrium, and correspondingly can be linked to the stimulated emission in equilibrium by thermodynamic arguments. Spontaneous emission does not occur in phase with any propagating waves in the system, and indeed can occur in the absence of such waves. Currently the optical transitions feature is dedicated to treating both stimulated and spontaneous emission in *direct band gap semiconductors.* Consequently the theory in the subsequent sections assumes a direct band gap at several points.

HAMILTONIAN IN THE PRESENCE OF AN ELECTROMAGNETIC WAVE

Stimulated emission is a quantum mechanical process that results from the change in the electron Hamiltonian due to the electromagnetic wave. The Hamiltonian appropriate for the motion of an electron in an electromagnetic field in the classical limit (Ref. 31, §16) is given by:

$$H = \frac{1}{2m_0}(\mathbf{p} - q\mathbf{A})^2 + V$$

where $\mathbf{A}$ is the magnetic vector potential and m_0 is the electron mass (*not* the effective mass).

The corresponding quantum mechanical operator is given by:

$$H = \frac{1}{2m_0}(-i\hbar\nabla - q\mathbf{A})^2 + V$$

$$= -\frac{\hbar^2}{2m_0}\nabla^2 + V + \frac{1}{2m_0}(i\hbar q\nabla \cdot \mathbf{A} + i\hbar q\mathbf{A} \cdot \nabla + q^2(\mathbf{A} \cdot \mathbf{A}))$$

For most practical optical applications $|q\mathbf{A}| \ll |\mathbf{p}|$ (Ref. 32) so the $q^2\mathbf{A}\cdot\mathbf{A}$ term can be neglected. When modeling electromagnetic fields in the frequency domain, COMSOL employs a gauge that ensures that the time varying electric potential is zero and the magnetic potential satisfies the equation $\nabla\cdot\mathbf{A}=0$ (see Magnetic and Electric Potentials in the *COMSOL Multiphysics Reference Manual* for further details on gauge fixing for electromagnetic waves). With this gauge for $\mathbf{A}$ the term $i\hbar q\nabla\cdot\mathbf{A}$ term is zero. Consequently the quantum mechanical Hamiltonian operator takes the form:

$$H = -\frac{\hbar^2}{2m_0}\nabla^2 + V + \frac{i\hbar q}{2m_0}\mathbf{A} \cdot \nabla = \frac{1}{2m_0}\mathbf{p}^2 + V + \frac{e}{2m_0}\mathbf{A} \cdot \mathbf{p}$$

Since $|q\mathbf{A}| \ll |\mathbf{p}|$ the time-dependent term that includes the vector potential can be treated as a small perturbation to the original stationary Hamiltonian H_0 such that:

$$H = H_0 + H'$$

where:

$$H_0 = \frac{1}{2m_0}\mathbf{p}^2 + V \tag{3-91}$$

$$H' = \frac{e}{2m_0}\mathbf{A} \cdot \mathbf{p} \tag{3-92}$$

Equation 3-91 is the Hamiltonian for the semiconductor in the absence of the field, which has eigenfunctions of the form given in Equation 3-14.

FERMI'S GOLDEN RULE AND CRYSTAL MOMENTUM CONSERVATION

Since the change to the electron Hamiltonian is small, time-dependent perturbation theory can be used to solve the problem (see Ref. 8 for an introduction to time-dependent perturbation theory that derives the main results used below). For small, oscillatory perturbations to a stationary Hamiltonian, a key result of time dependent perturbation theory (known as Fermi's golden rule) predicts that the probability of a transition from an occupied state (1) to an unoccupied state (2, in this case at a higher energy than state 1) per unit time, $W_{1 \to 2}$ is given by:

$$W_{1 \to 2} = \frac{2\pi}{\hbar}|H_{12}'|^2 \delta(E_2 - E_1 - \hbar\omega_0) \tag{3-93}$$

where E_1 and E_2 are the corresponding eigenvalues of the states, ω_0 is the angular frequency of the oscillation and H_{12}' is the matrix element corresponding to the oscillatory perturbation (H') to the original Hamiltonian:

$$H_{12} = \int \Psi_2^* H' \Psi_1 d^3x$$

Equation 3-93 gives the transition probability between two discrete states. The delta function indicates that the states must be separated by an energy equal to the photon energy, that is the transition must conserve energy. An additional requirement on the transition is that crystal momentum is conserved:

$$\mathbf{k}_2 = \mathbf{k}_1 + \mathbf{k}_{opt} \tag{3-94}$$

where $\mathbf{k}_{opt}$ is the photon wave vector. This requirement for crystal momentum conservation can be derived using a periodic expansion of the Bloch functions for the two wave functions in the matrix element H_{12}' with a plane wave excitation (see, for example, Ref. 32 and Ref. 33). However, the relation is in practice much more general since it results from fundamental symmetries of the system Hamiltonian (see Appendix M of Ref. 1). Typical optical wavelengths (400 to 700 nm in free space, dropping by a factor of order 10 inside the semiconductor) are significantly larger than the unit cell size of a semiconductor (typically less than 1 nm), which in turn determines the order

of the Bloch function wavelengths. Consequently $\mathbf{k}_{opt}$ is usually neglected in Equation 3-91 leading to $\mathbf{k}_2 = \mathbf{k}_1$.

The crystal momentum conservation requirement can therefore be rephrased as a requirement that optical transitions take place vertically in the $E\text{-}k$ diagram.

Equation 3-93 describes the transition rate from an unoccupied initial state to an occupied final state. To obtain the net rate of stimulated emission (including both upward and downward transitions) it is necessary to sum over all transitions from occupied to unoccupied states. Figure 3-11 shows the transitions of interest in a simple two-band model. Due to the spherical symmetry of the constant energy surfaces in k-space (in a direct band-gap semiconductor), upward transitions occur between states of fixed energy in the valence band (E_{1v}) and in the conduction band (E_{2c}).
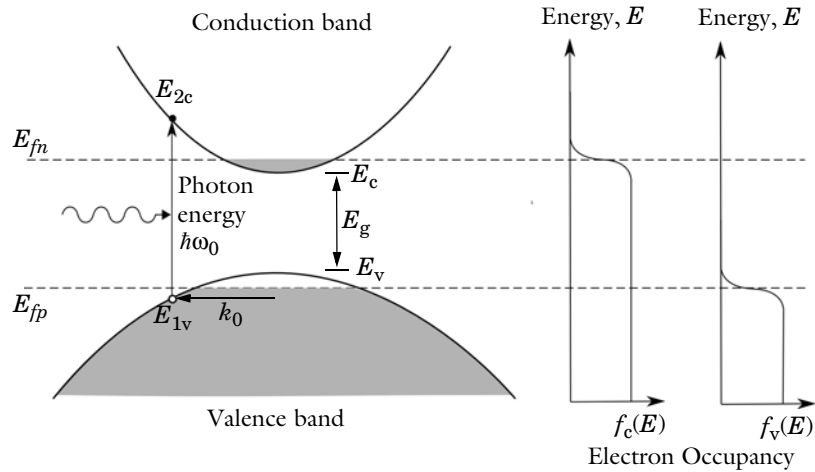
Figure 3-11: Diagram illustrating allowed optical transitions between the conduction and valence bands in a two band model of a direct band-gap semiconductor. The electron occupancy in the valence ($f_c(E)$) and conduction ($f_v(E)$) bands is also shown.

Assuming that the bands have a parabolic dispersion relation in the vicinity of k=0, E_{1v} and E_{2c} can be written as a function of the photon energy, $\hbar\omega_0$. The equations:

$$E_{1v} = E_v - \frac{\hbar k_0^2}{2m_h}$$

$$E_{2c} = \frac{\hbar k_0^2}{2m_e} + E_c$$

$$\hbar \omega_0 = E_{2c} - E_{1v}$$

can be rearranged into the form of a single quadratic equation for k_0. The equation has a single physically significant root (for positive k):

$$k_0 = \sqrt{\frac{2m_r}{\hbar^2}(\hbar \omega_0 - E_g)}$$

$$E_{1v} = E_v - \frac{m_r}{m_h}(\hbar \omega_0 - E_g)$$

$$E_{2c} = E_c + \frac{m_r}{m_e}(\hbar \omega_0 - E_g)$$ (3-95)

$$\frac{1}{m_r} = \frac{1}{m_e} + \frac{1}{m_h}$$

For states with a given magnitude of k we can define an average matrix element H_{12}^{av} which represents the averaged matrix element over all directions for a given excitation. For unpolarized light the random orientation of the polarization can also be accounted for in H_{12}^{av} (note that usually in the literature unpolarized light is assumed, and matrix elements quoted should be adjusted if polarized light is under consideration). Note also that the matrix element is in general a function of the magnitude of k, but for small values of k the assumption is generally made that it is independent of k.

Fermi's golden rule now takes the form:

$$W_{1 \to 2} = \frac{2\pi}{\hbar}\left|H_{12}^{av}\right|^2 \delta(E_2 - E_1 - \hbar\omega_0)$$ (3-96)

STIMULATED ABSORPTION

Equation 3-96 is the equation for the transition rate between a single pair of states. In a semiconductor, there are many states that satisfy Equation 3-95, and correspondingly it is necessary to integrate over pairs of states for which the transition can occur. Clearly an upward transition must take place from a full state into an empty state, so the occupancy of the states must also be accounted for. One of the assumptions underlying the drift diffusion equations is that the scattering within the

band occurs on a much smaller timescale than equilibrating processes that occur between the bands. Consequently stimulated electrons can be considered to equilibrate rapidly within the conduction band so that their distribution is described by the Fermi-Dirac function with the appropriate electron quasi-Fermi level. Correspondingly, the rate of stimulated absorption (the total number of upward transitions per unit volume per unit time, SI unit: $\text{m}^{-3}\text{s}^{-1}$) is given by:

$$G_{stim}^{1\to 2} = \iiint \frac{2\pi}{\hbar}\left|H_{12}^{av}\right|^2 g(k)f_v(1-f_c)\delta(E_{2c}-E_{1v}-\hbar\omega_0)d^3k$$

(3-97)

where $g(k)$ is the density of states in k-space ($1/4\pi^3$ from Equation 3-19) and the *electron* occupancy factors for the conduction and valence band, f_c and f_v, are given by:

$$f_c = \frac{1}{1+\exp\left(\dfrac{E_{2c}-E_{fn}}{k_B T}\right)}$$

$$f_v = \frac{1}{1+\exp\left(\dfrac{E_{1v}-E_{fp}}{k_B T}\right)}$$

(3-98)

E_{2c} and E_{1v} can be written in terms of k, leading to the equation:

$$G_{stim}^{1\to 2} = \iiint \frac{1}{2\pi^2\hbar}\left|H_{12}^{av}\right|^2 f_v(k)(1-f_c(k))\delta\left(\frac{\hbar^2 k^2}{2m_r}+E_g-\hbar\omega_0\right)d^3k$$

Transforming the integral to spherical polar coordinates and changing the integration variable gives:

$$G_{stim}^{1\to 2} = \int \frac{1}{2\pi^2\hbar}\left|H_{12}^{av}\right|^2 f_v(k)(1-f_c(k))\delta\left(\frac{\hbar^2 k^2}{2m_r}+E_g-\hbar\omega_0\right)4\pi k^2 dk$$

$$G_{stim}^{1\to 2} = \int \frac{2}{\pi\hbar}\left|H_{12}^{av}\right|^2 f_v(k)(1-f_c(k))\delta\left(\frac{\hbar^2 k^2}{2m_r}+E_g-\hbar\omega_0\right)\frac{m_r k}{\hbar^2}d\left(\frac{\hbar^2 k^2}{2m_r}\right)$$

$$G_{stim}^{1\to 2} = \frac{2m_r}{\pi\hbar^3}\left|H_{12}^{av}\right|^2 f_c(k_0)(1-f_v(k_0))k_0$$

$$G_{stim}^{1\to 2} = \frac{2\pi}{\hbar}\left|H_{12}^{av}\right|^2 f_v(\omega_0)(1-f_c(\omega_0))\frac{1}{2\pi^2}\frac{2m_r}{\hbar^2}\sqrt{\frac{2m_r}{\hbar^2}}(\hbar\omega_0-E_g)$$

Note that Equation 3-95 was used in the third and fourth steps. It is common to rewrite this expression in the form:

$$G_{stim}^{1 \to 2} = \frac{2\pi}{\hbar}\left|H_{12}^{av}\right|^2 f_v(1-f_c)g_{red}(\hbar\omega_0)$$

(3-99)

where the reduced density of states:

$$g_{red}(E) = \frac{1}{2\pi^2}\left(\frac{2m_r}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{(E-E_g)}$$

is defined by analogy with Equation 3-21 and where the functional dependence of f_c and f_v has been dropped.

PHYSICAL/THERMODYNAMIC CONSIDERATIONS, STIMULATED AND SPONTANEOUS EMISSION

The rate of stimulated absorption is directly related to the rate of stimulated and spontaneous emission as a result of physical and thermodynamic arguments originally due to Albert Einstein (Ref. 34). Historically Einstein argued for the existence of stimulated emission by means of an argument similar to the one presented here. In the argument that follows the existence of stimulated emission is assumed from the outset.

Consider the physics of a semiconductor interacting with a radiation field whose energy is distributed uniformly in frequency in the vicinity of the transition energy (that is the spectral width of the radiation field is large compared to the transition line width). In this case, a suitable phenomenological model for the rate of stimulated emission and absorption (at a particular value of the photon energy $E = \hbar\omega$, and in a range of photon energies, dE) is:

$$g_{stim}^{1 \to 2}dE = B_{12}n(\hbar\omega)f_v(1-f_c)g_{red}(\hbar\omega)dE$$
$$r_{stim}^{2 \to 1}dE = B_{21}n(\hbar\omega)f_c(1-f_v)g_{red}(\hbar\omega)dE$$

(3-100)

where B_{12} and B_{21} represent constants related to the semiconductor material and $n(\hbar\omega)$ is the mean number of photons per unit volume per unit photon energy (SI unit: $J^{-1}m^{-3}$).

The rate of spontaneous emission should not be directly dependent on the radiation field, so the following phenomenological model is adopted for this quantity:

$$r_{spon}^{2 \to 1}dE = A_{21}f_c(1-f_v)g_{red}(\hbar\omega)dE \tag{3-101}$$

where A_{21} is another constant. When the semiconductor is in equilibrium with the radiation field the two quasi-Fermi levels are equal and the emission and absorption rates must balance. Consequently, for the equilibrium case:

$$g_{stim}^{1 \to 2} = r_{stim}^{2 \to 1} + r_{spon}^{2 \to 1}$$

$$B_{12}n(\hbar\omega)f_v(1-f_c) = B_{21}n(\hbar\omega)f_c(1-f_v) + A_{21}f_c(1-f_v)$$

After a little algebra (using Equation 3-98 with $E_{fn}=E_{fp}=E_f$) the result is:

$$\frac{B_{12}n(\hbar\omega)}{A_{21}+n(\hbar\omega)B_{21}} = \exp\left(-\frac{\hbar\omega}{k_BT}\right) \tag{3-102}$$

It is instructive to consider the high temperature limit of this equation. In that limit the exponential term tends to unity and it is expected that stimulated emission dominates over spontaneous emission, since $n(\hbar\omega)$ becomes large whilst A_{21} is a constant. Consequently this limit implies that:

$$B_{12} = B_{21} \tag{3-103}$$

Next, substituting Equation 3-103 into Equation 3-102 and rearranging gives:

$$n(\hbar\omega) = \frac{A_{21}}{B_{12}}\left(\frac{1}{\exp\left(\dfrac{\hbar\omega}{k_BT}\right)-1}\right) \tag{3-104}$$

The form of Equation 3-104 is similar to that of the Planck blackbody radiation spectrum, which is observed to hold experimentally for many materials (for example, see Ref. 10 §63 or Ref. 32 section 9.2.1):

$$n(E) = \frac{n^3E^2}{\pi^2\hbar^3c^3}\left(\frac{1}{\exp\left(\dfrac{E}{k_BT}\right)-1}\right)$$

Note that this expression is modified slightly from the standard form usually seen in text books since the formula above gives the *number of photons* per unit photon *energy* rather than the *photon energy* per unit *frequency*.

Consequently a relationship between B_{12} and A_{21} is implied:

$$\frac{A_{21}}{B_{12}} = \frac{n^3 \omega_0^2}{\hbar \pi^2 c^3} \tag{3-105}$$

where the relation $E = \hbar\omega$ is used. Equation 3-103 and Equation 3-105 are derived assuming an exciting field with a distributed spectrum in thermal equilibrium. However the phenomenological models described by Equation 3-100 and Equation 3-101 are expected to apply away from equilibrium in the same form, so the relationships between $A_{21}, B_{12},$ and B_{21} are general. Equation 3-105, which describes spontaneous emission relates to a process that is entirely independent of the exciting radiation. Correspondingly, $A_{21} = 1/\tau_{spon}$ is written, which allows the phenomenological equations to be written in the following form:

$$g_{stim}^{1 \to 2} = \frac{\hbar \pi^2 c^3}{n^3 \omega_0^2 \tau_{spon}} n(\hbar\omega) f_v (1 - f_c) g_{red}(\hbar\omega)$$

$$r_{stim}^{2 \to 1} = \frac{\hbar \pi^2 c^3}{n^3 \omega_0^2 \tau_{spon}} n(\hbar\omega) f_c (1 - f_v) g_{red}(\hbar\omega) \tag{3-106}$$

$$r_{spon}^{2 \to 1} = \frac{1}{\tau_{spon}} f_c (1 - f_v) g_{red}(\hbar\omega)$$

These relationships apply for a *distributed* spectrum of incident radiation. In order to relate the present analysis to that in the preceding section, consider how to relate the case of a monochromatic field to that of a distributed spectrum, with a spectral width that is large compared to the transition width. One way this can be done is to consider the process of building up the distributed absorption rate $g_{stim}^{1 \to 2}(E)$ from the absorption rates due to a series of monochromatic fields, with appropriately scaled energy densities (Ref. 35). For some coefficient C, a single, monochromatic line spectrum at frequency ω_0 leads to the following frequency domain contribution to the rate of stimulated generation:

$$G_{stim}^{1 \to 2}(E) = Cn_E \delta(E - \hbar\omega_0)$$

where n_E (SI unit: m^{-3}) is the photon density at the photon energy $E = \hbar\omega_0$. To build up the corresponding distributed spectrum requires summing over a series of these line spectra, each with a different value for the driving photon energy E' and with, $n_{E'} = n(E')d(E')$. Correspondingly the sum can be transformed to an integral in the following way:

$$g_{stim}^{1 \to 2}(E) = \int n(E')C\delta(E - E')d(E') = Cn(E) \qquad (3\text{-}107)$$

Comparing Equation 3-107 with Equation 3-106 shows that:

$$C = \frac{\hbar \, \pi^2 c^3}{n^3 \omega_0^2 \tau_{spon}} f_v(1 - f_c)g_{red}(\hbar \, \omega)$$

The same argument can be applied to the rate of stimulated emission. Integrating the monochromatic rate over all frequencies gives the total generation/recombination rate due to the line source in both of these cases:

$$G_{stim}^{1 \to 2} = \frac{\hbar \, \pi^2 c^3 n_E}{n^3 \omega_0^2 \tau_{spon}} f_v(1 - f_c)g_{red}(\hbar \, \omega_0)$$

$$R_{stim}^{2 \to 1} = \frac{\hbar \, \pi^2 c^3 n_E}{n^3 \omega_0^2 \tau_{spon}} f_c(1 - f_v)g_{red}(\hbar \, \omega_0) \qquad (3\text{-}108)$$

With a monochromatic line source the stimulated emission must occur at the frequency of the source. In contrast, the spontaneous emission can occur at any frequency allowed by the band structure. The rate of spontaneous recombination is therefore computed by summing contributions from all possible transitions within the band, for the electron distribution. The radiation emitted is not in phase with any sources producing stimulated emission, and has a broader spectrum since transitions can occur between states separated by a range of energies.

The total recombination due to spontaneous emission is given by:

$$R_{spon} = \int_{E_g}^{\infty} \frac{1}{\tau_{spon}} f_c(1 - f_v)g_{red}(E)dE \qquad (3\text{-}109)$$

Note that f_c and f_v are both functions of E through Equation 3-98 and Equation 3-95.

Equation 3-108 and Equation 3-109 determine the rates of stimulated and spontaneous emission in terms of the spontaneous lifetime. The spontaneous lifetime can be related to the matrix element for the transition, discussed in the previous section. The energy density of the electromagnetic field for a traveling wave in a dielectric medium is $\varepsilon_0 \varepsilon_r' E_0^2 / 2$ where E_0 is the electric field norm and ε_r' is the real part of the medium permittivity. Correspondingly the number density of the photons is given by:

$$n_E = \frac{\varepsilon_0 \varepsilon_r' E_0^2}{2 \hbar \omega_0}$$

The following equation therefore applies for the rate of stimulated emission:

$$G_{stim}^{1 \to 2} = \frac{\pi^2 c^3 \varepsilon_0 \varepsilon_r' E_0^2}{2n^3 \omega_0^3 \tau_{spon}} f_v(1 - f_c) g_{red}(\hbar \omega_0)$$

Comparing this equation with Equation 3-99 shows that the following relationship exists between the matrix element and the spontaneous emission lifetime:

$$\tau_{spon} = \frac{\hbar \pi c^3 \varepsilon_0 \varepsilon_r' E_0^2}{4n^3 \omega_0^3 |H_{12}^{av}|^2} \tag{3-110}$$

As a result of Equation 3-110 the rates of spontaneous and stimulated emission can also be written in the form:

$$G_{stim}^{1 \to 2} = \frac{2\pi}{\hbar} |H_{12}^{av}|^2 f_v(1 - f_c) g_{red}(\hbar \omega_0)$$

$$R_{stim}^{2 \to 1} = \frac{2\pi}{\hbar} |H_{12}^{av}|^2 f_c(1 - f_v) g_{red}(\hbar \omega_0)$$

$$R_{spon} = \int_{E_g}^{\infty} \frac{4n^3}{\hbar^4 \pi c^3 \varepsilon_0} \frac{|H_{12}^{av}|^2}{E_0^2} E^3 f_c(1 - f_v) g_{red}(E) dE$$

Note that it is also common to define a net generation rate due to stimulated emission, given by:

$$G_{stim} = G_{stim}^{1 \to 2} - R_{stim}^{2 \to 1} = \frac{2\pi}{\hbar} |H_{12}^{av}|^2 (f_v - f_c) g_{red}(\hbar \omega_0) \tag{3-111}$$

THE MATRIX ELEMENT

The preceding section derived the rates of stimulated and spontaneous emission in terms of the perturbation to the Hamiltonian and the spontaneous emission lifetime.

Equation 3-92 showed the perturbation to the electric field could be written in the form:

$$H' = \frac{e}{2m_0} \mathbf{A} \cdot \mathbf{p}$$

The matrix element in this form depends on the magnitude of the magnetic vector potential. It is often more convenient to express the matrix element in terms of the amplitude of the electric field oscillation (E_0) and a unit vector in the direction of the electric field (**e**). With the frequency domain gauge for the oscillatory field in COMSOL Multiphysics, the electric field is related to the magnetic field by the equation:

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} = -i\omega\mathbf{A}$$

Writing the local electric field can be written in the form:

$$\mathbf{E} = E_0\mathbf{e}$$

gives:

$$\mathbf{A} = \frac{iE_0}{\omega}\mathbf{e}$$

Consequently Equation 3-92 can be written in the form:

$$H' = \frac{ieE_0}{2m_0\omega}\mathbf{e}\cdot\mathbf{p}$$

and:

$$|H'|^2 = \left(\frac{eE_0}{2m_0\omega}\right)^2|\mathbf{e}\cdot\mathbf{p}|^2 \tag{3-112}$$

The momentum matrix element between to states 1 and 2 (<2|**e·p**|1> using the bracket notation) is frequently referred to in the literature as M_{12}—a convention adopted by COMSOL Multiphysics.

An alternative form for the matrix element is sometimes used. As shown in section 9.1.3 of Ref. 32, an the Hamiltonian can also be expressed as:

$$H' = E_0\mathbf{e}\cdot\mu$$

where μ is the dipole matrix element ($\mu=q\mathbf{r}$ where **r** is the position vector) and correspondingly:

$$|H'|^2 = E_0^2|\mathbf{e}\cdot\mu|^2 \tag{3-113}$$

The matrix element $<2|\mathbf{e}\cdot\mu|1>$ is written in the form μ_{12} in the user interface.

The two forms of the matrix element given in Equation 3-112 and Equation 3-113 can be used to specify the matrix element in COMSOL Multiphysics. Note that the band averaged matrix element for the particular electric field orientation should be used (M_{12}^{av} or μ_{12}^{av}). As discussed in Ref. 36 and Ref. 38, the band-averaged matrix elements can be derived using a $\mathbf{k}\cdot\mathbf{p}$ perturbation method. For a simple 4-band model (Ref. 36), assuming unpolarized incident light, the matrix element takes the form (Ref. 37):

$$\left|M_{12}^{av}\right|^2 \;=\; \frac{m_0}{6}\left(\frac{m_0}{m^*}-1\right)\frac{E_g(E_g+\Delta)}{E_g+\frac{2}{3}\Delta}$$

where E_g is the gap energy and Δ is the spin orbital splitting energy of the valence band. m^* is the effective mass of electrons in the conduction band, but typically an experimentally determined value should be used rather than the theoretical value (see discussion in Ref. 37; for the case of GaAs, Ref. 38 provides values for other materials).

OPTICAL PROPERTIES

Poynting's theorem for electromagnetic fields can be written in the form (Ref. 33):

$$\int_S \mathbf{E}\times\mathbf{H}\cdot\mathbf{n}\,dS \;=\; \int_V \left(\mathbf{E}\cdot\mathbf{j}+\frac{\partial}{\partial t}\left(\frac{\varepsilon_0}{2}\mathbf{E}\cdot\mathbf{E}+\frac{\mu_0}{2}\mathbf{H}\cdot\mathbf{H}\right)+\mathbf{E}\cdot\frac{\partial\mathbf{P}}{\partial t}+\mu_0\mathbf{H}\cdot\frac{\partial\mathbf{M}}{\partial t}\right)dV$$

(3-114)

Here $\mathbf{E}$ is the electric field, $\mathbf{H}$ is the magnetic field strength, $\mathbf{P}$ is the material polarization, $\mathbf{M}$ is its magnetization, and V is an enclosed volume within the material, with surface S.

Each of the terms in Equation 3-114 has a physical interpretation that can be associated with the flow of energy through the volume. The $\mathbf{E}\times\mathbf{H}$ term on the left hand side of this equation describes the flow of energy out of the enclosed volume ($\mathbf{E}\times\mathbf{H}$ is known as Poynting's vector). The $\mathbf{E}\cdot\mathbf{j}$ term represents the energy expended on moving charges within the volume. The next term represents the rate of change of the stored electromagnetic energy in the vacuum and the final two terms represent the power per unit volume expended on the electric and magnetic dipoles present in the material.

For optical frequencies, the $\mathbf{E}\cdot\mathbf{j}$ term is of order ρE^2 for a material resistivity ρ (for heavily doped silicon ρ is of order 10^{-5} Ω/m). Most practical semiconductors are nonmagnetic, so the final term is usually not significant. In the frequency domain, the

term involving the polarization is of order $\omega\varepsilon_0 E^2$ (ω is of order 10^{15} rad/s for optical light, ε_0 is $8.85\cdot10^{-12}$ F/m so $\omega\varepsilon_0$ is of order 10^4 Ω/m). Consequently, when considering the interaction of semiconductors with propagating electromagnetic waves it is only necessary to consider the material polarization. In the frequency domain, power per unit volume lost to the material is given by the term:

$$P_v = i\omega\mathbf{E}\cdot\mathbf{P}$$

The polarization $\mathbf{P}$ is given by:

$$\mathbf{P} = \varepsilon_0\chi\mathbf{E} = \varepsilon_0(\chi' - i\chi'')\mathbf{E}$$

where χ is the (complex) material susceptibility, with real part χ' and imaginary part χ''. In the frequency domain $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{P}(\mathbf{r},t)$ take the form:

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}(\mathbf{r})e^{i\omega_0 t}$$

$$\mathbf{P}(\mathbf{r},t) = \mathbf{P}(\mathbf{r})e^{i\omega_0 t} = \varepsilon_0(\chi' - i\chi'')\mathbf{E}(\mathbf{r})e^{i\omega_0 t}$$

Consequently the time averaged dissipated power is given by:

$$\langle P_v \rangle = \frac{1}{2}\mathrm{Re}[i\omega_0\mathbf{E}^*(\mathbf{r})\cdot\mathbf{P}(\mathbf{r})] = \frac{1}{2}\omega_0\varepsilon_0\mathrm{Re}[i\mathbf{E}^*(\mathbf{r})\cdot\chi\mathbf{E}(\mathbf{r})]$$

For an isotropic material χ becomes a scalar value:

$$\langle P_v \rangle = \frac{1}{2}\mathrm{Re}[i\omega_0\varepsilon_0(\chi' - i\chi'')\mathbf{E}^*(\mathbf{r})\cdot\mathbf{E}(\mathbf{r})] = \frac{1}{2}\omega_0\varepsilon_0\chi''|\mathbf{E}(\mathbf{r})|^2 = \frac{1}{2}\omega_0\varepsilon_0\chi''E_0^2$$

(3-115)

Equation 3-115 shows how the imaginary part of the susceptibility is related to the power absorption by the material. Since each photon carries an energy $\hbar\omega$ the total power adsorbed is directly related to the net rate of stimulated emission (given by Equation 3-111).

$$\langle P_v \rangle = \hbar\,\omega_0 G_{stim} = \frac{1}{2}\omega_0\varepsilon_0\chi''E_0^2$$

Correspondingly:

$$\chi''(\omega_0) = \frac{2\,\hbar\,G_{stim}}{\varepsilon_0 E_0^2} = \frac{4\pi}{\varepsilon_0 E_0^2}\left|H_{12}^{av}\right|^2 (f_v^0 - f_c^0)g_{red}^0 \qquad (3\text{-}116)$$

where the superscript 0 has been added to f_v, f_c and g_{red} to indicate that these quantities are evaluated at the energy $\hbar\omega_0$ which corresponds to the excitation frequency.

Equation 3-116 shows how the imaginary part of the susceptibility is related to the rate of stimulated emission and correspondingly to the transition matrix element. Associated with the change in the imaginary part of the susceptibility is a small change in the real part. If the complete frequency spectrum of the susceptibility is known, it is possible to relate the imaginary part of the susceptibility to the real part using the Kramers-Kronig relations. The Kramers-Kronig relations result from the constraint that in the time domain, the equations for the susceptibility at time t can only depend on the electric field at times less than t (Ref. 39); that is, the equations are derived from considering the system to be causal. Alternatively, the equations can be derived by considering the analytic nature of the complex function χ for physical systems (see Ref. 32 or Ref. 33 for derivations of this form). The Kramers-Kronig relation for the susceptibility can be written in the form:

$$\chi'(\omega_0) = \frac{2}{\pi}P\int_0^\infty \frac{\omega\chi''(\omega)}{\omega^2 - \omega_0^2}d\omega \qquad (3\text{-}117)$$

Where the P indicates that the principle value of the integral is required. Equation 3-117 gives the real part of the susceptibility in terms of the imaginary part, provided that the entire frequency spectrum of the imaginary part is known. In practice it is not possible to determine the entire frequency spectrum of the imaginary part of the susceptibility, so instead a change in the imaginary part of the susceptibility is considered due to the rearrangement of the carriers in the band. Taking as a reference configuration for the semiconductor the case of an undoped semiconductor at equilibrium (at temperatures such that the occupancy of the conduction band is negligible) we define:

$$\chi_{ref}''(\omega_0) = \frac{4\pi}{\varepsilon_0 E_0^2}\left|H_{12}^{av}\right|^2 g_{red}^0 \qquad (3\text{-}118)$$

Equation 3-118 corresponds to a reference configuration in which the semiconductor has an empty conduction band and a full valence band. The real part of the susceptibility for the reference material can then be written as:

$$\chi_{ref}'(\omega_0) = \frac{2}{\pi}P\int_0^\infty \frac{\omega\chi_{ref}''(\omega)}{\omega^2 - \omega_0^2}d\omega$$

For a doped semiconductor at arbitrary temperature there is a change in the real and imaginary parts of the susceptibility:

$$\chi'(\omega) = \chi'_{\text{ref}}(\omega) + \Delta_{\text{ref}}\chi'(\omega)$$
$$\chi''(\omega) = \chi''_{\text{ref}}(\omega) + \Delta_{\text{ref}}\chi''(\omega)$$

(3-119)

where the subscript *ref* indicates a change from the reference configuration and where:

$$\Delta_{\text{ref}}\chi''(\omega) = \frac{4\pi}{\varepsilon_0 E_0^2}\left|H_{12}^{av}\right|^2 (f_v - f_c - 1)g_{\text{red}}$$

(3-120)

Substituting Equation 3-119 into Equation 3-117 gives:

$$\chi_{\text{ref}}'(\omega_0) + \Delta_{\text{ref}}\chi'(\omega_0) = \frac{2}{\pi}P\int_0^\infty \frac{\omega\chi_{ref}''(\omega)}{\omega^2 - \omega_0^2}d\omega + \frac{2}{\pi}P\int_0^\infty \frac{\omega\Delta_{ref}\chi''(\omega)}{\omega^2 - \omega_0^2}d\omega$$

The χ_0 terms can be eliminated using Equation 3-119 giving:

$$\Delta_{ref}\chi'(\omega_0) = \frac{2}{\pi}P\int_0^\infty \frac{\omega\Delta_{ref}\chi''(\omega)}{\omega^2 - \omega_0^2}d\omega$$

(3-121)

Equation 3-121 gives the change in the real part of the susceptibility from the reference material susceptibility, for a given carrier concentration. This makes the integral easier to perform in practice, since the changes in the susceptibility due to the carriers is small at energies far from the band gap.

Equation 3-121 can be used to compute the change in the real part of the susceptibility, given a knowledge of the susceptibility of the reference material. In COMSOL Multiphysics, the real part of the susceptibility of the reference material is treated as a user-specified material property (it is determined from the relative permittivity or refractive index). The change in the refractive index due to the excitation of carriers into the valence band (either as a result of doping or due to carrier injection) is then accounted for by means of Equation 3-121. Note that $\chi_{ref}''(\omega)$ is *not known* over all frequencies and the real part of the susceptibility is likely to have significant contributions from other processes that occur at frequencies away from those corresponding to the band gap. However, since it is possible to define $\Delta_{ref}\chi''(\omega)$ from Equation 3-120 we can compute the change in the real part of the susceptibility from Equation 3-121.

At the excitation frequency, ω_0, the imaginary part of the susceptibility due to optical transitions can be computed directly from Equation 3-118. Since the imaginary part

of the reference material susceptibility is not conveniently available as a material property, COMSOL Multiphysics calculates this part of the susceptibility directly. It is possible to include additional contributions to the imaginary part of the susceptibility from mechanisms other than the optical transitions, as discussed in the next section.

MATERIAL PROPERTY INPUTS AND OUTPUTS FOR THE OPTICAL TRANSITIONS FEATURE

The theory presented in the preceding section is focused on the determination of the complex susceptibility of the material. Practically speaking, values of the complex refractive index (n-ik) or the complex relative permittivity (ε_r'-$i\varepsilon_r''$) are more often available for a given material.

The permittivity is straightforwardly related to the susceptibility by the equations:

$$\varepsilon_r' = 1 + \chi'$$
$$\varepsilon_r'' = \chi''$$

The optical transitions feature computes changes in the material properties that result from the transitions occurring in the semiconductor. The real part of the material permittivity changes from an initial value $\varepsilon_{r,i}'$ to a modified value $\varepsilon_{r,i}'$ given by:

$$\varepsilon_{r,f}' = \varepsilon_{r,i}' + \Delta\varepsilon_r'$$

where in this case:

$$\varepsilon_{r,i}' = 1 + \chi'_{ref}(\omega_0)$$
$$\Delta\varepsilon_r' = \Delta_{ref}\chi'(\omega_0)$$

The results from the preceding section have been used in deriving the above equations. Note that for the real part of the permittivity, the initial permittivity value is the real part of the permittivity for the reference material at the excitation frequency ($\chi'_{ref}(\omega_0)$), and the change in the permittivity is the same as $\Delta_{ref}\chi'(\omega_0)$. However, this is *not* the case for the imaginary part of the susceptibility, because the reference material contribution to the imaginary part of the permittivity is not generally available as a a material property. The change in the imaginary part of the permittivity is given by:

$$\varepsilon_{r,f}'' = \varepsilon_{r,i}'' + \Delta\varepsilon_r''$$

Typically the initial value of the imaginary part of the permittivity ($\varepsilon_{r,i}''$) is zero. COMSOL Multiphysics allows for nonzero values of $\varepsilon_{r,i}''$ for cases in which there are

other loss mechanisms in the material besides the optical transitions, so it is possible to enter nonzero values for this parameter in the feature. These mechanisms contribute in an additive manner to the material losses (or gain). The change in the imaginary part of the permittivity is given by:

$$\Delta \varepsilon_r " = \chi "(\omega_0)$$

where $\chi "(\omega_0)$ is given by Equation 3-116.

In optical applications it is often more common to specify the real and imaginary parts of the refractive index (n-ik) than to specify the complex relative permittivity. Simple relationships exist relating these quantities, allowing the material properties to be expressed in either form. In general, the complex permittivity is equal to the square of the complex refractive index (see Ref. 32, Ref. 33, or Ref. 35), so that:

$$((n_i + \Delta n) - i(k_i + \Delta k))^2 = \varepsilon_{r,i}' + \Delta \varepsilon_r' - i(\varepsilon_{r,i}" + \Delta \varepsilon_r")$$

The relationships between these quantities can be obtained by expanding the left hand side and equating the real and imaginary parts of the equations. For the initial values of the permittivity and refractive index the following relationships hold:

$$\varepsilon_{r,i}' = n_i^2 - k_i^2$$
$$\varepsilon_{r,i}" = 2n_i k_i$$

Correspondingly, the remaining quantities are related by the equations:

$$\Delta \varepsilon_r' = 2n_i \Delta n + [\Delta n^2 - 2k_i \Delta k - \Delta k^2]$$
$$\Delta \varepsilon_r" = 2n_i \Delta k + [2k_i \Delta n + 2\Delta k \Delta n]$$

In practical semiconducting materials, k_i, Δk, and Δn are small in comparison to n_i, so the terms in the square brackets are small. This is assumed when generating the corresponding postprocessing variables.

Finally a further quantity, related to the imaginary part of the complex susceptibility, is important because it can be measured experimentally. The absorption coefficient (α) is given by:

$$\alpha = \frac{\omega}{cn} \chi "$$

The absorption coefficient is available as a postprocessing variable. In laser applications the gain ($\gamma = -\alpha$) is also frequently encountered.

Boundary Conditions

The Semiconductor interface includes boundary conditions appropriate for the Semiconductor Material Model feature. Additionally, if insulating regions are included within the model using the **Charge Conservation** feature, separate boundary conditions are available for these regions.

The theory for the following boundary conditions is discussed in the subsequent sections:

- Metal Contacts
- Thin Insulating Gates
- Continuity/Heterojunction
- Boundary Conditions for Charge Conservation

Metal Contacts

The Metal Contact boundary condition is used for modeling different types of metal-semiconductor junctions. The Ideal Ohmic and Ideal Schottky types of contact can be modeled with this feature.

IDEAL OHMIC

The *ohmic contact* option assumes local thermodynamic equilibrium at the contact. Note that in practice it is often used in nonequilibrium situations where the boundary condition imposed is no longer physical (for example in a forward biased p-n junction), which is reasonable provided that the junction is located some distance from the region of interest. Since equilibrium is assumed, both the hole and electron quasi-Fermi levels are equal at the boundary. Charge neutrality at the boundary is also assumed so there is no band bending and the band diagram takes the form shown in Figure 3-12.
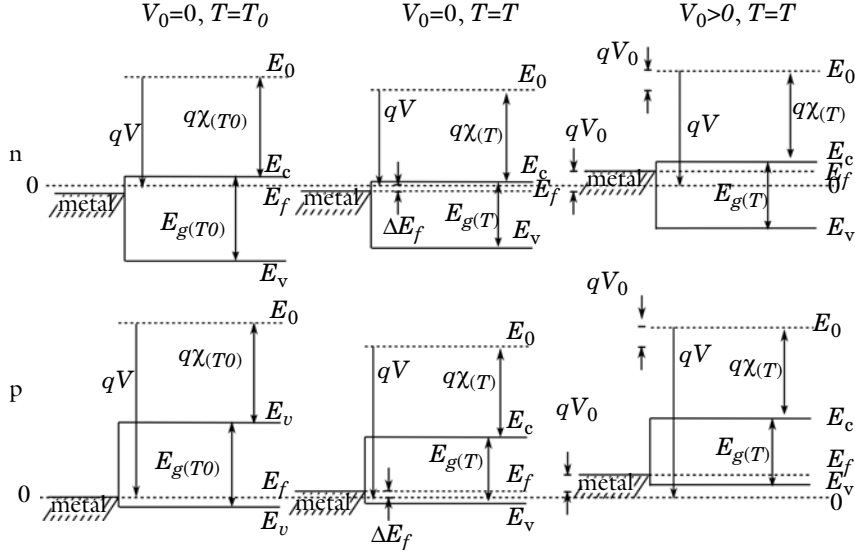
Figure 3-12: Energy band diagram for an ohmic contact with n-type (top) and p-type (bottom) semiconductors under different biasing and temperature conditions (left to right). On the left the semiconductor is in the reference configuration at the equilibrium temperature T_0 and at zero bias $V_0=0$. In the center, the temperature of the semiconductor is raised, changing the gap E_g and the electron affinity χ. Correspondingly, the energy of the conduction band edge E_c and of the valence band edge E_v, is shifted as is the Fermi level E_f. In this configuration the vacuum energy E_0 also changes as a result of differences in the space charge distribution in the device. On the right, in addition to the temperature change, a bias V_0 is applied to the metal, which shifts the entire band structure (as well as the vacuum level) up in energy by qV_0 from the configuration in the center.

Since equilibrium is assumed, Equation 3-49 is used for the carrier concentrations but it is useful to write it in the alternative forms:

$$n_{eq} = \gamma_n N_c \exp\left(-\frac{E_c - E_f}{k_b T}\right) = \gamma_n n_{i.eff} \exp\left(\frac{E_f - E_i}{k_b T}\right)$$

$$p_{eq} = \gamma_p N_v \exp\left(-\frac{E_f - E_v}{k_b T}\right) = \gamma_p n_{i.eff} \exp\left(\frac{E_i - E_f}{k_b T}\right)$$

(3-122)

where Equation 3-74 is used to derive the expressions for n and p in terms of the effective intrinsic carrier concentration. The charge neutrality condition states:

$$n_{eq} - p_{eq} + N_a^- - N_d^+ = 0$$

(3-123)

Solve Equation 3-122 and Equation 3-123 in a form convenient for numerical analysis by using the result $n_{eq}p_{eq}=\gamma_n\gamma_p n_{i,\text{eff}}^2$ (Equation 3-85). Using this result with Equation 3-123 gives:

$$(p_{eq}+(N_d^+-N_a^-))p_{eq}-\gamma_n\gamma_p n_{i,eff}^2 = 0$$

This quadratic equation can be solved for p_{eq} giving:

$$p_{eq} = -\frac{1}{2}(N_d^+-N_a^-)\pm\frac{1}{2}\sqrt{(N_d^+-N_a^-)^2+4\gamma_n\gamma_p n_{i,eff}^2}$$

p_{eq} must be positive therefore:

$$p_{eq} = -\frac{1}{2}(N_d^+-N_a^-)+\frac{1}{2}\sqrt{(N_d^+-N_a^-)^2+4\gamma_n\gamma_p n_{i,eff}^2}$$

$$n_{eq} = \frac{1}{2}(N_d^+-N_a^-)+\frac{1}{2}\sqrt{(N_d^+-N_a^-)^2+4\gamma_n\gamma_p n_{i,eff}^2}$$

(3-124)

From Equation 3-122 the difference between the intrinsic level and the Fermi level can be determined in the following manner:

$$E_f-E_i = k_BT\ln\left(\frac{n_{eq}}{\gamma_n n_{i,eff}}\right) = -k_BT\ln\left(\frac{p_{eq}}{\gamma_p n_{i,eff}}\right)$$

This result applies at arbitrary temperatures. Using Equation 3-85 and the above result, the conduction band energy level can be related to the intrinsic level and correspondingly to the equilibrium Fermi level in the following manner:

$$E_c = E_i+\frac{1}{2}E_g-\frac{kT}{2}\ln\left(\frac{N_v}{N_c}\right) = E_f-k_BT\ln\left(\frac{n_{eq}}{\gamma_n n_{i,eff}}\right)+\frac{1}{2}E_g-\frac{kT}{2}\ln\left(\frac{N_v}{N_c}\right)$$

where the result $E_v=E_c-E_g$ is used. The vacuum potential, V, is therefore:

$$V = -\left(\frac{1}{q}E_c+\chi\right) = \frac{k_BT}{q}\left(\ln\left(\frac{n_{eq}}{\gamma_n n_{i,eff}}\right)+\frac{1}{2}\ln\left(\frac{N_v}{N_c}\right)\right)-\frac{1}{q}\left(E_f+\frac{1}{2}E_g\right)-\chi \quad \text{(3-125)}$$

Equation 3-125 gives the vacuum potential relative to the Fermi level at an arbitrary temperature. However, it does not fix the vacuum potential on an absolute scale (the value of E_f is not known on this scale). As discussed in The Semiconductor Equations, COMSOL Multiphysics references the vacuum potential to the Fermi level in the equilibrium reference configuration (shown on the left of Figure 3-12). Since the vacuum level adjusts to accommodate the space charge layers that are created in the device, it does not remain constant when the temperature is changed away from

equilibrium. For an intrinsic semiconductor, however, the vacuum level remains constant when the temperature is changed. This is shown in Figure 3-13. E_f on the absolute scale must be set in a such a way that the limiting case of an intrinsic semiconductor is correct.
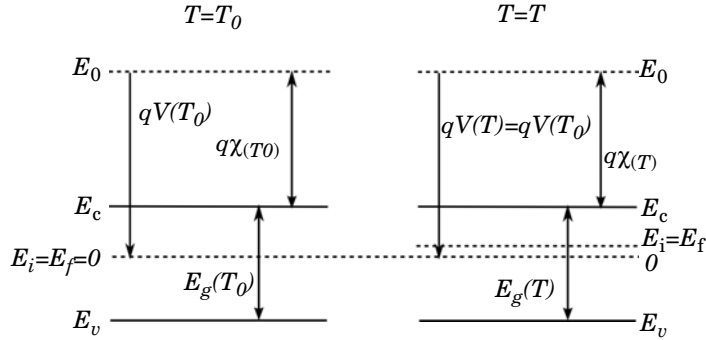
Figure 3-13: Diagram showing the band structure of an intrinsic semiconductor at the equilibrium reference temperature and at the local temperature (with no applied voltages). In this case the vacuum energy level does not change with a change in the local temperature.

For the particular case of the intrinsic semiconductor:

$$V(T) = V(T_0)$$

Using the above equation and Equation 3-125, and the fact that the intrinsic semiconductor has no band gap narrowing,

$$\frac{k_B T}{2q} \ln\left(\frac{N_v(T)}{N_c(T)}\right) - \frac{1}{q}\left(E_i(T) + \frac{1}{2}E_g^0(T)\right) - \chi^0(T)$$

$$= \frac{k_B T_0}{2q} \ln\left(\frac{N_v(T_0)}{N_c(T_0)}\right) - \frac{1}{q}\left(E_i(T_0) + \frac{1}{2}E_g^0(T_0)\right) - \chi^0(T_0)$$

where χ^0 is the electron affinity in the absence of band gap narrowing and E_g^0 is the energy gap in the absence of band gap narrowing. By definition $E_i(T_0)=E_f(T_0)=0$ therefore:

$$E_i(T) = E_f(T) = \frac{k_B}{2q}\left(T\ln\left(\frac{N_v(T)}{N_c(T)}\right) - T_0\ln\left(\frac{N_v(T_0)}{N_c(T_0)}\right)\right) + \chi^0(T_0) - \chi^0(T)$$
$$+ \frac{1}{2q}(E_g^0(T_0) - E_g^0(T)) \tag{3-126}$$

Equation 3-126 sets the value of the Fermi level relative to the zero in potential at temperature T for an intrinsic semiconductor. $E_f(T)$ is the offset in the energy scale relative to the equilibrium temperature for the particular case of an intrinsic semiconductor. Next consider a semiconductor with a nonuniform doping distribution but with a region of intrinsic semiconductor. The entire semiconductor is heated uniformly to raise its temperature from T_0 to T_1 (with no applied biases). The Fermi level in the intrinsic semiconductor changes according to Equation 3-126. Since the whole sample is still at equilibrium, the Fermi level everywhere else in the sample must also change by the same amount. Equation 3-126 gives the value of the Fermi level at equilibrium for any level of doping (in the absence of applied biases). The temperature-dependent (and doping-independent) offset is defined in the Fermi level:

$$\Delta E_f(T) = \frac{k_B}{2q}\left(T\ln\left(\frac{N_v(T)}{N_c(T)}\right) - T_0\ln\left(\frac{N_v(T_0)}{N_c(T_0)}\right)\right) + \chi^0(T_0) - \chi^0(T)$$
$$+ \frac{1}{2q}(E_g^0(T_0) - E_g^0(T)) \equiv V_{eq,adj} \tag{3-127}$$

Equation 3-125 can be written as:

$$V = \frac{k_B T}{q}\left(\ln\left(\frac{n_{eq}}{\gamma_n n_{i,eff}}\right) + \frac{1}{2}\ln\left(\frac{N_v}{N_c}\right)\right) - \frac{1}{q}\left(\Delta E_f + \frac{1}{2}E_g\right) - \chi \equiv V_{eq}$$

So with an applied bias V_0, the boundary condition on V should be:

$$V = \frac{k_B T}{q}\left(\ln\left(\frac{n_{eq}}{\gamma_n n_{i,eff}}\right) + \frac{1}{2}\ln\left(\frac{N_v}{N_c}\right)\right) - \frac{1}{q}\left(\Delta E_f + \frac{1}{2}E_g\right) - \chi + V_0 = V_{eq} + V_0 \tag{3-128}$$

The ohmic contact boundary condition imposes Equation 3-124 on the carrier concentrations and Equation 3-128 on the potential at the boundary. For the **Semiconductor Equilibrium** study step, only the constraint on the electric potential is applied. Note that all metal contacts attached to the same **Semiconductor Material Model** feature are biased at a common voltage, as dictated by the equilibrium condition. See Semiconductor Equilibrium Study Settings on how to set the common bias voltage.

IDEAL SCHOTTKY

The metal-semiconductor interface is one of the most challenging problems in the field of device physics. A variety of physical phenomena such as the influence of interface states, the effect of interfacial layers, scattering, potential fluctuations, interface roughness, image forces, and trap-assisted tunneling make practical detailed modeling of these devices complex. In practice, boundary conditions used in simulations must neglect much of the complexity of these devices.

The ideal Schottky option adopts a simplified model for *Schottky contacts*, which is based largely on the approach introduced by Crowell and Sze (Ref. 24). The semiconductor is assumed to be nondegenerate, since metal-degenerate semiconductor contacts are usually best represented by the Ideal Ohmic option.

The contact acts as a source or sink for carriers and consequently it can be treated as a surface recombination mechanism:

$$\mathbf{J}_n \cdot \mathbf{n} = -qv_n(n - n_0)$$
$$\mathbf{J}_p \cdot \mathbf{n} = qv_p(p - p_0)$$

Here, $\mathbf{n}$ is the outward normal of the semiconducting domain, v_n and v_p are the recombination velocities for holes and electrons, respectively, and n_0 and p_0 are the quasi-equilibrium carrier densities — that is, the carrier densities that would be obtained if it were possible to reach equilibrium at the contact without altering the local band structure. n_0 and p_0 are correspondingly defined as though the Fermi level of the semiconductor at the boundary is equal to that of the metal. From Figure 3-14 n_0 and p_0 are given by:

$$n_0 = N_c \exp\left(-\frac{E_c - E_{fm}}{k_B T}\right) = N_c \exp\left(-\frac{\Phi_B}{k_B T}\right) \tag{3-129}$$

$$p_0 = N_v \exp\left(-\frac{E_{fm} - E_v}{k_B T}\right) = N_v \exp\left(-\frac{E_g - \Phi_B}{k_B T}\right)$$

where:

$$\Phi_B = \Phi_m - \chi \tag{3-130}$$

Here, Φ_m is the metal work function, E_{fm} is the metal Fermi level, and Φ_B is the emission barrier height for electrons (from the metal). The observed barrier heights of Schottky junctions frequently do not conform to Equation 3-130, largely as a result of the complexities discussed previously. From a practical perspective, the value of Φ_B can

be determined experimentally and, consequently, can be considered as an input into the model (COMSOL Multiphysics makes it possible to directly enter the barrier height or to compute the ideal barrier height from the material properties).
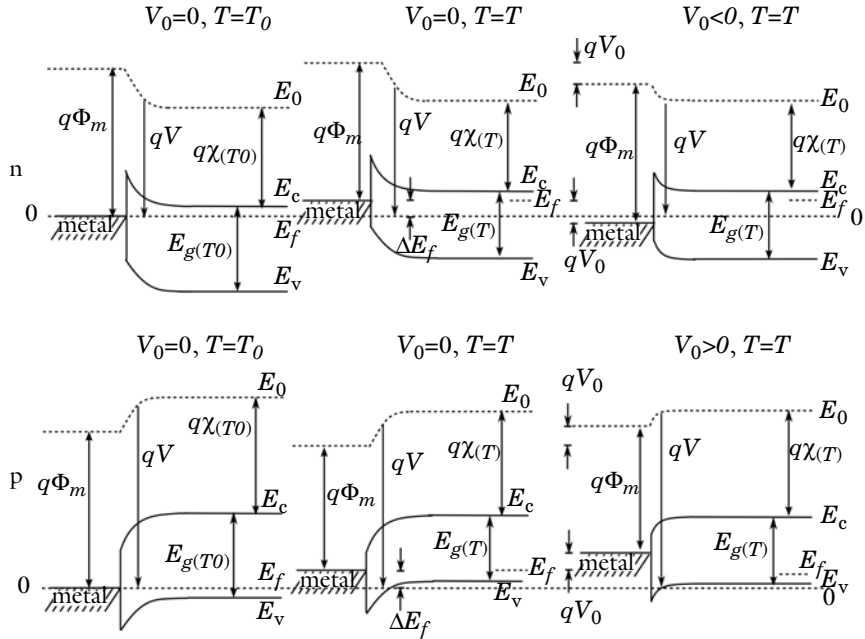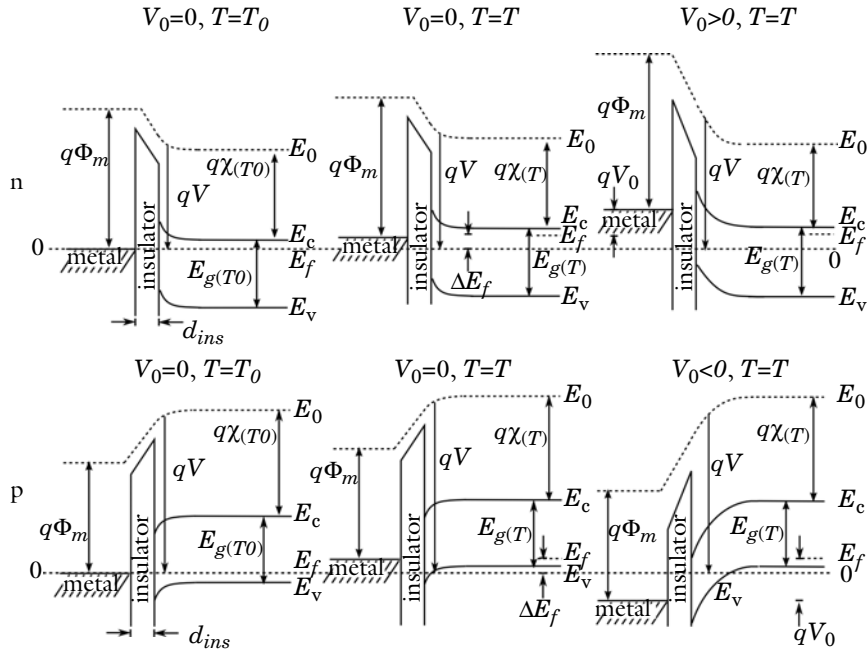

Figure 3-14: Energy band diagram for a Schottky contact with n-type (top) and p-type (bottom) semiconductors under different biasing and temperature conditions (left to right). On the left, the semiconductor is in the reference configuration at the equilibrium temperature T_0 and at zero bias $V_0=0$. In the center, the temperature of the semiconductor is raised, changing the gap E_g and the electron affinity χ. Correspondingly, the energy of the conduction band edge E_c and of the valence band edge E_v is shifted, as is the Fermi level E_f, in equilibrium regions of the device (indicated to the right of the band diagram). In this configuration the vacuum energy E_0 also changes as a result of differences in the space charge distribution in the device. On the right, in addition to the temperature change, a forward bias V_0 is applied to the metal.

The recombination velocities v_n and v_p are determined by assuming that the dominant source of current across the junction is thermionic emission. Ref. 3 provides a full derivation of this case, which shows that, if thermionic emission is dominant:

$$v_n = \frac{A_n^* T^2}{q N_c}$$

$$v_p = \frac{A_p^* T^2}{q N_v}$$
(3-131)

Here, A_n^* and A_p^* are the effective Richardson's constants for electrons and holes, respectively (these are essentially material properties related to the thermionic emission — Ref. 3 has details). The Schottky contact boundary condition allows the recombination velocities to be user defined or to be determined from Equation 3-131. In addition, an extra current contribution can be specified with either a user-defined scaling factor or the scaling factor computed using the WKB Tunneling Model.

Equation 3-129, Equation 3-130, and Equation 3-131 specify the boundary condition on the currents imposed at a Schottky contact. The boundary condition on the voltage can be determined from Figure 3-14:

$$V = -(\Phi_B + \chi) - \frac{\Delta E_f}{q} + V_0$$
(3-132)

Equation 3-132 is used by COMSOL Multiphysics to constrain the potential at the boundary. For the **Semiconductor Equilibrium** study step, only the constraint on the electric potential is applied. Note that all metal contacts attached to the same **Semiconductor Material Model** feature are biased at a common voltage, as dictated by the equilibrium condition. See Semiconductor Equilibrium Study Settings on how to set the common bias voltage.

Thin Insulating Gates

The band diagram for a thin insulating gate is shown in Figure 3-15. As for the ohmic contact, a change in the temperature of the device away from the equilibrium reference results in a shift of the metal and semiconductor Fermi levels (ΔE_f) on the absolute energy scale, given by Equation 3-127. An applied potential further shifts the metal Fermi level with respect to the semiconductor Fermi level (which can be defined in regions away from the contact where little current flows).

Figure 3-15: Energy band diagram for a thin insulating gate with n-type (top) and p-type (bottom) semiconductors under different biasing and temperature conditions (left to right). On the left, the semiconductor is in the reference configuration at the equilibrium temperature T_0 and at zero bias $V_0=0$. In the center, the temperature of the semiconductor is raised, changing the gap E_g and the electron affinity χ. Correspondingly, the energy of the conduction band edge E_c and of the valence band edge E_v is shifted, as is the Fermi level E_f, in equilibrium regions of the device (indicated to the right of the band diagram). In this configuration the vacuum energy E_0 also changes as a result of differences in the space charge distribution in the device. On the right, in addition to the temperature change, a bias V_0 is applied to the metal, leading to an inversion layer under the gate.

When the Thin Insulator Gate boundary condition is used, the thin insulating layer is not included in the COMSOL Multiphysics model but its effect is included in the formulation of the boundary condition. The insulator is assumed to be so thin that the electric field (which must be perpendicular to the metal surface) is to a good approximation also perpendicular to the insulator-semiconductor boundary. When this is the case, the normal electric displacement field ($\mathbf{D}$) at the insulator-semiconductor interface can be written as:

$$\mathbf{n} \cdot \mathbf{D} = -\varepsilon_{ins}\varepsilon_0 \frac{V_g - V}{d_{ins}}$$

where V_g is the potential on the gate, V is the potential at the insulator-semiconductor interface, d_{ins} is the thickness of the insulator, ε_{ins} is the relative dielectric permittivity of the insulator, ε_0 is the permittivity of free space, and $\mathbf{n}$ is the outward normal of the semiconductor domain. From Figure 3-15, the gate voltage with applied potential V_0 is given by:

$$V_g \;=\; -\Phi_m + V_0 - \frac{\Delta E_f}{q}$$

where Φ_m is the metal work function. ΔE_f is given by Equation 3-127. Therefore:

$$\mathbf{n} \cdot \mathbf{D} \;=\; \varepsilon_{ins}\varepsilon_0 \frac{V + \Phi_m - V_0 + \dfrac{\Delta E_f}{q}}{d_{ins}} \qquad (3\text{-}133)$$

The electron and hole currents flowing into the insulator must be zero therefore:

$$\begin{aligned}
\mathbf{n} \cdot \mathbf{J}_n &= 0 \\
\mathbf{n} \cdot \mathbf{J}_p &= 0
\end{aligned} \qquad (3\text{-}134)$$

The thin insulating gate applies the Neumann boundary conditions given by Equation 3-133 and Equation 3-134.

TRAPS ON THE SEMICONDUCTOR/INSULATOR BOUNDARY

When traps are present on the gate the traps accumulate charge as described in the Traps section. As a result of the charge on the boundary the electric displacement field is discontinuous across the interface and consequently:

$$\mathbf{n} \cdot \mathbf{D} \;=\; -\varepsilon_{ins}\varepsilon_0 \frac{V_g - V}{d_{ins}} - Q$$

where Q is the surface charge density due to the traps, given by Equation 3-83 or Equation 3-84. Consequently the form of Equation 3-133 is modified so that:

$$\mathbf{n} \cdot \mathbf{D} \;=\; \varepsilon_{ins}\varepsilon_0 \frac{V + \Phi_m - V_0 + \dfrac{\Delta E_f}{q}}{d_{ins}} - Q$$

Similarly, in a transient study, the traps can provide a sink for electrons or holes and Equation 3-134 is changed such that:

$$\mathbf{n} \cdot \mathbf{J}_n = R_e$$
$$\mathbf{n} \cdot \mathbf{J}_p = R_h$$

where R_e and R_h are given by Equation 3-82.

Continuity/Heterojunction

Space charge regions develop at the interface between two different semiconductors, as a result of the change in the band structure that occurs at the junction. Such interfaces are referred to as heterostructures. COMSOL Multiphysics handles all interior boundaries in a model using the Continuity/Heterojunction feature, which automatically detects whether a change in the band structure occurs at the interface. For interior boundaries within a single material, the electron and hole densities are continuous and the boundary has no effect on the solution. When a heterostructure is present, one of the following Continuity model options should be selected from the Heterojunction settings:

- Continuous quasi-Fermi levels
- Thermionic emission

The boundary conditions for these two options are described in more detail below.

CONTINUOUS QUASI-FERMI LEVELS

This boundary condition enforces continuity of the quasi-Fermi levels at the junction:

$$E_{fn1} = E_{fn2} \qquad E_{fp1} = E_{fp2}$$

where E_{fn1} and E_{fp1} are the electron and hole quasi-Fermi levels in material 1 and E_{fn2} and E_{fp2} are the electron and hole quasi-Fermi levels in material 2.

This is an approximate boundary condition, and applies when the junction has negligible resistivity.

> 📄 Fermi-Dirac statistics are currently not supported in the finite volume method when the thermionic emission boundary condition is used.

THERMIONIC EMISSION

The thermionic emission boundary condition is based on Ref. 25.

In the limit of no tunneling, the normal currents across the junction are given by:

$$\mathbf{n}_1 \cdot \mathbf{J}_{n1} = \begin{cases} -q(v_{n1}n_1 e^{-(E_{c2}-E_{c1})/(k_BT)} - v_{n2}n_2) & E_{c2} \geq E_{c1} \\ q(v_{n2}n_2 e^{-(E_{c1}-E_{c2})/(k_BT)} - v_{n1}n_1) & E_{c2} < E_{c1} \end{cases}$$

$$\mathbf{n}_1 \cdot \mathbf{J}_{p1} = \begin{cases} q(v_{p1}p_1 e^{-(E_{v1}-E_{v2})/(k_BT)} - v_{p2}p_2) & E_{v1} \geq E_{v2} \\ -q(v_{p2}p_2 e^{-(E_{v2}-E_{v1})/(k_BT)} - v_{p1}p_1) & E_{v1} < E_{v2} \end{cases}$$

$$\mathbf{n}_2 \cdot \mathbf{J}_{n2} = -\mathbf{n}_1 \cdot \mathbf{J}_{n1} \qquad\qquad \mathbf{n}_2 \cdot \mathbf{J}_{p2} = -\mathbf{n}_1 \cdot \mathbf{J}_{p1}$$

(3-135)

where $\mathbf{n}_1 \cdot \mathbf{J}_{n1}$ is the outward normal electron current from material 1, $\mathbf{n}_2 \cdot \mathbf{J}_{n2}$ is the normal electron current leaving material 2, $\mathbf{n}_1 \cdot \mathbf{J}_{p1}$ is the outward normal hole current from material 1, $\mathbf{n}_2 \cdot \mathbf{J}_{p2}$ is the normal hole current leaving material 2. v_{n1}, v_{n2}, v_{p1}, and v_{p2} are the electron and hole recombination velocities for each material at the boundary. n_1, n_2, p_1, and p_2 are the electron and hole concentrations on each side of the boundary. Other quantities are defined in Figure 3-16. The recombination velocities are given by:

$$v_{n1} = \frac{A_{n1}{}^*T^2}{qN_{c1}} \qquad v_{n2} = \frac{A_{n2}{}^*T^2}{qN_{c2}}$$

$$v_{p1} = \frac{A_{p1}{}^*T^2}{qN_{v1}} \qquad v_{p2} = \frac{A_{p2}{}^*T^2}{qN_{v2}}$$

where the effective Richardson's coefficients $A_{n1}{}^\star$, $A_{n2}{}^\star$, $A_{p1}{}^\star$, and $A_{p2}{}^\star$ are given by:

$$A_{n1}{}^* = \frac{4\pi m_{e1}{}^* k_B{}^2}{h^3}q \qquad A_{n2}{}^* = \frac{4\pi m_{e2}{}^* k_B{}^2}{h^3}q$$

$$A_{p1}{}^* = \frac{4\pi m_{h1}{}^* k_B{}^2}{h^3}q \qquad A_{p2}{}^* = \frac{4\pi m_{h2}{}^* k_B{}^2}{h^3}q$$

The effective masses in the above equations are assigned the smaller value of the density of states effective mass between the 2 domains according to Ref. 25. The effective mass can be altered in the equation view if required.
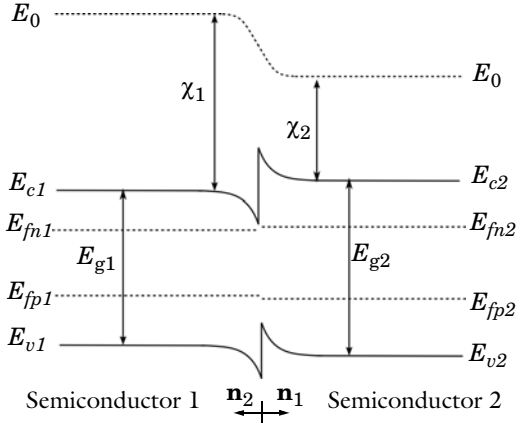
Figure 3-16: Heterostructure band diagram showing the vacuum energy level, E_0, and the conduction (E_{c1}, E_{c2}) and valence band (E_{v1}, E_{v2}) energies for the two materials. The electron (E_{fn1}, E_{fn2}) and hole (E_{fp1}, E_{fp2}) quasi-Fermi levels are also shown, as are the material band gaps (E_{g1}, E_{g2}) and affinities (χ_1, χ_2).

WKB Tunneling Model

The effect of tunneling can be accounted for by including an extra proportional factor δ in the thermionic current density, using the formulas derived in Ref. 25 (based on the WKB approximation).

The electron and hole normal current densities given in Equation 3-135 are multiplied by a factor of $(1+\delta_{nJn})$ and $(1+\delta_{nJp})$, respectively. The extra current factors δ_{nJn} and δ_{nJp} are given by the double integration along the electrical field line (dl) and along the energy axis (dV_x):

$$\delta = \frac{q}{k_B T} e^{\frac{qV_{max}}{k_B T}} \int_{V_{min}}^{V_{max}} e^{-\frac{qV_x}{k_B T}} e^{\frac{-4\pi}{h}\int_1^2 \sqrt{max(0,\, 2m(E_b - qV_x))}\,dl}\, dV_x \qquad (3\text{-}136)$$

where h is the Plank constant, the limits of the energy axis integration are given by

$$V_{min} = max(E_{b1}, E_{b2})/q$$
$$V_{max} = max(E_b)/q$$

where the max function of the second equation is taken within the domain selection of the potential barrier, and the potential barrier variable E_b is given by

$$E_b = \begin{cases} E_c & electrons \\ -E_v & holes \end{cases}$$

and E_{b1} and E_{b2} are the values of E_b at the two opposite boundaries 1 and 2 across the potential barrier and connected by an electric field line, evaluated on the side of each boundary that is (immediately) outside of the potential barrier domain selection. The integral $\int_1^2 \dots dl$ is the line integral along the electric field line between the two opposite boundaries 1 and 2 across the potential barrier domain selection.

Boundary Conditions for Charge Conservation

When a charge conservation domain is added to a model all the boundary conditions available for electrostatics can be applied to exterior boundaries of the domain (boundaries adjacent to the semiconductor and interior boundaries automatically obtain the correct boundary conditions). These boundary conditions include a work function offset for the electric potential where appropriate. However, ΔE_f is not added automatically to the model. For this reason, it is recommended that for isothermal models the equilibrium reference temperature (set this in the Semiconductor interface Settings window under Reference Temperature) is set to the same temperature as the model temperature. For nonisothermal models, ΔE_f can be included in the work function in the following manner:

$$\Phi_m = \Phi_{m0} + \texttt{intop1(semi.V\_eq\_adj)}$$

where is Φ_{m0} the metal work function and an integration coupling operator (`intop1`) has been added on a point within the semiconducting domain adjacent to the insulator (if more than one Semiconductor interface is added to the domain, the prefix `semi` in the variable within the integration operator might need to be incremented).

Tunneling

Equation 3-37 in the section Electrons in a Perturbed Periodic Potential describes the transport of both electrons and holes in a semiconductor with a potential that varies in space. In many circumstances the potential varies slowly in space and wave packets move according to the classical Hamiltonian, so correspondingly their dynamics is determined by the semiclassical model, from which both the drift diffusion equations follow. However, since Equation 3-37 is essentially a Schrödinger equation for electrons and holes, it allows for quantum mechanical phenomena, such as tunneling which are outside of the scope of the semiclassical model.

Tunneling occurs when an electron or hole wave packet is incident on a narrow potential barrier with a barrier height greater than the energy associated with the group velocity of the wave packet. A classical particle would be reflected at the boundary, but in the solutions of the Schrödinger equation the envelope function $\Psi_m(\mathbf{r})$ associated with the wave packet decays exponentially inside the barrier. For thin barriers $\Psi_m(\mathbf{r})$ is significant on the opposite side of the barrier and correspondingly there is a transmission probability associated with transport through the potential barrier. Since the tunneling probability must be computed for wave packets with a range of energies or k-vectors, it is usually only possible to solve the tunneling problem in 1D. Consequently, the approaches adopted are necessarily phenomenological in nature. The nature of the approximations required to arrive at the theory of tunneling is discussed in detail in section 4 of Ref. 40. Since much of the underlying theory is approximate in nature, it is sensible to favor numerically lighter solutions over more detailed approaches.

Tunneling commonly occurs in semiconductor devices at a variety of locations, including:

• Tunneling through the barrier formed at a Schottky diode when the semiconductor is heavily doped underneath the metal contact (this is one way to produce an ohmic contact).

• Tunneling through the potential barrier formed by the depletion layer associated with a heterojunction.

• Direct tunneling through thin layers of oxide in very thin gates.

• Tunneling into the conduction band of an oxide material when a high bias is applied to a thicker gate oxide (Fowler-Nordheim tunneling).

Note that for tunneling through direct band gap oxide barriers (such as silicon oxide) in indirect band gap semiconductors (such as silicon), an additional complication is encountered due to the band structure mismatch that occurs as a result of the change in the material at the interface. This mismatch is not usually observed in practice — for reasons that are currently not fully understood (see the discussion in chapter 5 of Ref. 43). In this case the phenomenological perspective adopted in Ref. 40 is usually employed, and tunneling through the barrier is treated without accounting for the band structure mismatch, since this approach best describes the experimental results.

In COMSOL Multiphysics, features enabling the modeling of Fowler-Nordheim tunneling are available.

FOWLER-NORDHEIM TUNNELING

When large fields are applied across an oxide layer, tunneling can occur directly into the conduction band of the oxide, as shown in Figure 3-17 below.
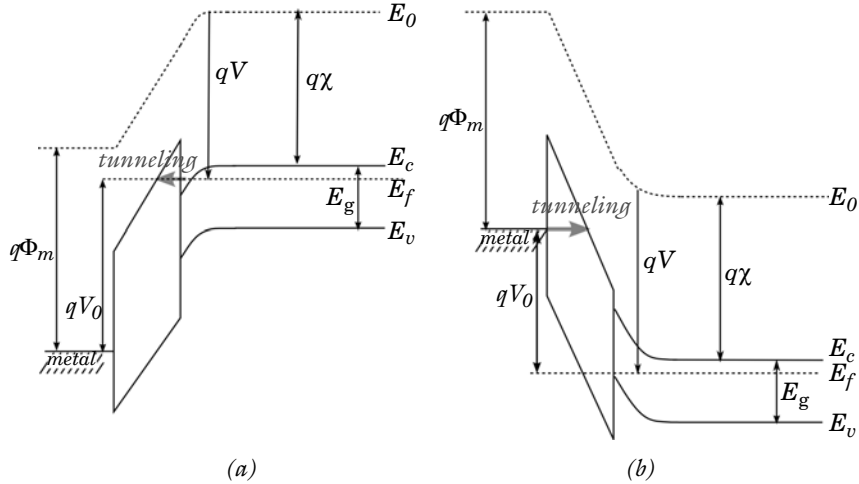
Figure 3-17: Band diagrams showing Fowler-Nordheim electron tunneling into the conduction band of an oxide. E_g is the band gap of the semiconductor, χ. is the electron affinity and Φ_m is the work function of the metal. The energy of the conduction band edge in the semiconductor is E_c, that of the valence band edge is E_v, the vacuum level is E_0 and the Fermi level is E_f. In both (a) and (b) the temperature of the device is the same as the equilibrium reference temperature (temperature changes would cause an additional shift in the Fermi-level which are not shown in the figure - see for example, Figure 3-15). In (a) a large potential V_0 is applied to the semiconductor. The band structure of the insulator is such that electrons can tunnel through the triangular barrier formed by the conduction band edge in the insulator, into the insulator conduction band. In (b) the potential V_0 is applied to the metal, and consequently electrons from the metal can tunnel into the insulator conduction band. Once the electrons tunnel into the conduction band of the insulator they are transported via drift diffusion into the metal (case (a)) or semiconductor (case (b)). Note that the tunnel barrier presented to the electrons is triangular in shape in both cases.

Fowler and Nordheim originally treated tunneling through triangular barriers (Ref. 41) in the context of the Sommerfeld model. Their analysis was applied to tunneling in oxides within a semiconductor device context by Lenzlinger and Snow (Ref. 42). It is worth noting that Fowler and Nordheim did not make a WKB approximation in their original analysis, but instead approximated the final form of the analytic solution (a WKB approximation was used in Ref. 42 but for this reason is not strictly necessary). The original result due to Fowler and Nordheim showed that the tunnel current through a triangular barrier for electrons (J_{FN}^n) and/or holes (J_{FN}^p) takes the form:

$$J_{FN}^n = A_{FN}^n E_{ins}^2 \exp\left(-\frac{B_{FN}^n}{E_{ins}}\right)$$

(3-137)

$$J_{FN}^p = A_{FN}^p E_{ins}^2 \exp\left(-\frac{B_{FN}^p}{E_{ins}}\right)$$

where E_{ins} is the electric field in the insulator and A_{FN}^n, A_{FN}^p, B_{FN}^n, and B_{FN}^p are constants related to the material properties of the insulator and semiconductor. For the commonly encountered case of the silicon/silicon oxide system, only electron tunneling needs to be considered because the barrier for hole tunneling is significantly higher than that for electrons.

Ref. 42 provides a detailed derivation of Equation 3-137, for the case of a semiconductor-oxide system at finite temperature. The effect of a finite temperature was shown to be equivalent to a change in the values of the constants A_{FN}^n and B_{FN}^n. Similarly image force lowering effects at the barrier also caused an effective change in these constants. Since using the derivative material properties does not lead to a fully consistent description of the tunneling current as a function of both electric field and temperature, it is customary to simply treat A_{FN}^n and B_{FN}^n as inputs to a model of the tunneling process at a particular temperature. These values can be extracted from a plot of $\log(J_{FN}^n / E_{ins}^2)$ versus $1/E_{ins}$.

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The Semiconductor Optoelectronics, Beam Envelopes Interface

> ⚠ This physics interface requires a Wave Optics Module license. For theory and physics interface feature descriptions relating to the Beam Envelopes interface, see the *Wave Optics Module User's Guide*.

The **Semiconductor Optoelectronics, Beam Envelopes** interface (🔔) is used to model the interaction of electromagnetic waves with semiconductors. This multiphysics interface adds Electromagnetic Waves, Beam Envelopes and Semiconductor interfaces. By default an Optical Transitions node is added to the Semiconductor interface. The multiphysics couplings add the stimulated and/or spontaneous generation rates to the semiconductor and account for the electromagnetic gain or loss due to absorption or emission of light by the material.

Combinations of frequency-domain modeling for the Electromagnetic Waves, Beam Envelopes interface and stationary modeling for the Semiconductor interface, called frequency-stationary and, similarly, frequency-transient modeling, are supported in 2D and 3D.

When a predefined **Semiconductor Optoelectronics, Beam Envelopes** interface is added from the **Semiconductor** branch (🔳) of the **Model Wizard** or **Add Physics** windows, **Semiconductor** and **Electromagnetic Waves, Beam Envelopes** interfaces are added to the Model Builder.

In addition, a **Multiphysics Couplings** node is added, which automatically includes the multiphysics coupling feature **Semiconductor-Electromagnetic Waves Coupling**.

On the Constituent Physics Interfaces
The Semiconductor interface solves Poisson's equation for the electric potential and the drift-diffusion equations for electrons and holes in a semiconductor material.

The Electromagnetic Waves, Beam Envelopes interface computes electric and magnetic field distributions for systems and devices where the field amplitude varies slowly on a wavelength scale. The physics interface can be used efficiently for unidirectional and bidirectional propagation of electromagnetic beams. In this physics interface the electric field is factored into a product of a slowly varying envelope function (slowly on the scale of a wavelength) and a rapidly varying phase function.

The phase function is a priori prescribed, so the physics interface solves the time-harmonic wave equation for the slowly varying envelope function.

COUPLING FEATURES

If a multiphysics interface is added from the Model Wizard or using the Add Physics window, then the appropriate coupling feature is automatically added to the model builder tree structure. Alternatively, the physics interfaces can be added one at a time, followed by the coupling features.

For example, if single **Semiconductor** and **Electromagnetic Waves, Beam Envelopes** interfaces are added, then COMSOL Multiphysics adds an empty **Multiphysics Couplings** node. You can then choose the coupling feature: **Semiconductor-Electromagnetic Waves Coupling**.

💡	Coupling features are available from the context menu (right-click the **Multiphysics Couplings** node) or from the **Physics** toolbar, **Multiphysics** menu.

PHYSICS INTERFACES AND COUPLING FEATURES

💡	Use the online help in COMSOL Multiphysics to locate and search all the documentation. All these links also work directly in COMSOL Multiphysics when using the Help system.

Coupling Features
The Semiconductor-Electromagnetic Waves Coupling node is described in the section Semiconductor-Electromagnetic Waves Coupling below.

Physics Interface Features
Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

💡	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

The available physics features for The Semiconductor Interface are listed in the section Domain, Edge, Boundary, Pair, and Point Nodes for the Semiconductor Interface.

> [!] The available physics features for The Electromagnetic Waves, Beam Envelopes Interface are listed in the section Domain, Boundary, Edge, and Point Nodes for the Electromagnetic Waves, Beam Envelopes Interface. As this physics interface requires the Wave Optics Module these links do not work in the PDF but they do work in the on line help.

Semiconductor-Electromagnetic Waves Coupling

The **Semiconductor-Electromagnetic Waves Coupling** ( ) node passes the optical field intensity from an electromagnetic waves interface to the **Optical Transitions** feature in the **Semiconductor** interface. The change in the complex refractive index or permittivity that results from the absorption in the semiconductor is then passed back to the electromagnetic waves interface.

SETTINGS
The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. The software refer to variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is semc1.

DOMAIN SELECTION
The default setting is **All domains** which couples all domains in the **Semiconductor** interface that have an active **Optical Transitions** feature with the corresponding domains in the electromagnetic waves interface.

COUPLED INTERFACES
This section defines the physics involved in the coupling. By default, the software selects an appropriate physics interface for you from the **Semiconductor** and **Electromagnetic waves** lists. These selections determine the two interfaces that are coupled by the feature.

The Semiconductor Optoelectronics, Frequency Domain Interface

> ! This physics interface requires a Wave Optics Module license. For theory and physics interface feature descriptions relating to the Electromagnetic Waves, Frequency Domain interface, see the *Wave Optics Module User's Guide*.

The **Semiconductor Optoelectronics, Frequency Domain** interface (👤) is used to model the interaction of electromagnetic waves with semiconductors. This multiphysics interface adds Electromagnetic Waves, Frequency Domain and Semiconductor interfaces. By default an Optical Transitions node is added to the Semiconductor interface. The multiphysics couplings add the stimulated and/or spontaneous generation rates to the semiconductor and account for the electromagnetic gain or loss, due to absorption or emission of light by the material.

Combinations of frequency-domain modeling for the Electromagnetic Waves, Frequency Domain interface and stationary modeling for the Semiconductor interface, called frequency-stationary and, similarly, frequency-transient modeling, are supported in 2D and 3D.

When a predefined **Semiconductor Optoelectronics, Frequency Domain** interface is added from the **Semiconductor** branch (🏭) of the **Model Wizard** or **Add Physics** windows, **Semiconductor** and **Electromagnetic Waves, Frequency Domain** interfaces are added to the Model Builder.

In addition, a **Multiphysics Couplings** node is added, which automatically includes the multiphysics coupling feature **Semiconductor-Electromagnetic Waves Coupling**.

On the Constituent Physics Interfaces
The Semiconductor interface solves Poisson's equation for the electric potential and the drift-diffusion equations for electrons and holes in a semiconductor material.

The Electromagnetic Waves, Frequency Domain interface computes electric and magnetic field distributions for systems and devices where the field amplitude varies slowly on a wavelength scale. The physics interface can be used efficiently for unidirectional and bidirectional propagation of electromagnetic beams. In this physics interface the electric field is factored into a product of a slowly varying envelope

function (slowly on the scale of a wavelength) and a rapidly varying phase function. The phase function is a priori prescribed, so the physics interface solves the time-harmonic wave equation for the slowly varying envelope function.

COUPLING FEATURES

If a multiphysics interface is added from the Model Wizard or using the Add Physics window, then the appropriate coupling feature is automatically added to the model builder tree structure. Alternatively, the physics interfaces can be added one at a time, followed by the coupling features.

For example, if single **Semiconductor** and **Electromagnetic Waves, Frequency Domain** interfaces are added, then COMSOL Multiphysics adds an empty **Multiphysics Couplings** node. You can then choose the coupling feature: **Semiconductor-Electromagnetic Waves Coupling**..

💡	Coupling features are available from the context menu (right-click the **Multiphysics Couplings** node) or from the **Physics** toolbar, **Multiphysics** menu.

PHYSICS INTERFACES AND COUPLING FEATURES

💡	Use the online help in COMSOL Multiphysics to locate and search all the documentation. All these links also work directly in COMSOL Multiphysics when using the Help system.

Coupling Features
The Semiconductor-Electromagnetic Waves Coupling node is described in The Semiconductor Optoelectronics, Beam Envelopes Interface section.

Physics Interface Features
Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

💡	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

The available physics features for The Semiconductor Interface are listed in the section Domain, Edge, Boundary, Pair, and Point Nodes for the Semiconductor Interface.

	The available physics features for The Electromagnetic Waves, Frequency Domain Interface are listed in the section Domain, Boundary, Edge, Point, and Pair Nodes for the Electromagnetic Waves, Frequency Domain Interface. As this physics interface requires the Wave Optics Module these links do not work in the PDF but they do work in the on line help.

4

The AC/DC Branch

This chapter describes the theory for the physics interfaces found under the AC/DC branch (⚡).

In this chapter:

- The Electrostatics Interface
- The Electrical Circuit Interface
- Theory for the Electrostatics Interface
- Theory for the Electrical Circuit Interface

See The Electromagnetics Interfaces in the *COMSOL Multiphysics Reference Manual* for other AC/DC interface and feature node settings.

The Electrostatics Interface

The **Electrostatics (es)** interface (⚡), found under the **AC/DC** branch (⚡) when adding a physics interface, is used to compute the electric field, electric displacement field, and potential distributions in dielectrics under conditions where the electric charge distribution is explicitly prescribed. The formulation is stationary except for use together with other physics interfaces. Eigenfrequency, frequency-domain, small-signal analysis, and time-domain modeling are supported in all space dimensions.

The physics interface solves Gauss' Law for the electric field using the scalar electric potential as the dependent variable.

Charge Conservation is the main node, which adds the equation for the electric potential and has a Settings window for defining the constitutive relation for the electric displacement field and its associated properties such as the relative permittivity.

When this physics interface is added, these default nodes are also added to the **Model Builder** — **Charge Conservation**, **Zero Charge** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and space charges. You can also right-click **Electrostatics** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is es.

CROSS-SECTION AREA (1D COMPONENTS)

For 1D components, enter a default value for the **Cross-section area** A (SI unit: m^2). The default value of 1 is typically not representative for a thin domain. Instead it describes a unit thickness that makes the 1D equation identical to the equation used for 3D components. See also Change Cross Section.

THICKNESS (2D COMPONENTS)

For 2D components, enter a default value for the **Out-of-plane thickness** d (SI unit: m). The default value of 1 is typically not representative for a thin dielectric medium, for example. Instead it describes a unit thickness that makes the 2D equation identical to the equation used for 3D components. See also Change Thickness (Out-of-Plane).

PHYSICS-CONTROLLED MESH

Select the **Enable** check box to allow the physics interface to control the meshing process. Information from the physics, such as the presence of an infinite elements domain or periodic condition, will be used to set up automatically an appropriate mesh sequence.

DEPENDENT VARIABLES

The dependent variable is the **Electric potential** V. You can change its name, which changes both the field name and the variable name. If the new name coincides with the name of another electric potential field in the model, the physics interfaces shares degrees of freedom. The new name must not coincide with the name of a field of another type or with a component name belonging to some other field.

DISCRETIZATION

❗	In the *COMSOL Multiphysics Reference Manual*, see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

▥	*Electric Sensor*: Application Library path **COMSOL_Multiphysics/Electromagnetics/electric_sensor**

Domain, Boundary, Edge, Point, and Pair Nodes for the Electrostatics Interface

The Electrostatics interface has these domain, boundary, edge, point, and pair nodes available.

ABOUT THE BOUNDARY CONDITIONS

The relevant physics interface condition at interfaces between different media is

$$\mathbf{n}_2 \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_s$$

In the absence of surface charges, this condition is fulfilled by the natural boundary condition

$$\mathbf{n} \cdot [(\varepsilon_0 \nabla V - \mathbf{P})_1 - (\varepsilon_0 \nabla V - \mathbf{P})_2] = -\mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = 0$$

AVAILABLE NODES

These nodes, listed in alphabetical order, are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users). Also see Table 4-1 for a list of interior and exterior boundary conditions, including edge, point, and pair availability.

> In general, to add a node, go to the **Physics** toolbar no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Change Cross Section
- Change Thickness (Out-of-Plane)
- Charge Conservation
- Charge Conservation, Piezoelectric[1]
- Dielectric Shielding
- Distributed Capacitance
- Electric Displacement Field
- Electric Potential
- Electrostatic Point Dipole
- External Surface Charge Accumulation
- Floating Potential
- Ground

- Initial Values
- Line Charge
- Line Charge (on Axis)
- Line Charge (Out-of-Plane)
- Periodic Condition
- Point Charge
- Point Charge (on Axis)
- Space Charge Density
- Surface Charge Density
- Terminal
- Thin Low Permittivity Gap
- Zero Charge (the default boundary condition)

[1] This feature is available with the Piezoelectric Devices interface, which requires the Acoustics Module, MEMS Module, or the Structural Mechanics Module.

Table 4-1 lists the interior and exterior boundary conditions available with this physics interface. It also includes edge, point, and pair availability.

TABLE 4-1: INTERIOR AND EXTERIOR BOUNDARY CONDITIONS (INCLUDING EDGE, POINT, AND PAIR AVAILABILITY) FOR THE ELECTROSTATICS INTERFACE

NODE	INTERIOR	EXTERIOR	ALSO AVAILABLE FOR
Change Cross Section	x	x	pairs
Change Thickness (Out-of-Plane)	x	x	pairs
Dielectric Shielding	x	x	pairs
Distributed Capacitance	x	x	pairs
Electric Displacement Field	x	x	pairs
Electric Potential	x	x	edges, points, and pairs
External Surface Charge Accumulation		x	pairs
Floating Potential	x	x	pairs
Ground	x	x	edges, points, and pairs
Periodic Condition		x	not applicable
Surface Charge Density	x	x	pairs
Terminal	x	x	domains
Thin Low Permittivity Gap	x		not applicable
Zero Charge (the default)	x	x	pairs

For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node to the model that is valid on the axial symmetry boundaries only. There are also **Line Charge (on Axis)** and **Point Charge (on Axis)** available.

In the *COMSOL Multiphysics Reference Manual*, see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Charge Conservation

The **Charge Conservation** node adds the equations for charge conservation according to Gauss' law for the electric displacement field. It provides an interface for defining the constitutive relation and its associated properties such as the relative permittivity.

MATERIAL TYPE

The **Material type** setting decides how materials behave and how material properties are interpreted when the mesh is deformed. Select **Solid** for materials whose properties change as functions of material strain, material orientation, and other variables evaluated in a material reference configuration (material frame). Select **Non-solid** for materials whose properties are defined only as functions of the current local state at each point in the spatial frame, and for which no unique material reference configuration can be defined. Select **From material** to pick up the corresponding setting from the domain material on each domain.

ELECTRIC FIELD

Select a **Constitutive relation** to describe the macroscopic properties of the medium (relating the electric displacement $\mathbf{D}$ with the electric field $\mathbf{E}$) and the applicable material properties, such as the relative permittivity. Select:

- **Relative permittivity** (the default) to use the constitutive relation $\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E}$. Then the default is to take the **Relative permittivity** ε_r (dimensionless) values **From material**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** and enter values or expressions in the field or matrix. The default is 1.

- **Polarization** to use the constitutive relation $\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P}$. Then enter the components based on space dimension for the **Polarization** vector $\mathbf{P}$ (SI unit: C/m^2). The defaults are 0 C/m^2.

- **Remanent electric displacement** to use constitutive relation $\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E} + \mathbf{D}_r$, where $\mathbf{D}_r$ is the remanent displacement (the displacement when no electric field is present). Then the default is to take the **Relative permittivity** ε_r (dimensionless) values **From material**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** and enter values or expressions in the field or matrix. Then enter the components based on space dimension for the **Remanent electric displacement** $\mathbf{D}_r$ (SI unit: C/m^2). The defaults are 0 C/m^2.

Initial Values

The **Initial Values** node adds an initial value for the electric potential V that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter a value or expression for the initial value of the **Electric potential** V (SI unit: V). The default value is 0 V.

Space Charge Density

The **Space Charge Density** node adds a space charge density ρ, which appears on the right-hand side of the equation that the physics interface defines.

SPACE CHARGE DENSITY

Enter a value or expression for the **Space charge density** ρ_v (SI unit: C/m^3). The default is 0 C/m^3.

Zero Charge

The **Zero Charge** node adds the condition that there is zero charge on the boundary so that $\mathbf{n} \cdot \mathbf{D} = 0$. This boundary condition is also applicable at symmetry boundaries where the potential is known to be symmetric with respect to the boundary. This is the default boundary condition at exterior boundaries. At interior boundaries, it means that no displacement field can penetrate the boundary and that the electric potential is discontinuous across the boundary.

Ground

The **Ground** node implements ground (zero potential) as the boundary condition $V = 0$.

Ground means that there is a zero potential on the boundary. This boundary condition is also applicable at symmetry boundaries where the potential is known to be antisymmetric with respect to the boundary.

For some physics interfaces, also select additional **Ground** nodes from the **Edges** (3D components) or **Points** (2D and 3D components) submenus. For 2D axisymmetric components, it can be applied on the Symmetry axis.

> ⚠ Beware that constraining the potential on edges or points in 3D or on points in 2D usually yields a current outflow that is mesh dependent.

GROUND

Enter a value for the **Contact work function** Φ_c (SI unit: V). The default is 4 V.

CONSTRAINT SETTINGS

To display this section, click the **Show** button (👁) and select **Advanced Physics Options**.

Electric Potential

The **Electric Potential** node provides an electric potential V_0 as the boundary condition $V = V_0$.

Because the electric potential is being solved for in the physics interface, the value of the potential is typically defined at some part of the geometry. For some physics interfaces, also select additional **Electric Potential** nodes from the **Edges** (3D components) or **Points** (2D and 3D components) submenus. For 2D axisymmetric components, it can be applied on the symmetry axis.

BOUNDARY, EDGE, OR POINT SELECTION

> ⚠ Beware that constraining the potential on edges or points in 3D or on points in 2D usually yields a current outflow that is mesh dependent.

ELECTRIC POTENTIAL

Enter the value or expression for the **Electric potential** V_0 (SI unit: V). The default is 0 V.

Enter a value for the **Contact work function** Φ_c (SI unit: V). The default is 4 V.

CONSTRAINT SETTINGS

To display this section, click the **Show** button (👁) and select **Advanced Physics Options**.

Surface Charge Density

The **Surface Charge Density** node provides the following surface-charge boundary condition for exterior boundaries (left) and interior boundaries (right):

$$-\mathbf{n} \cdot \mathbf{D} = \rho_s, \qquad \mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_s$$

Specify the surface charge density ρ_s at an outer boundary or at an interior boundary between two nonconducting media.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or click **Harmonic Perturbation** on the **Physics** toolbar. For more information, see Harmonic Perturbation — Exclusive and Contributing Nodes in the *COMSOL Multiphysics Reference Manual*.

SURFACE CHARGE DENSITY

Enter the value or expression for the **Surface charge density** ρ_s (SI unit: C/m^2).

External Surface Charge Accumulation

The **External Surface Charge Accumulation** node implements the boundary condition

$$-\mathbf{n} \cdot \mathbf{D} = \rho_s$$

where ρ_s is the solution of the following distributed ODE on the boundary:

$$\frac{d\rho_s}{dt} = \mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e$$

where $\mathbf{n} \cdot \mathbf{J}_i$ is the normal component of the total ion current density on the wall and $\mathbf{n} \cdot \mathbf{J}_e$ is the normal component of the total electron current density on the wall, which are feature inputs.

MATERIAL TYPE

The **Material type** setting decides how materials behave and how material properties are interpreted when the mesh is deformed. Select **Solid** for materials whose properties change as functions of material strain, material orientation, and other variables evaluated in a material reference configuration (material frame). Select **Non-solid** for materials whose properties are defined only as functions of the current local state at each point in the spatial frame, and for which no unique material reference

configuration can be defined. Select **From material** to pick up the corresponding setting from the domain material on each domain.

EXTERNAL SURFACE CHARGE ACCUMULATION

Enter values or expressions for the **Normal ion current density** $\mathbf{n} \cdot \mathbf{J}_i$ (SI unit: A/m^2) and the **Normal electron current density** $\mathbf{n} \cdot \mathbf{J}_e$ (SI unit: A/m^2).

Electric Displacement Field

The **Electric Displacement Field** node adds the following electric-displacement boundary condition:

$$\mathbf{n} \cdot \mathbf{D} = \mathbf{n} \cdot \mathbf{D}_0$$

It specifies the normal component of the electric displacement field at a boundary.

ELECTRIC DISPLACEMENT FIELD

Enter the coordinates of the **Boundary electric displacement field** $\mathbf{D}_0$ (SI unit: C/m^2).

Periodic Condition

The **Periodic Condition** node defines periodicity or antiperiodicity between two boundaries. If required, activate periodic conditions on more than two boundaries, in which case the Periodic Condition tries to identify two separate surfaces that can each consist of several connected boundaries. For more complex geometries, it might be necessary to use the **Destination Selection** subnode. With this subnode the boundaries which constitute the source and destination surfaces can be manually specified. The **Destination Selection** subnode is available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu.

📄 | When this feature is used in conjunction with a Sector Symmetry feature on connected boundaries, wherever the sector symmetry boundaries connect with the periodic boundaries, the same periodic condition feature cannot be used on both sides. At least two periodic condition features are required for the model to compute correctly.

When using nonconforming meshes on the source and destination of a periodic boundary pair, for numerical stability, a finer mesh should be applied on the destination side. Use conforming meshes if possible.

PERIODIC CONDITION

Select a **Type of periodicity** — **Continuity** (the default), **Antiperiodicity**, or **Floquet periodicity**. Select:

- **Continuity** to make the electric potential periodic (equal on the source and destination),

- **Antiperiodicity** to make it antiperiodic, or

- **Floquet periodicity** (only available with products supporting piezoelectric modeling). Specify the components of the **k-vector for Floquet periodicity $\mathbf{k}_F$** (SI unit: rad/m).

CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.

For information about the Orientation of Source section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

Thin Low Permittivity Gap

Use the **Thin Low Permittivity Gap** node

$$\mathbf{n} \cdot \mathbf{D}_1 = \frac{\varepsilon_0 \varepsilon_r}{d_s}(V_1 - V_2)$$

$$\mathbf{n} \cdot \mathbf{D}_2 = \frac{\varepsilon_0 \varepsilon_r}{d_s}(V_2 - V_1)$$

to model a thin gap of a material with a small permittivity compared to the adjacent domains. The layer has the thickness d_s and the relative permittivity ε_r. The indices 1 and 2 refer to the two sides of the boundary.

THIN LOW PERMITTIVITY GAP

The default is to take the **Relative permittivity** ε_r (dimensionless) values **From material**. For **User defined**, enter a different value or expression. Enter a **Surface thickness** d_s (SI unit: m). The default is 5 mm.

Dielectric Shielding

The **Dielectric Shielding** node adds dielectric shielding as a boundary condition. It describes a thin layer with thickness d_s and a bulk relative permittivity; ε_r that shields the electric field:

$$\mathbf{n} \cdot \mathbf{D} = -\nabla_t \cdot \varepsilon_0 \varepsilon_{rs} d_s \nabla_t V$$

Use this boundary condition when approximating a thin domain with a boundary to reduce the number of mesh elements.

MATERIAL TYPE

The **Material type** setting decides how materials behave and how material properties are interpreted when the mesh is deformed. Select **Solid** for materials whose properties change as functions of material strain, material orientation and other variables evaluated in a material reference configuration (material frame). Select **Non-solid** for materials whose properties are defined only as functions of the current local state at each point in the spatial frame, and for which no unique material reference configuration can be defined. Select **From material** to pick up the corresponding setting from the domain material on each domain.

ELECTRIC SHIELDING

The default is to take the **Relative permittivity** ε_r (dimensionless) values **From material**. It takes it from the adjacent domains if not explicitly defined. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** and enter values or expressions in the field or matrix. Enter a **Surface thickness** d_s (SI unit: m) of the shielding. The default is 1 m.

Terminal

The **Terminal** node provides a boundary or domain condition for connection to external circuits, to transmission lines, or with a specified voltage or charge. By specifying zero charge, a floating potential condition is obtained.

The **Terminal** node also enables the computation of the lumped parameters of the system, such as capacitance

TERMINAL

Specify the terminal properties. Enter a unique **Terminal name** that will be used to identify the global variables (such as the terminal voltage or current) that are defined

by the terminal. The **Terminal name** can contain alphanumeric characters, but it should be numeric when performing terminal sweeps.

Enter a value for the **Contact work function** Φ_c(SI unit: V). The default is 4 V.

Select a **Terminal type** — **Charge** (the default), **Voltage**, **Circuit**, or **Terminated**. Select:

- **Charge** to prescribe the total charge deposited on the terminal boundaries. Enter the total charge Q_0. The default is 0 C, which corresponds to a uncharged floating electrode.

- **Voltage** to specify a fixed electric potential at the terminal. Enter an electric potential V_0. The default is 1 V.

- **Circuit** to specify a terminal connected to an Electrical Circuit physics interface that models an external circuit. The Terminal node provides a current-voltage characteristic to the circuit.

> **!** The Electrical Circuit interface requires a current from the Terminal, so the **Circuit** terminal type can only be used in Time Dependent or Frequency Domain studies, in which the current can be computed as the time derivative of the charge.
>
> The **Circuit** type cannot be used together with a terminal sweep.

- **Terminated** to connect the terminal to an impedance that might represent a load or a transmission line. When **Terminated** is selected, the scattering parameters (S-parameters) are computed. The **Terminated** setting can only be used in frequency-domain studies.

  - Enter a **Terminal power** P_0 to specify the input power at this terminal from the transmission line. This excitation can be toggled using a port sweep.

  - Select an option from the **Characteristic impedance from** list to define the value of the impedance — **Physics interface** or **User defined**. For **Physics interface** the **Reference impedance** Z_{ref} defined on the **Settings** window for the physics under Sweep Settings is used. For **User defined** enter a specific impedance Z_{ref} for this terminal. The default is 50 Ω.

Initial values
The initial values subsection is used to provide initial values for the internal state variables in the Terminal. These settings can be useful to provide an initial guess to the nonlinear solver or the initial value in a time-dependent study.

The **Initial value for voltage** is available for all Terminal types except Voltage. Enter an **Initial value for voltage** V_{init}.

The **Initial value for charge** is available for the Circuit excitation. It specifies the initial charge on the terminal when the circuit is connected. Enter an **Initial value for charge** Q_{init}.

CONSTRAINT SETTINGS

To display this section, click the **Show** button (![show icon]) and select **Advanced Physics Options**.

🔍   Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

Floating Potential

The **Floating Potential** node is used when modeling a metallic electrode at floating potential. It applies a constant voltage V_0 on the boundary (for domain features, this is the boundary enclosing the selected domain), such that the total normal electric displacement field **D** equals a specific charge Q_0:

$$V = V_0$$

$$\int_{\partial\Omega} (\mathbf{D} \cdot \mathbf{n})dS = Q_0,$$

where Ω represents the boundary and **n** refers to the surface normal. The constant boundary voltage implies the tangential electric field equals zero; the electric field will be perpendicular to the boundary:

$$-\nabla_t V = \mathbf{E}_t = 0$$
$$\mathbf{n} \times \mathbf{E} = 0.$$

In case of $Q_0 = 0$ (the default case), the boundary will behave as an unconnected, neutrally charged, good conductor under electrostatic conditions (a floating equipotential). Although locally the displacement field may vary, the total electric displacement field entering or leaving the boundary equals zero.

If the floating potential touches a point, boundary or domain feature that is not floating (a **Terminal** or **Ground** feature), the floating potential will acquire that feature's potential. If the floating potential is set to a certain charge, or connected to a circuit, it behaves like a terminal.

The **Floating potential identifier** text area shows the unique identifier for the floating potential feature. It is used to identify the global variables created by the node, such as the voltage. The **Floating potential group** check box on the **Settings** window for **Floating Potential** controls how potentials are assigned to boundary segments in the feature's boundary selection. If this check box is not selected, a single potential is applied to all boundaries in the selection. If the check box is selected, each group of contiguous boundaries in the selection is given a unique potential. This simplifies the setup of models with many floating electrodes. The values of the potential at each group of boundaries are then made available in postprocessing, collected in a vector variable.

The following options are not available if the **Floating potential group** check box is selected. Select a specification for the **Electric charge** — choose **User defined** to specify a total **Charge** Q_0 deposited on the surface. Select **Circuit** to connect the floating potential to an Electrical Circuit. Enter a value for the **Contact work function** Φ_c (SI unit: V). The default is 4 V.

	The Electrical Circuit interface requires a current from the Floating Potential, so the **Circuit** terminal type can only be used in Time Dependent or Frequency Domain studies, in which the current can be computed as the time derivative of the charge.

Initial Values

The initial values subsection is used to provide initial values for the internal state variables in the Floating potential. These settings can be useful to provide an initial guess to the nonlinear solver or the initial value in a time-dependent study.

Enter an **Initial value for voltage** V_{init}.

The **Initial value for charge** is available for the Circuit excitation. It specifies the initial charge on the floating potential when the circuit is connected. Enter an **Initial value for charge** Q_{init}.

C O N S T R A I N T   S E T T I N G S

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.

	Settings and Properties Windows for Feature Nodes in the *COMSOL Multiphysics Reference Manual*

Distributed Capacitance

The **Distributed Capacitance** node adds a distributed capacitance boundary condition according to the following equations for exterior boundaries (left) and interior boundaries (right):

$$-\mathbf{n} \cdot \mathbf{D} = \varepsilon_0 \varepsilon_r \frac{V_{\text{ref}} - V}{d_s} \qquad \mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \varepsilon_0 \varepsilon_r \frac{V_{\text{ref}} - V}{d_s}$$

Use this boundary condition to model a thin sheet or film of a dielectric material. The sheet has the relative permittivity ε_r and the surface thickness d_s, and it is connected to the reference potential V_{ref}.

DISTRIBUTED CAPACITANCE

Enter the values or expressions for **Relative permittivity** ε_r (dimensionless), **Surface thickness** d_s (SI unit: m), and **Reference potential** V_{ref}. The default value for the surface thickness is 10^{-3} m (1 mm) and 0 V for the reference potential.

Enter a value for the **Contact work function** Φ_c(SI unit: V). The default is 4 V.

Line Charge

For 3D components, use the **Line Charge** node to specify line charges along the edges of a geometry. Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** on the **Physics** toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the *COMSOL Multiphysics Reference Manual*.

EDGE SELECTION

> ⚠ Beware that constraining the potential on edges usually yields a current outflow that is mesh dependent.

LINE CHARGE

Enter a value or expression to apply a **Line charge** Q_L (SI unit: C/m). This source represents electric charge per unit length and the default is 0 C/m.

⊙	Line Charge (on Axis) and Line Charge (Out-of-Plane)

Line Charge (on Axis)

For 2D axisymmetric components, use the **Line Charge (on Axis)** node to specify line charges along the symmetry axis.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or click **Harmonic Perturbation** on the **Physics** toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the *COMSOL Multiphysics Reference Manual*.

LINE CHARGE (ON AXIS)

Enter a value or expression to apply a **Line charge** Q_L (SI unit: C/m). This source represents electric charge per unit length and the default is 0 C/m.

⊙	Line Charge and Line Charge (Out-of-Plane)

Line Charge (Out-of-Plane)

For 2D and 2D axisymmetric components, points are selected and this is the same as a line out-of-plane.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** on the **Physics** toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the *COMSOL Multiphysics Reference Manual*.

Use the **Line Charge (Out-of-Plane)** node to specify line charges along the points of a geometry for 2D and 2D axisymmetric components.

> ⚠️ Beware that constraining the potential on points usually yields a current outflow that is mesh dependent.

LINE CHARGE (OUT-OF-PLANE)

Enter a value or expression to apply a **Line charge** Q_L (SI unit: C/m). This source represents electric charge per unit length and the default is 0 C/m.

> 🔍 Line Charge and Line Charge (on Axis)

Point Charge

The **Point Charge** node adds a point source to 3D components. The point charge represents an electric displacement field flowing out of the point.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** on the **Physics** toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the *COMSOL Multiphysics Reference Manual*.

POINT SELECTION

> ⚠️ Beware that constraining the potential on points usually yields a current outflow that is mesh dependent.

POINT CHARGE

Enter a value or expression to apply a **Point charge** Q_P (SI unit: C) to points. This source represents an electric displacement field flowing out of the point. The default is 0 C.

> 🔍 Point Charge (on Axis) and Line Charge (Out-of-Plane)

Point Charge (on Axis)

The **Point Charge (on Axis)** node adds a point source to 2D axisymmetric components. The point charge represents an electric displacement field flowing out of the point.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** on the **Physics** toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the *COMSOL Multiphysics Reference Manual*.

POINT SELECTION

⚠️ Beware that constraining the potential on points usually yields a current outflow that is mesh dependent.

POINT CHARGE (ON AXIS)

Enter a value or expression to apply a **Point charge** Q_P (SI unit: C) to points on an axis. This source represents an electric displacement field flowing out of the point. The default is 0 C.

🔍 Point Charge and Line Charge (Out-of-Plane)

Change Cross Section

This node is available with 1D components. This setting overrides the global **Cross-Section Area** setting made in any physics interface that uses this feature. For 2D components, see Change Thickness (Out-of-Plane).

Use the **Change Cross-Section** node to set the cross-section area for specific geometric entities.

CHANGE CROSS SECTION

Enter a value or expression for the **Cross-section area** A. The default value of 1 unit length is typically not representative for a thin domain. Instead it describes a unit thickness that makes the 1D equation identical to the equation used for 3D components.

Change Thickness (Out-of-Plane)

This node is available for 2D components. This setting overrides the global **Thickness** setting made in any physics interface that uses this node. For 1D components, see Change Cross Section.

Use the **Change Thickness (Out-of-Plane)** node to set the out-of-plane thickness for specific geometric entities.

CHANGE THICKNESS (OUT-OF-PLANE)

Enter a value or expression for the **Out-of-plane thickness** d (SI unit: m). The default value is, in most cases, 1 unit length, which is typically not representative for a thin domain. Instead it describes a unit thickness that makes the 2D equation identical to the equation used for 3D components.

Charge Conservation, Piezoelectric

📋 This feature is available with the Piezoelectric Devices interface, which requires the Acoustics Module, MEMS Module, or the Structural Mechanics Module. See the individual documentation for information.

The **Charge Conservation, Piezoelectric** node is normally used together with a **Piezoelectric Effect** multiphysics coupling node and a corresponding **Piezoelectric Material** node in the **Solid Mechanics** interface. The node is added by default to the **Electrostatics** interface when adding a Piezoelectric Devices interface. It is also available from the context menu (right-click the **Electrostatics** interface parent node) or from the **Physics** toolbar.

⚠️ When the **Charge Conservation, Piezoelectric** node is added to the electrostatics interface in the absence of an active **Piezoelectric Effect** multiphysics coupling node, the material behaves similarly to a Charge Conservation node, with electric properties corresponding to the relative permittivity entered (see below). The piezoelectric effect is *not* included in the corresponding equation system.

ELECTRIC DISPLACEMENT

If the node is used together with an active **Piezoelectric Effect** multiphysics coupling node, then these settings are locked. Note that if they are unlocked, then the material

behaves like a dielectric and *not* a piezoelectric. In this case, the default is to take the **Relative permittivity** ε_{rS} (dimensionless) values **From material**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** and enter values or expressions in the field or matrix.

Electrostatic Point Dipole

Add an **Electrostatic Point Dipole** node to 3D and 2D components. Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or click **Harmonic Perturbation** on the **Physics** toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the *COMSOL Multiphysics Reference Manual*.

The **Electrostatic Point Dipole** represents the limiting case of zero separation distance between two equally strong point sources of opposing signs while maintaining the product between separation distance and source strength at a fixed value (p). The dipole moment is a vector entity with positive direction from the negative charge to the positive one.

ELECTROSTATIC POINT DIPOLE

Select a **Dipole specification** — **Magnitude and direction** (the default) or **Electric dipole moment**.

- For **Magnitude and direction** enter coordinates for the **Electric dipole moment direction** $\mathbf{n}_p$ (dimensionless) and the **Electric dipole moment, magnitude** p.

- For **Electric dipole moment** enter coordinates for the **Electric dipole moment** $\mathbf{p}$.

The Electrical Circuit Interface

The **Electrical Circuit (cir)** interface (⬚), found under the **AC/DC** branch (⚡) when adding a physics interface, is used to model currents and voltages in circuits including voltage and current sources, resistors, capacitors, inductors, and semiconductor devices. Models created with the Electrical Circuit interface can include connections to distributed field models. The physics interface supports stationary, frequency-domain and time-domain modeling and solves Kirchhoff's conservation laws for the voltages, currents and charges associated with the circuit elements.

When this physics interface is added, it adds a default **Ground Node** feature and associates that with node zero in the electrical circuit.

> ⚠ Circuit nodes are nodes in the electrical circuit (electrical nodes) and should not be confused with nodes in the Model Builder tree of the COMSOL Multiphysics software. Circuit node names are not restricted to numerical values but can contain alphanumeric characters.

DEVICE NAMES

Each circuit component has an associated **Device name**, which is constructed from a prefix identifying the type of the device and a string. The string can be specified in the feature's **Settings** window. The **Device name** is used to identify variables defined by the component, and for the SPICE Import and Export functionality.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `cir`.

RESISTANCE IN PARALLEL TO PN JUNCTIONS

For numerical stability, a large resistance is added automatically in parallel to the pn junctions in diodes and BJT devices. Enter a default value for the **Resistance in parallel to pn junctions** R_j (SI unit: Ω). The default value is $1 \cdot 10^{12}$ Ω.

CREATE UNIQUE NODES FOR NEW DEVICES

When this setting is selected (the default), newly added devices will be assigned unused node names. The devices will be disconnected from the rest of the circuit and the nodes should be updated to reflect the actual circuit connections. When the this setting is deselected, new devices will be connected to the lowest-numbered nodes starting from 0.

ELECTRICAL CIRCUIT TOOLBAR

The following nodes are available from the **Electrical Circuit** ribbon toolbar (Windows users), **Electrical Circuit** context menu (Mac or Linux users), or right-click to access the context menu (all users).:

For step-by-step instructions and general documentation descriptions, this is the **Electrical Circuit** toolbar.

- Ground Node
- Voltmeter
- Ampère Meter
- Resistor
- Capacitor
- Inductor
- Voltage Source
- Current Source
- Diode
- Voltage-Controlled Voltage Source[1]
- Voltage-Controlled Current Source[1]
- Current-Controlled Voltage Source[1]
- Current-Controlled Current Source[1]
- Subcircuit Definition
- Subcircuit Instance
- Mutual Inductance
- Transformer
- NPN BJT and PNP BJT[2]
- n-Channel MOSFET and p-Channel MOSFET[2]
- External I vs. U[3]
- External U vs. I[3]
- External I-Terminal[3]
- SPICE Circuit Import
- SPICE Circuit Export

[1] Selected from the **Dependent Sources** submenu when you right-click main node.

[2] Selected from the **Transistors** submenu when you right-click main node.

[3] Selected from the **External Couplings** submenu when you right-click main node.

Ground Node

The **Ground Node** (⏚) feature adds a ground node with the default node number zero to the electrical circuit. This is the default node in the Electrical Circuit interface. More ground nodes can be added but those must have unique node numbers and are by default given higher node numbers.

GROUND CONNECTION

Set the **Node name** for the ground node in the circuit. The convention is to use 0 (zero) for the ground node. If adding more ground nodes. each must have a unique node name (number).

Voltmeter

The **Voltmeter** (⦵) feature connects a voltmeter (voltage measurement device) between two nodes in the electrical circuit. A voltmeter behaves electrically as an open circuit. The voltmeter node adds a Probe sampling the voltage across it.

DEVICE NAME

Enter a **Device name** for the voltmeter. The name is also used in the probe.

NODE CONNECTIONS

Set the two **Node names** for the connecting nodes for the resistor.

Ampère Meter

The **Ammeter** (⊕) feature connects an ammeter (current measurement device) between two nodes in the electrical circuit. An ammeter behaves electrically as a short circuit. The ammeter node adds a Probe sampling the current through it.

DEVICE NAME

Enter a Device name for the ammeter. The name is also used in the probe.

NODE CONNECTIONS

Set the two **Node names** for the connecting nodes for the resistor.

DEVICE PARAMETERS

Enter the **Resistance** of the resistor.

Resistor

The **Resistor** (▭) feature connects a resistor between two nodes in the electrical circuit.

DEVICE NAME

Enter a **Device name** for the resistor. The prefix is R.

NODE CONNECTIONS

Set the two **Node names** for the connecting nodes for the resistor.

DEVICE PARAMETERS

Enter the **Resistance** of the resistor.

Capacitor

The **Capacitor** (⊣⊢) feature connects a capacitor between two nodes in the electrical circuit.

DEVICE NAME

Enter a **Device name** for the capacitor. The prefix is C.

NODE CONNECTIONS

Set the two **Node names** for the connecting nodes for the capacitor.

DEVICE PARAMETERS

Enter the **Capacitance** of the capacitor.

Inductor

The **Inductor** (⟋) feature connects an inductor between two nodes in the electrical circuit.

DEVICE NAME

Enter a Device name for the inductor. The prefix is L.

NODE CONNECTIONS

Set the two **Node names** for the connecting nodes for the inductor.

DEVICE PARAMETERS

Enter the **Inductance** of the inductor.

Voltage Source

The **Voltage Source** (⊙) feature connects a voltage source between two nodes in the electrical circuit.

DEVICE NAME

Enter a **Device name** for the voltage source. The prefix is V.

NODE CONNECTIONS

Set the two **Node names** for the connecting nodes for the voltage source. The first node represents the positive reference terminal.

Enter the **Source type** that should be adapted to the selected study type. It can be **DC-source**, **AC-source**, or a time-dependent **Sine source** or **Pulse source**. Depending on the choice of source, also specify the following parameters:

- For a DC-source, the **Voltage V$_{src}$** (default value: 1 V). DC-sources are active in Stationary and Time-Dependent studies.

- For an AC-source: the **Voltage V$_{src}$** (default value: 1 V) and the **Phase** Θ (default value: 0 rad). AC-sources are active in Frequency Domain studies only.

- For a sine source: the **Voltage V$_{src}$** (default value: 1 V), the **Offset V$_{off}$** (default value: 0 V), the **Frequency** (default value: 1 kHz), and the **Phase** Θ (default value: 0 rad). The sine sources are active in Time-Dependent studies and also in Stationary studies, providing that a value for t has been provided as a model parameter or global variable.

- For a pulse source: the **Voltage V$_{src}$** (default value: 1 V), the **Offset V$_{off}$** (default value: 0 V), the **Delay t$_d$** (default value: 0s), the **Rise time t$_r$** and **Fall time t$_f$** (default values: 0 s), the **Pulse width p$_w$** (default value: 1 µs), and the **Period T$_{per}$** (default value: 2 µs). The pulse sources are active in Time-Dependent studies and also in Stationary studies, providing that a value for t has been provided as a model parameter or global variable.

All values are peak values rather than RMS.

📋	For the AC source, the frequency is a global input set by the solver. AC sources should be used in Frequency-domain studies only. Do not use the **Sine source** unless the model is time-dependent.

Current Source

The **Current Source** (⏀) feature connects a current source between two nodes in the electrical circuit.

DEVICE NAME

Enter a **Device name** for the current source. The prefix is I.

Set the two **Node names** for the connecting nodes for the current source. The first node represents the positive reference terminal from where the current flows through the source to the second node.

DEVICE PARAMETERS

Enter the **Source type** that should be adapted to the selected study type. It can be **DC-source**, **AC-source**, or a time-dependent **Sine source** or **Pulse source**. Depending on the choice of source, also specify the following parameters:

- For a DC-source, the **Current i_{src}** (default value: 1 A). DC-sources are active in Stationary and Time-Dependent studies.

- For an AC-source: the **Current i_{src}** (default value: 1 A) and the **Phase Θ** (default value: 0 rad). AC-sources are active in Frequency Domain studies only.

- For a sine source: the **Current i_{src}** (default value: 1 A), the **Offset i_{off}** (default value: 0 A), the **Frequency** (default value: 1 kHz), and the **Phase Θ** (default value: 0 rad). The sine sources are active in Time-Dependent studies and also in Stationary studies, providing that a value for t has been provided as a model parameter or global variable.

- For a pulse source: the **Current i_{src}** (default value: 1 A), the **Offset i_{off}** (default value: 0 A), the **Delay t_d** (default value: 0 s), the **Rise time t_r** and **Fall time t_f** (default values: 0 s), the **Pulse width p_w** (default value: 1 μs), and the **Period T_{per}** (default value: 2 μs). The pulse sources are active in Time-Dependent studies and also in Stationary studies, providing that a value for t has been provided as a model parameter or global variable.

All values are peak values rather than RMS.

	For the AC source, the frequency is a global input set by the solver. AC sources should be used in Frequency-domain studies only. Do not use the **Sine source** unless the model is time-dependent.

Voltage-Controlled Voltage Source

The **Voltage-Controlled Voltage Source** (◈) feature connects a voltage-controlled voltage source between two nodes in the electrical circuit. A second pair of nodes define the input control voltage.

DEVICE NAME

Enter a **Device name** for the voltage-controlled voltage source. The prefix is E.

NODE CONNECTIONS

Specify four **Node names**: the first pair for the connection nodes for the voltage source and the second pair defining the input control voltage. The first node in a pair represents the positive reference terminal.

DEVICE PARAMETERS

Enter the voltage **Gain**. The resulting voltage is this number multiplied by the control voltage.

Voltage-Controlled Current Source

The **Voltage-Controlled Current Source** (⬦) feature connects a voltage-controlled current source between two nodes in the electrical circuit. A second pair of nodes define the input control voltage.

DEVICE NAME

Enter a **Device name** for the voltage-controlled current source. The prefix is G.

NODE CONNECTIONS

Specify four **Node names**: the first pair for the connection nodes for the current source and the second pair defining the input control voltage. The first node in a pair represents the positive voltage reference terminal or the one from where the current flows through the source to the second node.

DEVICE PARAMETERS

Enter the source **Gain** (SI units: S). The resulting current is this number multiplied by the control voltage. It represents the transconductance of the source.

Current-Controlled Voltage Source

The **Current-Controlled Voltage Source** (⬦) feature connects a current-controlled voltage source between two nodes in the electrical circuit. The input control current is the one flowing through a two-pin device.

DEVICE NAME

Enter a **Device name** for the current-controlled voltage source. The prefix is H.

Set two **Node names** for the connection nodes for the voltage source. The first node in a pair represents the positive reference terminal.

D E V I C E   P A R A M E T E R S

Enter the voltage **Gain** and select the **Device** whose current is taken as the control current. The resulting voltage is this number multiplied by the control current through the named **Device** (any two-pin device). Thus it formally has the unit of resistance.

Current-Controlled Current Source

The **Current-Controlled Current Source** (◈) feature connects a current-controlled current source between two nodes in the electrical circuit. The input control current is the one flowing through a named device that must be a two-pin device.

D E V I C E   N A M E

Enter a **Device name** for the current-controlled current source. The prefix is F.

N O D E   C O N N E C T I O N S

Specify two **Node names** for the connection nodes for the current source. The first node in a pair represents the positive reference terminal from where the current flows through the source to the second node.

D E V I C E   P A R A M E T E R S

Enter the current **Gain** and select the **Device** whose current is taken as the control current. The resulting current is this number multiplied by the control current through the **Device**.

Subcircuit Definition

The **Subcircuit Definition** (▥) feature is used to define subcircuits, which can be inserted as devices into the main circuit using Subcircuit Instance nodes. Create the subcircuit by adding subnodes to the **Subcircuit Definition** node, either by using the **Physics** toolbar, or by right-clicking the **Subcircuit Definition**.

S U B C I R C U I T   P I N S

Define the **Pin names** at which the subcircuit connects to the main circuit or to other subcircuits when referenced by a Subcircuit Instance node. The **Pin names** refer to circuit nodes in the subcircuit. The order in which the **Pin names** are defined is the

order in which they are referenced by a Subcircuit Instance node. The devices constistuting the subcircuit should be connected only to the subcircuit's pins and to themselves.

Subcircuit Instance

The **Subcircuit Instance** (⊞) feature represents an instance of a subcircuits defined by a Subcircuit Definition feature.

DEVICE NAME
Enter a **Device name** for the subcircuit instance. The prefix is X.

NODE CONNECTIONS
Select the **Name of subcircuit link** from the list of defined subcircuits in the circuit model and the circuit **Node names** at which the subcircuit instance connects to the main circuit or to another subcircuit if used therein.

NPN BJT and PNP BJT

The **NPN BJT** (⊕) and the **PNP BJT** (⊕) device models are large-signal models for bipolar junction transistors (BJT). It is an advanced device model and no thorough description and motivation of the many input parameters are attempted here. Many device manufacturers provide model input parameters for this BJT model. For any particular make of BJT, the device manufacturer should be the primary source of information.

DEVICE NAME
Enter a **Device name** for the BJT. The prefix is Q.

NODE CONNECTIONS
Specify three **Node names** for the connection nodes for the **BJT** device. These represent the *collector*, *base*, and *emitter* nodes for the **NPN** transistor, and the *emitter*, *base*, and *collector* nodes for the **PNP** transistor.

MODEL PARAMETERS

Specify the **Model Parameters**. Reasonable defaults are provided but for any particular BJT, the device manufacturer should be the primary source of information.

🔍	The interested reader is referred to Ref. 1 for more details on semiconductor modeling within circuits.
	For an explanation of the **Model Parameters** see Bipolar Transistors.

n-Channel MOSFET and p-Channel MOSFET

The **n-Channel MOSFET** (⊕) and the **p-Channel MOSFET** (⊕) device models are large-signal models for, respectively, an n-Channel MOS field-effect transistor (MOSFET) and p-Channel MOSFET. These are advanced device models and no thorough description and motivation of the many input parameters are attempted here. Many device manufacturers provide model parameters for the MOSFET models. For any particular make of MOSFET, the device manufacturer should be the primary source of information.

DEVICE NAME

Enter a **Device name** for the MOSFET. The prefix is M.

NODE CONNECTIONS

Specify four **Node names** for the connection nodes for the **n-Channel MOSFET** or **p-Channel MOSFET** device. These represent the *drain*, *gate*, *source*, and *bulk* nodes, respectively.

MODEL PARAMETERS

Specify the **Model Parameters**. Reasonable defaults are provided but for any particular MOSFET, the device manufacturer should be the primary source of information.

🔍	The interested reader is referred to Ref. 1 for more details on semiconductor modeling within circuits.
	For an explanation of the **Model Parameters** see MOSFET Transistors.

Mutual Inductance

The **Mutual Inductance** allows specifying a coupling between two existing Inductor features in the circuit. The mutual inductance of the coupling is

$$M = k \sqrt{L_1 L_2}$$

where k is the coupling factor and L_1 and L_2 are the inductances of the inductors.

DEVICE PARAMETERS

Enter values or expressions for the:

- **Coupling factor** k (dimensionless). The value must be between 0 and 1, and the default is 0.98.
- **First inductance** L_1 (SI unit: H) and **Second inductance** L_2 (SI unit: H). These must be set to two different Inductor features in the circuit.

Transformer

The **Transformer** feature represents either a combination of two Inductor and a Mutual Inductance features, or an ideal transformer.

NODE CONNECTIONS

Enter or edit the table in the **Node names** column for the **primary** and **secondary** node connections.

DEVICE PARAMETERS

Chose a **Transformer model**—**Specify inductors** (the default) or **Ideal transformer**.

For **Specify inductors** enter values or expressions for the:

- **Coupling factor** k (dimensionless). The default is 0.98.
- **First inductance** L_1 (SI unit: H). The default is 1 mH.
- **Second inductance** L_2 (SI unit: H). The default is 1 mH.

For **Ideal transformer** enter values or expressions for the **Winding ratio** N_1/N_2 (dimensionless). The default is 10.

Diode

The **Diode** device model (⊣◁⊢) is a large-signal model for a diode. It is an advanced device model and no thorough description and motivation of the many input parameters are attempted here. The interested reader is referred to Ref. 1Ref. 1 for more details on semiconductor modeling within circuits. Many device manufacturers provide model parameters for this diode model. For any particular make of diode, the device manufacturer should be the primary source of information.

DEVICE NAME

Enter a **Device name** for the diode. The prefix is D.

NODE CONNECTIONS

Specify two **Node names** for the positive and negative nodes for the **Diode** device.

MODEL PARAMETERS

Specify the **Model Parameters**. Reasonable defaults are provided but for any particular diode, the device manufacturer should be the primary source of information.

🔍	For an explanation of the **Model Parameters** see Diode.

External I vs. U

The **External I vs. U** (⊣⊙⊢) feature connects an arbitrary voltage measurement (for example, a circuit terminal or circuit port boundary or a coil domain from another physics interface) as a voltage source between two nodes in the electrical circuit. The resulting circuit current from the first node to the second node is typically coupled back as a prescribed current source in the context of the voltage measurement.

DEVICE NAME

Enter a **Device name** for the External I vs. U node.

NODE CONNECTIONS

Specify the two **Node names** for the connecting nodes for the voltage source. The first node represents the positive reference terminal.

EXTERNAL DEVICE

Enter the source of the **Voltage**. If circuit or current excited terminals or circuit ports are defined on boundaries or domains or a multiturn coil domains is defined in other physics interfaces, these display as options in the **Voltage** list. Also select the **User defined** option and enter your own voltage variable, for example, using a suitable coupling operator. For inductive or electromagnetic wave propagation models, the voltage measurement must be performed as an integral of the electric field because the electric potential only does not capture induced EMF. Also the integration must be performed over a distance that is short compared to the local wavelength.

!	Except when coupling to a circuit terminal, circuit port, or coil, the current flow variable must be manually coupled back in the electrical circuit to the context of the voltage measurement. This applies also when coupling to a current excited terminal. The name of this current variable follows the convention `cirn.IvsUm_i`, where `cirn` is the tag of the Electrical Circuit interface node and `IvsUm` is the tag of the **External I vs. U** node. The tags are typically displayed within curly brackets {} in the Model Builder.

🔍	Component Couplings and Coupling Operators in the *COMSOL Multiphysics Reference Manual*

External U vs. I

The **External U vs. I** (🔲) feature connects an arbitrary current measurement (for example, a coil domain from another physics interface) as a current source between two nodes in the electrical circuit. The resulting circuit voltage between the first node and the second node is typically coupled back as a prescribed voltage source in the context of the current measurement.

DEVICE NAME

Enter a **Device name** for the External U vs. I node.

NODE CONNECTIONS

Specify the two **Node names** for the connecting nodes for the current source. The current flows from the first node to the second node.

EXTERNAL DEVICE

Enter the source of the **Current**. Voltage excited terminals or lumped ports defined on boundaries in other physics interfaces are natural candidates but do not appear as options in the **Voltage** list because those do not have an accurate built-in current measurement variable. A **User defined** option must be selected and a current variable entered, for example, using a suitable coupling operator.

⚠	The voltage variable must be manually coupled back in the electrical circuit to the context of the current measurement. This applies also when coupling to a voltage excited terminal or lumped port. The name of this voltage variable follows the convention `cirn.UvsIm_v`, where `cirn` is the tag of the Electrical Circuit interface node and `UvsIm` is the tag of the **External U vs. I** node. The tags are typically displayed within curly brackets {} in the Model Builder.

🔍	Component Couplings and Coupling Operators in the *COMSOL Multiphysics Reference Manual*

External I-Terminal

The **External I-Terminal** (⬗) feature connects an arbitrary voltage-to-ground measurement (for example, a circuit terminal from another physics interface) as a voltage-to-ground assignment to a node in the electrical circuit. The resulting circuit current from the node is typically coupled back as a prescribed current source in the context of the voltage measurement. This node does not apply when coupling to inductive or electromagnetic wave propagation models because then voltage must be defined as a line integral between two points rather than a single point measurement of electric potential. For such couplings, use the External I vs. U node instead.

DEVICE NAME

Enter a **Device name** for the External I-terminal.

NODE CONNECTIONS

Set the **Node name** for the connecting node for the voltage assignment.

Enter the source of the **Voltage**. If circuit- or current-excited terminals are defined on boundaries in other physics interfaces, these display as options in the **Voltage** list. Also select the **User defined** option and enter a voltage variable, for example, using a suitable coupling operator.

> ⚠ Except when coupling to a circuit terminal, the current flow variable must be manually coupled back in the electrical circuit to the context of the voltage measurement. This applies also when coupling to a current excited terminal. The name of this current variable follows the convention `cirn.termIm_i`, where `cirn` is the tag of the Electrical Circuit interface node and `termIm` is the tag of the **External I-Terminal** node. The tags are typically displayed within curly brackets `{}` in the Model Builder.

> 🔍 Component Couplings and Coupling Operators in the *COMSOL Multiphysics Reference Manual*.

SPICE Circuit Import

Right-click the **Electrical Circuit** ( ) feature node to import an existing SPICE netlist (select **Import Spice Netlist**). A window opens—enter a file location or browse your directories to find one. The default file extension for a SPICE netlist is `.cir`. The SPICE circuit import translates the imported netlist into Electrical Circuit interface nodes so these define the subset of SPICE features that can be imported.

> 🔍 See SPICE Import and Export about the supported SPICE commands.

SPICE Circuit Export

Right-click the **Electrical Circuit** ( ) feature node to export the current circuit to the SPICE netlist file format (select **Export Spice Netlist**). A window opens—enter a file location or browse your directories to find one. The default file extension for a SPICE netlist is `.cir`. The compatible circuit nodes are exported as SPICE devices

See SPICE Export for more details on the supported SPICE commands.

Theory for the Electrostatics Interface

The Electrostatics Interface is available for 3D, 2D in-plane, and 2D axisymmetric components. Applications with electrostatic equations include high-voltage apparatus, electronic devices, and capacitors. The term "statics" is not to be interpreted literally—it is the observation time, or time scale at which the applied excitation changes, that is short compared to the charge relaxation time; also, the electromagnetic wavelength and skin depth are very large compared to the size of the domain of interest.

If you do not know whether to use the Electric Currents or the Electrostatics interface, which both solve for the scalar electric potential V, consider using an explicit charge transport model. See Charge Relaxation Theory.

Charge Relaxation Theory

COMSOL Multiphysics includes physics interfaces for the modeling of static electric fields and currents. Deciding what specific physics interface and study type to select for a particular modeling situation requires a basic understanding of the charge dynamics in conductors.

The different physics interfaces involving only the scalar electric potential can be interpreted in terms of the charge relaxation process. The fundamental equations involved are *Ohm's law* for the conduction current density

$$\mathbf{J}_c = \sigma\mathbf{E}$$

the *equation of continuity*

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{J}_c = 0$$

and *Gauss' law*

$$\nabla\cdot(\varepsilon\mathbf{E}) = \rho$$

By combining these, one can deduce the following differential equation for the space charge density in a homogeneous medium

$$\frac{\partial \rho}{\partial t} + \frac{\sigma}{\varepsilon} \rho = 0$$

This equation has the solution

$$\rho(t) = \rho_0 e^{-t/\tau}$$

where

$$\tau = \frac{\varepsilon}{\sigma}$$

is called the charge relaxation time. For a good conductor like copper, τ is of the order of 10^{-19} s, whereas for a good insulator like silica glass, it is of the order of 10^3 s. For a pure insulator, it becomes infinite.

When modeling real-world devices, there is not only the *intrinsic time scale* of the charge relaxation time but also an *external time scale* t at which a device is energized or the observation time. It is the relation between the external time scale and the charge relaxation time that determines what physics interface and study type to use. The results are summarized in Table 4-2 below,

TABLE 4-2: SUITABLE PHYSICS INTERFACE AND STUDY TYPE FOR DIFFERENT TIME-SCALE REGIMES.

CASE	PHYSICS INTERFACE	STUDY TYPE
$\tau \gg t$	Electrostatics	Stationary
$\tau \ll t$	Electric Currents	Stationary
$\tau \sim t$	Electric Currents	Time Dependent orFrequency Domain

FIRST CASE: $\tau \gg T$

If the external time scale is short compared to the charge relaxation time, the charges do not have time to redistribute to any significant degree. Thus the charge distribution can be considered as a given model input. The best approach is to solve the Electrostatics formulation using the electric potential V.

By combining the definition of the potential with Gauss' law, you can derive the classical Poisson's equation. Under static conditions, the electric potential V is defined by the equivalence $\mathbf{E} = -\nabla V$. Using this together with the constitutive relation $\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P}$ between $\mathbf{D}$ and $\mathbf{E}$, you can rewrite Gauss' law as a variant of Poisson's equation

$$-\nabla \cdot (\varepsilon_0 \nabla V - \mathbf{P}) = \rho$$

This equation is used in the Electrostatics interface. It is worth noting that Gauss' law does not require the charge distribution to be static. Thus, provided dynamics are slow enough that induced electric fields can be neglected and hence a scalar electric potential is justified, the formulation can be used also in the Time Dependent study type. That typically involves either prescribing the charge dynamics or coupling a separate formulation for this.

> Such separate charge transport formulations can be found in the Plasma Module, the Semiconductor Module, and the Chemical Reaction Engineering Module.

SECOND CASE: $\tau \ll T$

If the external time scale is long compared to the charge relaxation time, the stationary solution to the equation of continuity has been reached. In a stationary coordinate system, a slightly more general form of Ohm's law than above states that

$$\mathbf{J}_c = \sigma\mathbf{E} + \mathbf{J}_e$$

where $\mathbf{J}_e$ is an externally generated current density. The static form of the equation of continuity then reads

$$\nabla \cdot \mathbf{J}_c = -\nabla \cdot (\sigma\nabla V - \mathbf{J}_e) = 0$$

To handle current sources, the equation can be generalized to

$$-\nabla \cdot (\sigma\nabla V - \mathbf{J}_e) = Q_j$$

This equation is used in the static study type for the Electric Currents interface.

GENERAL CASE: CHARGE DYNAMICS

If the charge relaxation time is comparable to the external time scale, the Time Dependent or Frequency Domain study types for the Electric Currents interface must be used.

Combining the time-harmonic equation of continuity

$$\nabla \cdot \mathbf{J}_c = \nabla \cdot (\sigma\mathbf{E} + \mathbf{J}_e) = -j\omega\rho$$

with the equation ($\nabla \cdot \mathbf{D} = \rho$) yields the following equation for the frequency domain study type:

$$-\nabla \cdot ((\sigma + j\omega\varepsilon_0)\nabla V - (\mathbf{J}_e + j\omega\mathbf{P})) = 0$$

For the Time Dependent study type, use the transient equation of continuity

$$\nabla \cdot \mathbf{J}_c = \nabla \cdot (\sigma\mathbf{E} + \mathbf{J}_e) = -\frac{\partial\rho}{\partial t}$$

and the resulting equation becomes

$$-\nabla \cdot \frac{\partial}{\partial t}(\varepsilon_0\nabla V + \mathbf{P}) - \nabla \cdot (\sigma\nabla V - \mathbf{J}_e) = 0$$

These dynamic formulations are valid as long as induced electric fields can be ignored and hence the electric field is essentially curl free. This condition is fulfilled provided that skin effect and wave propagation effects can be ignored. The skin depth must be much larger than the geometrical dimensions of the modeled device and so must the wavelength. Note also that these formulations can be used to model dielectric regions of capacitive/resistive devices even though the interior of electrodes sometimes does not meet the large skin depth condition. In that case, the electrodes must only be represented as boundary conditions (fixed or floating potential). The interior, metallic domains are not included in the analysis. Obviously, this is only a valid approach for devices where metallic electrodes do not entirely bypass (short circuit) the capacitive/resistive layers. If metallic electrodes short circuit the capacitive/resistive layers, the time evolution of the current is determined by inductive and resistive effects with very little influence from the capacitive layers. Then the Magnetic Fields interface is the appropriate modeling tool.

Electrostatics Equations

Under static conditions, the electric potential, V, is defined by the relationship:

$$\mathbf{E} = -\nabla V$$

Combining this equation with the constitutive relationship $\mathbf{D} = \varepsilon_0\mathbf{E} + \mathbf{P}$ between the electric displacement $\mathbf{D}$ and the electric field $\mathbf{E}$, it is possible to represent Gauss' law as the following equation:

$$-\nabla \cdot (\varepsilon_0\nabla V - \mathbf{P}) = \rho$$

In this equation, the physical constant, ε_0 (SI unit: F/m) is the permittivity of vacuum, $\mathbf{P}$ (SI unit: C/m^2) is the electric polarization vector, and ρ (SI unit: C/m^3) is a space charge density. This equation describes the electrostatic field in dielectric materials.

For in-plane 2D modeling, the Electrostatics interface assumes a symmetry where the electric potential varies only in the x and y directions and is constant in the z direction. This implies that the electric field, $\mathbf{E}$, is tangential to the xy-plane. With this symmetry, the same equation is solved as in the 3D case. The physics interface solves the following equation where d is the thickness in the z direction:

$$-\nabla \cdot d(\varepsilon_0 \nabla V - \mathbf{P}) = \rho$$

The axisymmetric version of the physics interface considers the situation where the fields and geometry are axially symmetric. In this case, the electric potential is constant in the φ direction, which implies that the electric field is tangential to the rz-plane.

The Electrostatics Interface in Time Dependent or Frequency Domain Studies

The Electrostatics Interface can also be solved in a dynamic study (Time Dependent or Frequency Domain). The equation system solved, however, is typically always the one presented in the previous section for the stationary case, in which no transient electromagnetic effects are taken into account. The difference is that the sources of the problem (charge densities, electric potential) are assumed to be time-varying (in a Time Dependent study) or time-harmonic (in a Frequency Domain study).

The support for dynamic studies simplifies the coupling of the Electrostatics interface with other physics interfaces. Using the physics interface in a dynamic study is a valid approximation only if the time-scale (or the frequency) of the study is so slow that transient electromagnetic effects can be neglected; for example, in acoustic or structural problems.

Most of the features in the Electrostatics interface have the same behavior in all study types, with the important exception of the Terminal node.

The Electrostatics interface also supports the small-signal analysis study sequence, which can be used when a time-harmonic perturbation is superposed on a static bias charge or voltage.

Theory for the Electrical Circuit Interface

The Electrical Circuit Interface theory is discussed in this section:

- Electric Circuit Modeling and the Semiconductor Device Models
- Bipolar Transistors
- MOSFET Transistors
- Diode
- Reference for the Electrical Circuit Interface

🔍	Connecting to Electrical Circuits

Electric Circuit Modeling and the Semiconductor Device Models

Electrical circuit modeling capabilities are useful when simulating all sorts of electrical and electromechanical devices ranging from heaters and motors to advanced plasma reactors in the semiconductor industry. There are two fundamental ways that an electrical circuit model relates to a physical field model.

- The field model is used to get a better, more accurate description of a single device in the electrical circuit model.
- The electrical circuit is used to drive or terminate the device in the field model in such a way that it makes more sense to simulate both as a tightly coupled system.

The Electrical Circuit interface makes it possible to add nodes representing circuit elements directly to the Model Builder tree in a COMSOL Multiphysics model. The circuit variables can then be connected to a physical device model to perform co-simulations of circuits and multiphysics. The model acts as a device connected to the circuit so that its behavior is analyzed in larger systems.

The fundamental equations solved by the Electrical Circuit interface are Kirchhoff's circuit laws, which in turn can be deduced from Maxwell's equations. The supported study types are Stationary, Frequency Domain, and Time Dependent.

There are three more advanced large-signal semiconductor device features available in the Electrical Circuit interface. The equivalent circuits and the equations defining their non-ideal circuit elements are described in this section. For a more complete treatise on semiconductor device modeling see Ref. 1.

Bipolar Transistors

Figure 4-1 illustrates the equivalent circuit for the npn bipolar junction transistor.
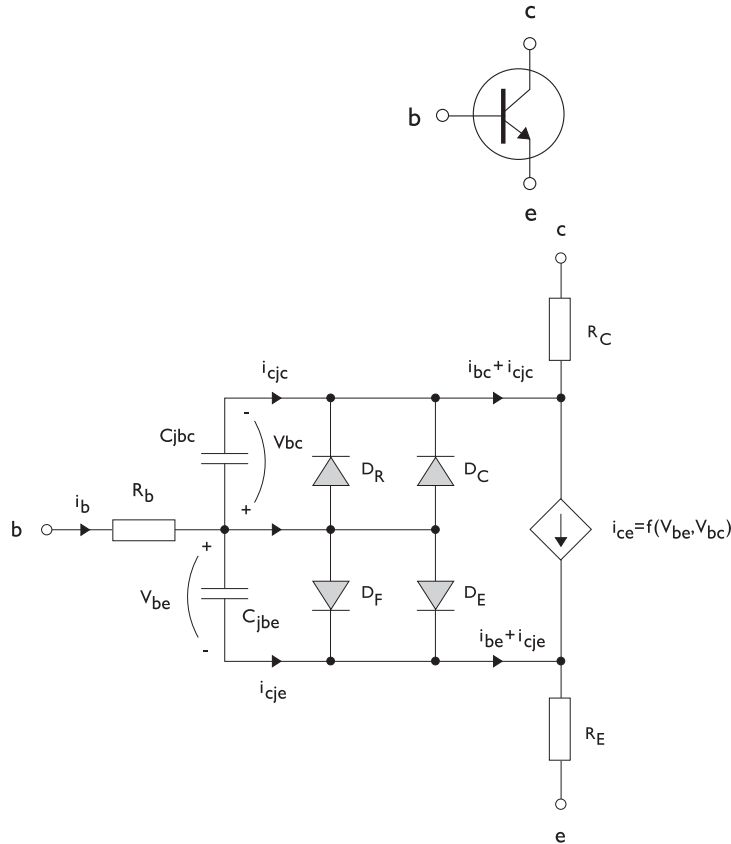
Figure 4-1: A circuit for the bipolar transistor.

The pnp transistor model is similar in all regards to the npn transistor, with the difference that the polarities of the currents and voltages involved are reversed. The following equations are used to compute the relations between currents and voltages in the circuit.

$$v_{rb} = \frac{1}{A}\left(R_{BM} - \frac{R_B - R_{BM}}{f_{bq}}\right)i_b$$

$$f_{bq} = \frac{1}{2\left(1 - \frac{v_{bc}}{V_{AF}} - \frac{v_{be}}{V_{AR}}\right)}\left(1 + \sqrt{1 + 4I_S\left(\frac{e^{\frac{v_{be}}{N_F V_T}} - 1}{I_{KF}A} + \frac{e^{\frac{v_{bc}}{N_R V_T}} - 1}{I_{KR}A}\right)}\right)$$

$$i_{be} = A\left(\frac{I_S}{B_F}\left(e^{\frac{v_{be}}{N_F V_T}} - 1\right) + I_{SE}\left(e^{\frac{v_{be}}{N_E V_T}} - 1\right)\right)$$

$$i_{bc} = A\left(\frac{I_S}{B_R}\left(e^{\frac{v_{bc}}{N_R V_T}} - 1\right) + I_{SC}\left(e^{\frac{v_{bc}}{N_C V_T}} - 1\right)\right)$$

$$i_{ce} = A\left(\frac{I_S}{f_{bq}}\left(e^{\frac{v_{be}}{N_F V_T}} + e^{\frac{v_{bc}}{N_C V_T}}\right)\right)$$

$$V_T = \frac{k_B T_{NOM}}{q}$$

There are also two capacitances that use the same formula as the junction capacitance of the diode model. In the parameter names below, replace x with C for the base-collector capacitance and E for the base-emitter capacitance.

$$C_{jbx} = AC_{Jx} \times \begin{cases} \left(1 - \frac{v_{bx}}{V_{Jx}}\right)^{-M_{Jx}} & v_{bx} < F_C V_{Jx} \\ (1 - F_C)^{-1 - M_{Jx}}\left(1 - F_C(1 + M_{Jx}) + M_{Jx}\frac{v_{bx}}{V_{Jx}}\right) & v_{bx} \geq F_C V_{Jx} \end{cases}$$

The model parameters are listed in the table below.

TABLE 4-1: BIPOLAR TRANSISTOR MODEL PARAMETERS

PARAMETER	DEFAULT	DESCRIPTION
B_F	100	Ideal forward current gain
B_R	1	Ideal reverse current gain
C_{JC}	0 F/m^2	Base-collector zero-bias depletion capacitance
C_{JE}	0 F/m^2	Base-emitter zero-bias depletion capacitance
F_C	0.5	Breakdown current
I_{KF}	Inf (A/m^2)	Corner for forward high-current roll-off

TABLE 4-1: BIPOLAR TRANSISTOR MODEL PARAMETERS

PARAMETER	DEFAULT	DESCRIPTION
I_{KR}	Inf (A/m^2)	Corner for reverse high-current roll-off
I_S	1e-15 A/m^2	Saturation current
I_{SC}	0 A/m^2	Base-collector leakage saturation current
I_{SE}	0 A/m^2	Base-emitter leakage saturation current
M_{JC}	1/3	Base-collector grading coefficient
M_{JE}	1/3	Base-emitter grading coefficient
N_C	2	Base-collector ideality factor
N_E	1.4	Base-emitter ideality factor
N_F	1	Forward ideality factor
N_R	1	Reverse ideality factor
R_B	0 Ωm^2	Base resistance
R_{BM}	0 Ωm^2	Minimum base resistance
R_C	0 Ωm^2	Collector resistance
R_E	0 Ωm^2	Emitter resistance
T_{NOM}	298.15 K	Device temperature
V_{AF}	Inf (V)	Forward Early voltage
V_{AR}	Inf (V)	Reverse Early voltage
V_{JC}	0.71 V	Base-collector built-in potential
V_{JE}	0.71 V	Base-emitter built-in potential

MOSFET Transistors

Figure 4-2 illustrates an equivalent circuit for the n-channel MOSFET transistor. The p-channel MOSFET transistor is treated similarly, but the polarities of the involved voltages are reversed.
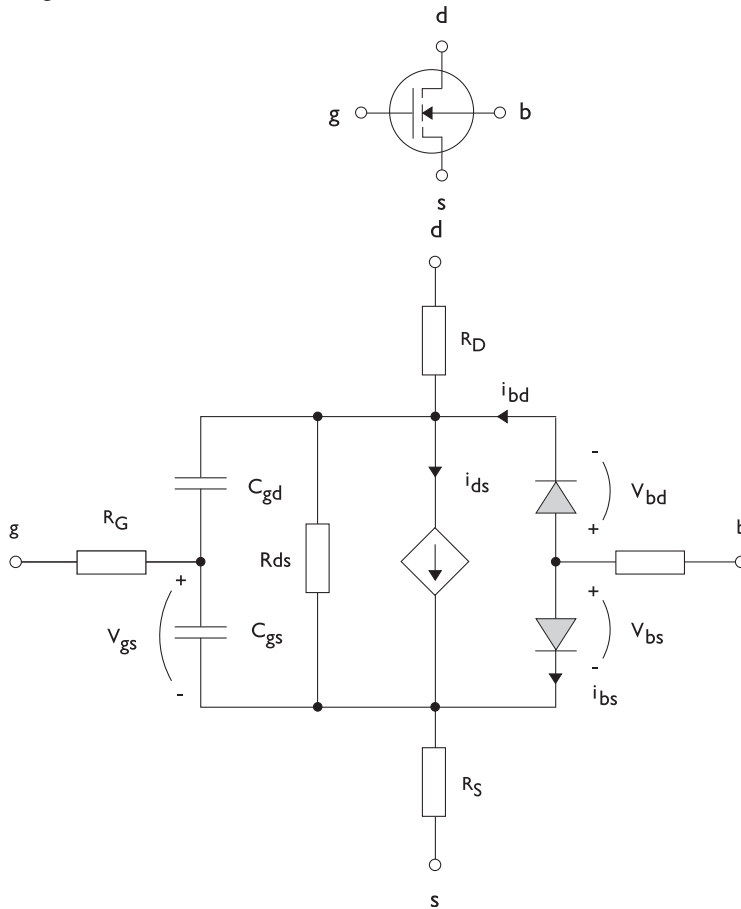
Figure 4-2: A circuit for the MOSFET transistor.

The following equations are used to compute the relations between currents and voltages in the circuit.

$$i_{ds} = \begin{cases} \dfrac{W}{L}\dfrac{K_P}{2}(1 + \Lambda v_{ds})v_{ds}(2v_{th} - v_{ds}) & v_{ds} < v_{th} \\[2ex] \dfrac{W}{L}\dfrac{K_P}{2}(1 + \Lambda v_{ds})v_{th}^2 & v_{ds} \geq v_{th} \\[2ex] 0 & v_{ds} < v_{th} \leq 0 \end{cases}$$

$$v_{th} = v_{gs} - (V_{TO} + \Gamma(\sqrt{\Phi - v_{bs}} - \sqrt{\Phi}))$$

$$i_{bd} = I_S\left(e^{\frac{v_{bd}}{NV_T}} - 1\right)$$

$$i_{bs} = I_S\left(e^{\frac{v_{bs}}{NV_T}} - 1\right)$$

$$V_T = \frac{k_B T_{NOM}}{q}$$

There are also several capacitances between the terminals

$$C_{gd} = C_{gd0}W$$
$$C_{gs} = C_{gs0}W$$

$$C_{jbd} = C_{BD} \times \begin{cases} \left(1 - \dfrac{v_{bd}}{P_B}\right)^{-M_J} & v_{bx} < F_C P_B \\[2ex] (1 - F_C)^{-1 - M_J}\left(1 - F_C(1 + M_J) + M_J\dfrac{v_{bx}}{P_B}\right) & v_{bx} \geq F_C P_B \end{cases}$$

The model parameters are as follows:

TABLE 4-2: MOSFET TRANSISTOR MODEL PARAMETERS

PARAMETER	DEFAULT	DESCRIPTION
C_{BD}	0 F/m	Bulk-drain zero-bias capacitance
C_{GDO}	0 F/m	Gate-drain overlap capacitance
C_{GSO}	0 F/m	Gate-source overlap capacitance
F_C	0.5	Capacitance factor
I_S	1e-13 A	Bulk junction saturation current
K_P	2e-5 A/V^2	Transconductance parameter
L	50e-6 m	Gate length
M_J	0.5	Bulk junction grading coefficient

TABLE 4-2: MOSFET TRANSISTOR MODEL PARAMETERS

PARAMETER	DEFAULT	DESCRIPTION
N	1	Bulk junction ideality factor
P_B	0.75 V	Bulk junction potential
R_B	0 Ω	Bulk resistance
R_D	0 Ω	Drain resistance
R_{DS}	Inf (Ω)	Drain-source resistance
R_G	0 Ω	Gate resistance
R_S	0 Ω	Source resistance
T_{NOM}	298.15 K	Device temperature
V_{TO}	0 V	Zero-bias threshold voltage
W	50e-6 m	Gate width
Γ (GAMMA)	1 $V^{0.5}$	Bulk threshold parameter
Φ (PHI)	0.5 V	Surface potential
Λ (LAMBDA)	0 1/V	Channel-length modulation

Diode

Figure 4-3 illustrates equivalent circuit for the diode.
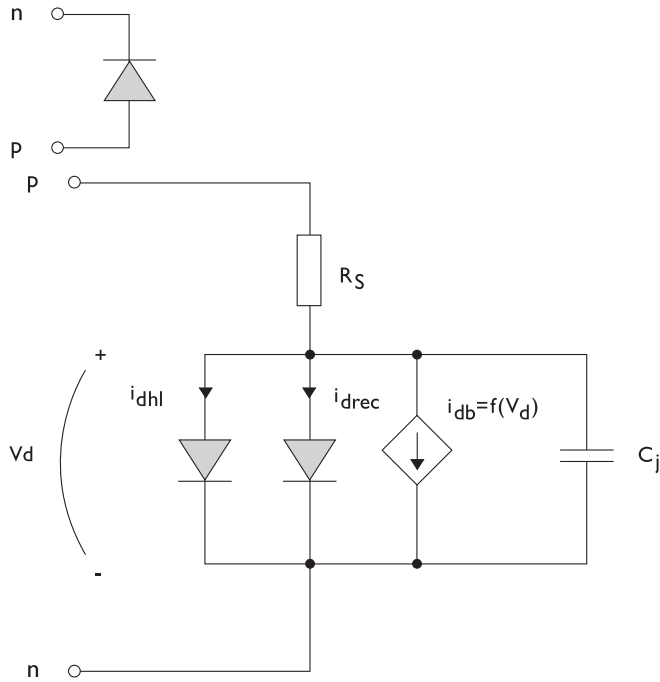
Figure 4-3: A circuit for the diode.

The following equations are used to compute the relations between currents and voltages in the circuit.

$$i_d = i_{dhl} + i_{drec} + i_{db} + i_c$$

$$i_{dhl} = I_S\left(e^{\frac{v_d}{NV_T}} - 1\right)\frac{1}{\sqrt{1 + \frac{I_S}{I_{KF}}\left(e^{\frac{v_d}{NV_T}} - 1\right)}}$$

$$i_{drec} = I_{SR}\left(e^{\frac{v_d}{N_R V_T}} - 1\right)$$

$$i_{db} = I_{BV}e^{-\frac{v_d + B_V}{N_{BV}V_T}}$$

$$C_j = C_{J0} \times \begin{cases} \left(1 - \dfrac{v_d}{V_J}\right)^{-M} & v_d < F_C V_J \\[2mm] (1 - F_C)^{-1-M}\left(1 - F_C(1+M) + M\dfrac{v_d}{V_J}\right) & v_d \geq F_C V_J \end{cases}$$

$$V_T = \frac{k_B T_{NOM}}{q}$$

where the following model parameters are required

TABLE 4-3: DIODE TRANSISTOR MODEL PARAMETERS

PARAMETER	DEFAULT	DESCRIPTION
B_V	Inf (V)	Reverse breakdown voltage
C_{J0}	0 F	Zero-bias junction capacitance
F_C	0.5	Forward-bias capacitance coefficient
I_{BV}	1e-09 A	Current at breakdown voltage
I_{KF}	Inf (A)	Corner for high-current roll-off
I_S	1e-13 A	Saturation current
M	0.5	Grading coefficient
N	1	Ideality factor
N_{BV}	1	Breakdown ideality factor
N_R	2	Recombination ideality factor
R_S	0 Ω	Series resistance
T_{NOM}	298.15 K	Device temperature
V_J	1.0 V	Junction potential

Reference for the Electrical Circuit Interface

1. P. Antognetti and G. Massobrio, *Semiconductor Device Modeling with Spice*, 2nd ed., McGraw-Hill, 1993.

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Schrödinger Equation Interfaces

This chapter describes the **Schrödinger Equation** interface (⬢) and the
Schrödinger-Poisson Equation multiphysics interface (⬢).

In this chapter:

- The Schrödinger Equation Interface
- Theory for the Schrödinger Equation Interface
- The Schrödinger-Poisson Equation Multiphysics Interface

The Schrödinger Equation Interface

The **Schrödinger Equation (schr)** interface ( ), found under the **Semiconductor** branch ( ) when adding a physics interface, solves the Schrödinger equation for the wave function of a single particle in an external potential. By default, the Schrödinger equation is added to all the domain selections of the interface.

When this physics interface is added, these default nodes are added to the Model Builder: **Effective Mass**, **Electron Potential Energy**, **Zero Flux**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions or additional contributions to the potential energy. You can also right-click **Schrödinger Equation** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `schr`.

MODEL PROPERTIES

Use **Model properties** to set the particle type and study-specific variables in the model.

Particle type
Select an option from the **Particle type** list: **Electrons** (the default) or **Holes**.

- For electron-like particles, the direction of lower energy is in the negative direction of the electron potential energy. Pictorially, this type of particles tend to fall down to the bottom of an electron potential energy well.

- For hole-like particles, the direction of lower energy is in the positive direction of the electron potential energy. Pictorially, this type of particles tend to float up to the top of an electron potential energy peak.

Azimuthal quantum number
For axisymmetric models, enter an integer for the azimuthal quantum number m (unitless). The default is 0.

Eigenvalue scale

• Enter a constant value for the **Eigenvalue scale** λ_{scale} (J) for eigenvalue studies. The eigenenergy is defined as the product of the eigenvalue scale and the eigenvalue (dimensionless). The default is 1 eV, so that the eigenvalue will be the numerical value of the eigenenergy in unit of eV.

Energy

Enter a constant value or a global parameter for the **Energy** E (J) for stationary studies. This specifies the total energy of the stationary Schrödinger equation.

DISCRETIZATION

Use this section to change the discretization of the Schrödinger equation.

DEPENDENT VARIABLES

The dependent variable (field variable) is for the particle **Wave function** psi. The name can be changed but the names of fields and dependent variables must be unique within a model.

🔍	• Domain and Boundary Nodes for the Schrödinger Equation Interface • Theory for the Schrödinger Equation Interface

Domain and Boundary Nodes for the Schrödinger Equation Interface

The Schrödinger Equation Interface has these domain and boundary nodes available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking the main physics interface node to access the context menu (all users).

💡	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

❗	In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

	• The Schrödinger Equation Interface
Ⓠ	• Theory for the Schrödinger Equation Interface

These nodes and subnodes are described in this section and listed in alphabetical order:

- Effective Mass
- Electron Potential Energy
- Initial Values
- Open Boundary

- Periodic Condition
- Zero Flux
- Zero Probability

Effective Mass

Use the **Effective Mass** node to set the effective mass of the particle. The default is 0.067*me_const for electron-like particles and 0.45*me_const for hole-like particles.

It is common for electrons or holes to have different effective masses in different regions of a heterostructure. This can be easily specified by using multiple **Effective Mass** nodes. Later nodes overrides earlier nodes in the Model Builder tree.

Electron Potential Energy

The **Electron Potential Energy** feature adds contribution to the total potential energy experienced by the particle. The contribution from all **Electron Potential Energy** nodes are summed up to give the total potential energy. This makes it easy to construct complicated potential profiles by employing a number of nodes.

ELECTRON POTENTIAL ENERGY

Select a profile option for the **Electron Potential Energy** V_e (for electrons) or V_h (for holes): **Simple harmonic potential** (the default), **Quantum well**, or **User defined**.

Simple harmonic potential
For this profile, enter the

- **Angular frequency** ω_0 (rad/s). The default is 1[eV]/hbar_const.
- **Center of potential** $\mathbf{r}_0$ (m). The default is the origin of the geometry. For axisymmetric models, the center of potential is fixed at the origin (not editable).
- **Constant offset** V_0 (J). The default is 0[eV].

The contribution to the total electron potential energy is

$$V_0 \pm \frac{1}{2}m_{eff}\omega_0^2|\mathbf{r} - \mathbf{r}_0|^2$$

where the plus sign is for electrons and minus sign for holes.

Quantum well
For this profile, enter the

- **Width of quantum well** d_0 (m). The default is 10[nm].
- **Depth of quantum well** V_w (J). The default is 100[meV].
- **Center of potential** $\mathbf{r}_0$ (m). The default is the origin of the geometry. For axisymmetric models, the center of potential is fixed at the origin (not editable).
- **Constant offset** V_0 (J). The default is 0[eV].

The contribution to the total electron potential energy is

$$V_0 \pm V_w\left(|\mathbf{r} - \mathbf{r}_0| > \frac{1}{2}d_0\right)$$

where the plus sign is for electrons and minus sign for holes.

If the effective mass of the particle varies from the well region to the barrier region, as is very often the case, then it will be easier to not use this option. Instead, define different domains for the well and barrier regions and use the **User defined** option to specify the potential and effective mass in each domain.

User defined
For this option, enter the contribution to the electron potential energy in the input field. The default is 0.5*schr.meff*((1[eV]/hbar_const)^2)*(x^2) for electrons and -0.5*schr.meff*((1[eV]/hbar_const)^2)*(x^2) for holes.

Initial Values

The **Initial Values** node provides initial values for the wave function. The default is 0.

Zero Flux

The **Zero Flux** node is the default boundary condition for external boundaries where the normal component of the probability current density is set to zero by the nature of the equation system.

Zero Probability

Use the **Zero Probability** node to constrain the value of the wave function to zero at a boundary.

Periodic Condition

The **Periodic Condition** allows modeling just one unit cell of a periodic structure, such as superlattices.

PERIODICITY SETTINGS

Select an option from the **Type of periodicity** drop down menu: **Continuity** (the default) or **Floquet-Bloch periodicity**.

• For **Floquet-Bloch periodicity**, enter the **k-vector for Floquet periodicity** $\mathbf{k}_F$ (rad/m). The default is the null vector, reducing the condition to be equivalent to **Continuity**. For time dependent studies, the **Floquet-Bloch periodicity** option does not apply. If erroneously selected, it will be reduced to the continuity condition.

DESTINATION SELECTION (SUBNODE)

If desired, use this subnode to manually select the destination boundary for the periodic condition.

Open Boundary

The **Open Boundary** condition allows outgoing waves leave the modeling domain without being reflected back from the external boundary. It allows an optional incoming wave to be specified by the user. An advanced physics option allows the reversal of the open boundary condition: an unspecified incoming wave comes into the modeling domain through the boundary and no outgoing wave leaves the domain through the boundary.

	For stationary studies, an alternative for modeling nonreflecting outgoing waves is to use an exterior domain specified as a **Perfectly Matched Layer** to absorb the outgoing waves.

WAVE TYPE

This setting specifies the outgoing wave type. Depending on the spatial dimension of the geometry, one or more of the following outgoing wave types may be supported:

Plane wave, **Cylindrical wave** and **Spherical wave**. If only one wave type is supported by the geometry, the drop down menu is grayed out and displays the supported wave type. If more than one is supported, the drop down menu is active and allows the user to make a selection.

The "no reflection" condition works well only if the outgoing wave propagating direction is normal to the boundary, otherwise some reflection will occur. Therefore for the **Plane wave** type, the wave vector is assumed to be in the direction of the outgoing normal of the boundary.

For the **Cylindrical wave** type, enter the **Axial direction of cylindrical wave** and one **Point on center axis of cylindrical wave**.

For the **Spherical wave** type, enter the **Center of spherical wave**.

INCOMING WAVE

This setting specifies an optional incoming wave if the check box is checked. The following settings may appear only if the check box is checked.

Incoming wave type

If more than one wave type is supported by the spatial dimension of the geometry, then the **Incoming wave type** drop down menu appears and allow the user to make a selection.

For any incoming wave type, enter the **Incoming wave amplitude** ψ_0. The default is 1.

For incoming **Plane wave**, enter the **Incoming wave direction**.

For incoming **Cylindrical wave**, enter the **Axial direction of incoming cylindrical wave** and one **Point on center axis of incoming cylindrical wave**.

For incoming **Spherical wave**, enter the **Center of incoming spherical wave**.

OPEN BOUNDARY TYPE

This setting is available if the **Advanced Physics Options** is enabled by clicking the **Show** button (🕶) and selecting **Advanced Physics Options**. Select either **Outgoing** or **Incoming**.

Outgoing

This is the default. The open boundary allows outgoing waves leave the modeling domain without being reflected back from the boundary.

Incoming

This reverses the usual open boundary condition: an unspecified incoming wave comes into the modeling domain through the boundary and no outgoing wave leaves the

domain through the boundary. This particular option is mainly for analyzing resonant tunneling conditions, see the Double Barrier 1D tutorial in the Application Libraries.

Theory for the Schrödinger Equation Interface

For an introduction to the Schrödinger equation and its application in quantum confined semiconductor systems, the user is encouraged to consult textbooks such as Ref. 1 and Ref. 2. This section is not meant to be a replacement for general textbooks on the subject. Only those parts of the theory pertaining to the usage of the physics interface will be covered.

In this section:

- Sign Convention and Energy Units
- Units of Wave Functions
- Sign Convention of the Electron Potential Energy
- References for the Schrödinger Equation Interface

Sign Convention and Energy Units

The single-particle Schrödinger Equation implemented in the physics interface reads

$$-\hbar^2 \nabla \bullet \left(\frac{\nabla \psi(\mathbf{r}, t)}{2m_{eff}(\mathbf{r})} \right) + V(\mathbf{r}, t)\psi(\mathbf{r}, t) = -i\hbar \frac{\partial}{\partial t}\psi(\mathbf{r}, t) \tag{5-1}$$

Note that the energy operator on the right-hand side of the equation takes an opposite sign convention as the one adopted in most textbooks of quantum mechanics. This is because COMSOL Multiphysics takes the engineering convention of $\exp(+i\omega t)$ for time-harmonic solutions, as opposed to the physics convention of $\exp(-i\omega t)$. The engineering convention is adopted for the Schrödinger Equation interface so that the sign convention is consistent within the COMSOL product family. Under this unusual sign convention, the momentum operator also acquires an opposite sign, since a plane wave is now $\exp(-ikx+i\omega t)$, not $\exp(+ikx-i\omega t)$ as in most textbooks.

The stationary Schrödinger Equation reads

$$-\hbar^2 \nabla \bullet \left(\frac{\nabla \psi(\mathbf{r})}{2m_{eff}(\mathbf{r})} \right) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{5-2}$$

For stationary studies, where the total energy E is a known quantity, enter a constant value or a global parameter for the **Energy** E (J) in the physics interface settings window (see section Energy).

For eigenvalue studies, where the eigenenergy E is unknown and to be solved for, enter a constant value for the **Eigenvalue scale** λ_{scale} (J) in the physics interface settings window (see section Eigenvalue scale). The eigenenergy E is given by the product of the eigenvalue scale λ_{scale} and the eigenvalue λ (dimensionless). The default value for λ_{scale} is 1 eV, so that the eigenvalue λ takes on the numerical value of the eigenenergy E in units of eV.

Units of Wave Functions

Since COMSOL does not allow fractional units, the wave functions in all spatial dimensions are set to unitless. The built-in variable for the probability density (`schr.Pr` by default) has the unit of $1/m$ in 1D, $1/m^2$ in 2D or 1D axisymmetry, and $1/m^3$ in 3D or 2D axisymmetry.

Sign Convention of the Electron Potential Energy

The sign convention for the **Electron Potential Energy** domain condition follows the one adopted by the Semiconductor Interface:

• For electron-like particles, the direction of lower energy is in the negative direction of the electron potential energy. Pictorially, this type of particles tend to fall down to the bottom of an electron potential energy well.

• For hole-like particles, the direction of lower energy is in the positive direction of the electron potential energy. Pictorially, this type of particles tend to float up to the top of an electron potential energy peak.

References for the Schrödinger Equation Interface

1. L. I. Schiff, *Quantum Mechanics*, 3rd edition (1968), Mcgraw-Hill.

2. P. Harrison, *Quantum Wells, Wires and Dots*, 3rd edition (2009), Wiley.

The Schrödinger-Poisson Equation Multiphysics Interface

The **Schrödinger-Poisson Equation** multiphysics interface creates a bidirectional coupling between an **Electrostatics** physics interface and a **Schrödinger Equation** physics interface, to model charge carriers in quantum-confined systems. The electric potential from the Electrostatics contributes to the potential energy term in the Schrödinger Equation. A statistically weighted sum of the probability densities from the eigenstates of the Schrödinger Equation contributes to the space charge density in the Electrostatics. All spatial dimensions (1D, 1D axial symmetry, 2D, 2D axial symmetry, and 3D) are supported. A dedicated **Schrödinger-Poisson** study type is available for automated generation of self-consistent iterations in the solver sequence.

When a predefined **Schrödinger-Poisson Equation** multiphysics interface is added from the **Semiconductor** branch (![icon]) of the **Model Wizard** or **Add Physics** windows, **Schrödinger Equation** and **Electrostatics** interfaces are added to the Model Builder.

In addition, a **Multiphysics Couplings** node is added, which automatically includes the multiphysics coupling feature **Schrödinger-Poisson Coupling**.

On the constituent physics interfaces
The **Schrödinger Equation** interface solves the Schrödinger equation for general quantum mechanical problems, as well as for the electron and hole wave functions in quantum-confined semiconductors under the assumption of the envelope function approximation.

The **Electrostatics** interface is used to compute the electric field, the electric displacement field and potential distributions in dielectrics under conditions where the electric charge distribution is explicitly prescribed. The formulation is stationary but for use together with other physics, also eigenfrequency, frequency-domain, small-signal analysis and time-domain modeling are supported in all space dimensions. The physics interface solves Gauss' Law for the electric field using the scalar electric potential as the dependent variable.

COUPLING FEATURES

If a multiphysics interface is added from the Model Wizard or using the Add Physics window, then the appropriate coupling feature is automatically added to the model

builder tree structure. Alternatively, the physics interfaces can be added one at a time, followed by the coupling features.

For example, if single **Electrostatics** and **Schrödinger Equation** interfaces are added, then COMSOL Multiphysics adds an empty **Multiphysics Couplings** node. You can then choose the coupling feature: **Schrödinger-Poisson Coupling**.

	Coupling features are available from the context menu (right-click the **Multiphysics Couplings** node) or from the **Physics** toolbar, **Multiphysics** menu.

PHYSICS INTERFACES AND COUPLING FEATURES

	Use the online help in COMSOL Multiphysics to locate and search all the documentation. All these links also work directly in COMSOL Multiphysics when using the Help system.

Coupling Features
The Schrödinger-Poisson Coupling node is described in the section Schrödinger-Poisson Coupling below.

Physics Interface Features
Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

The available physics features for The Schrödinger Equation Interface are listed in the section Domain and Boundary Nodes for the Schrödinger Equation Interface.

For theory and physics interface feature descriptions relating to the Electrostatics interface, see the *COMSOL Multiphysics Reference Manual*.

Schrödinger-Poisson Coupling

The **Schrödinger-Poisson Coupling** ( ) node takes user inputs to generate the variables and equations necessary for the bi-directional coupling between the **Electrostatics** physics interface and the **Schrödinger Equation** physics interface, to model charged particles in quantum-confined systems.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. The software refer to variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `schrp1`.

DOMAIN SELECTION

The default setting is **All domains** which couples all domains in the selected **Schrödinger Equation** physics interface that overlap with the domain selection of the selected **Electrostatics** interface.

COUPLED INTERFACES

This section defines the physics involved in the coupling. By default, the software selects an appropriate physics interface for you from the **Schrödinger Equation** and **Electrostatics** lists. These selections determine the two physics interfaces that are coupled by this feature.

MODEL INPUT

Enter the temperature T (K) of the system to be modeled. The default value is `293.15[K]`.

PARTICLE DENSITY COMPUTATION

From the **Particle density computation** drop-down menu, select **Fermi-Dirac statistics, parabolic band** (the default) or **User defined**.

Fermi-Dirac statistics, parabolic band
This option computes the statistically weighted effective density of states for each eigenstate, assuming Fermi-Dirac statistics and parabolic band approximation. See the

Equation section of the user interface for the formula used, which varies according to the spatial dimension.

Enter the Fermi energy level E_f (J), density-of-state effective mass m_d (kg), and the degeneracy factor g_i (dimensionless). The default values are 0[eV], 0.067*me_const, and 1, respectively.

User defined

Directly enter the formula for the statistically weighted effective density of states N_i (1/m^2 in 1D, 1/m in 2D and 1D axial symmetry, dimensionless in 3D and 2D axial symmetry). The default expression is 0.

CHARGE DENSITY COMPUTATION

Enter the charge number z_q (dimensionless) for the particle, for example, -1 for electrons and 1 for positrons. The default value is -1.

From the **Charge density computation** list, select **Modified Gummel iteration** (the default), **Damped iteration**, or **User defined**.

If the **Minimization of global variable** option is used in the Schrödinger-Poisson study step settings, enter the formula for the **Global error variable** (dimensionless). The default expression is (schrp1.max(abs(V-schrp1.V_old)))/1[V], which computes the max difference between the electric potential profiles from the two most recent iterations, scaled by 1 V.

Modified Gummel iteration

This option updates the space charge density contribution from the sum of the statistically weighted probability density profile for each eigenstate, by making a prediction based on the high temperature limit (Maxwell-Boltzmann statistics). See the **Equation** section of the user interface for the formula used.

An additional tuning parameter α (dimensionless) can be entered to either accelerate the convergence at low temperatures using positive values, or provide extra damping using negative values. The default value is 0.

Damped iteration

This option updates the space charge density contribution from the sum of the statistically weighted probability density profile for each eigenstate, by adding a fractional contribution to the space charge density from the previous iteration (with the same fraction removed from the previous charge density). See the **Equation** section of the user interface for the formula used.

The fraction is specified by the damping factor α (dimensionless). The default value is `0.1`.

User defined
Directly enter the formula for the space charge density ρ_v (C/m^3). The default expression is `0`.

Schrödinger-Poisson Study Step

The dedicated Schrödinger-Poisson study step automatically generates the iterations in the solver sequence for the self-consistent solution of the fully coupled Schrödinger-Poisson equation.

To take advantage of the default settings detailed below, use the **Model Wizard** or the **Add Study** button in the ribbon/toolbar of the graphical user interface. A study step added by right-clicking a Study node does not include any default settings suggested by the physics.

STUDY SETTINGS
The default option for the **Eigenfrequency (Eigenvalue) search method** drop-down menu is **Manual**, because for a completely new problem, it is often necessary to use this option to find the range of the eigenenergies and a rough estimate of the number of eigenstates. Make sure that the **Unit** drop-down menu is left as blank (default).

Once the range and number are found, switch to the **Region** search option with appropriate settings for the range and number of eigenvalues, in order to ensure that all significant eigenstates are found by the solver.

Search region (Region search option)
Make sure the **Unit** drop-down menu is left as blank (default).

The real and imaginary parts of the input fields refer to the real and imaginary parts of the eigenvalue, respectively (not the real and imaginary part of the eigenfrequency). So, to look for the eigenenergies of bound states, set the input fields for the real parts to the expected energy ranges, and set the input fields for the imaginary parts to a small range around zero to capture numerical noise or slightly leaky quasi-bound states.

PHYSICS AND VARIABLES SELECTION
If there are extra domain or boundary conditions used to obtain the initial value for the fully coupled problem, remember to disable them here. For example, see the tutorial model schrodinger_poisson_nanowire, where the Thomas-Fermi solution is

used as the initial condition, and the space charge density contribution from the Thomas-Fermi approximation is disabled here.

ITERATIONS

The default option for the **Termination method** drop-down menu is **Minimization of global variable**, which updates a table displaying the history of a global error variable after each iteration during the solution process. This provides a good indication of the solution process to monitor whether the iteration is converging.

The default expression for the **Global variable** input field uses the built-in global error variable schrp1.global_err, which computes the max difference between the electric potential fields from the two most recent iterations, in the unit of V, as discussed in the section Charge Density Computation for the Schrödinger-Poisson Coupling multiphysics node earlier. Note that the prefix for the variable, in this case schrp1, should match the **Name** input field of the Schrödinger-Poisson Coupling multiphysics node. (See section Settings) Setting the **Absolute tolerance** to 1e-6 thus means the iteration ends after the max difference is less than 1 uV.

VALUES OF DEPENDENT VARIABLES

Use this section to configure the initial conditions for the study step. Consult the COMSOL Multiphysics Reference Manual for details.

STUDY EXTENSIONS

Use the **Auxiliary sweep** option to solve for a set of parameters, for example, in the schrodinger_poisson_nanowire tutorial model, it is used to solve for a set of azimuthal quantum numbers.

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Glossary

This Glossary of Terms contains modeling terms relevant to Semiconductor modeling. For mathematical terms as well as geometry and CAD terms specific to the COMSOL Multiphysics® software and documentation, see the glossary in the *COMSOL Multiphysics Reference Manual*. For references to more information about a term, see the index.

Glossary of Terms

acceptor Dopant atoms that, when added to the semiconductor, have the effect of removing free electrons from the system at sufficiently high temperatures.

Auger recombination Auger recombination becomes important at high nonequilibrium carrier densities since the process requires three carriers. For example, when two electrons collide the collision can result in the recombination of one of the electrons with a hole. The energy released by the transition is transferred to the surviving electron, which subsequently returns to equilibrium as it undergoes collisions with the lattice.

avalanche breakdown See *impact ionization*.

band A collection of states that can be occupied by electrons, spanning a discrete range of energies.

band bending A shift in the energy levels associated with the band structure as a function of position in space. Band bending is usually caused by electric fields originating from space charge layers in the semiconductor.

band gap A range of energies in which no states are available for electrons to occupy.

band gap narrowing A reduction in the band gap of a heavily doped semiconductor resulting from the merging of the impurity band with the conduction or valence band.

base (transistor) See *bipolar transistor*.

basis The specific pattern of atoms that is repeated periodically at each point in a lattice.

bipolar transistor/bipolar junction transistor/BJT A transistor that uses two back to back p-n junctions to achieve power amplification. These transistors can be of the type PNP or NPN. There are three terminals in a bipolar transistor: the emitter, the base, and the collector, each of which is connected to one of the differently doped regions of the semiconductor (the base is connected to the region between the collector and emitter). During operation, a small current flowing between the base and the emitter usually controls a much larger current between the collector and emitter terminals, either to amplify a signal or to implement a switch.

Bloch's theorem A theorem that describes restrictions on the form of the electron wave function in a periodic potential.

Bloch wave function/Bloch state A wave function that satisfies Bloch's theorem.

Boltzmann equation A partial differential equation that, for semiconductors, describes the evolution of the hole and electron distribution functions.

body (transistor) See *field effect transistor*.

collector (transistor) See *bipolar transistor*.

conduction band A band with a range of energies that lie just above the band gap in which the Fermi level lies.

degenerate semiconductor A semiconductor where Fermi-Dirac statistics are required to describe the carrier distribution functions.

depletion region A region of the semiconductor, usually at a p-n junction or metal semiconductor contact, in which the carrier concentration is greatly suppressed at equilibrium. There is usually a space charge and corresponding electric field associated with the depletion region.

density of states The number of states per unit energy (or, in some cases, per unit volume of k-space) that can be occupied by electrons.

diode A two terminal device with much lower resistance when current flows in one direction (the forward direction) than when it flows in the other direction (the reverse direction).

direct recombination This recombination process is possible in direct band gap semiconductors and occurs when electron-hole pairs recombine with the emission of photons (with an energy close to the band gap).

donors Dopant atoms which, when added to the semiconductor, have the effect of adding additional free electrons to the system at sufficiently high temperatures.

dopants Impurities that are deliberately added to a semiconductor in order to modify the conductivity of the material.

drain (transistor) See *field effect transistor*.

drift-diffusion equations Equations describing the migration and diffusion of electrons and holes in a semiconductor under the influence of applied fields, temperature gradients, or concentration gradients.

electron distribution function A function that determines the fraction of available states that are full as a function of energy.

electron quasi-Fermi level See *quasi-Fermi level.*

electrons An elementary particle with a negative elementary electric charge.

emitter (transistor) See *bipolar transistor.*

Fermi-Dirac distribution The general form of the electron (or hole) distribution function in equilibrium.

Fermi-Dirac statistics Electron or hole statistics that are described by the Fermi-Dirac distribution.

Fermi level The energy associated with states which, at a specified temperature, have a 50% probability of being occupied. The Fermi level is the chemical potential for electrons.

Fermi surface The surface in k-space that corresponds to the Fermi level.

field effect transistor A transistor that uses an electric field to alter the geometry of a conducting channel adjacent to the surface of a semiconductor. Usually the field is applied to the surface of a semiconductor in an oppositely doped region (sometimes connected to the body terminal) between two doped-like regions of semiconductor (connected to the source and the drain terminals). The field results from a voltage applied to a terminal referred to as the gate. In a MOSFET, the field produces band bending near the surface of the semiconductor, resulting in an inversion layer, which produces a conducting channel between the source and the drain. The extent of the channel is controlled by the applied field allowing the channel resistance to be modulated. For a *JFET* or *MESFET*, the field is applied to a p-n junction or a Schottky contact, altering the size of the depletion layer and consequently modifying the channel thickness.

Gaussian doping A distribution of dopants where the concentration decays from a peak value following a Gaussian distribution.

Generation A process by which electron hole pairs are created.

gate (transistor) See *field effect transistor*.

heterojunction An interface between two different semiconductors.

hole distribution function A function which determines fraction of available states which are empty as a function of energy.

hole quasi-Fermi level See *quasi-Fermi level*.

holes Particles evoked to simplify the computation of current from bands that are almost completely full of electrons.

impact ionization A carrier generation mechanism that occurs when the carriers are accelerated by the electric field in between collisions to velocities where the energies are greater than the gap energy, these can dissipate enough energy during collisions that additional electron hole pairs can be generated. This process is referred to as impact ionization and is responsible for the phenomenon of avalanche breakdown.

incomplete ionization For semiconductors with a wide band gap or for conventional semiconductors at low temperatures, the thermal energy is not sufficient to completely ionize the dopant atoms and only a fraction of the dopants are ionized. This situation is referred to as incomplete ionization.

insulator A solid that has no observable conductivity at temperatures below its melting point. The band structure of insulators is such that there are only completely full or completely empty bands, and a band gap of sufficient size exists between the full and empty bands that there is negligible thermal excitation.

inversion layer A layer of semiconductor in which band bending leads to a change of the material from n-type to p-type or vice versa.

JFET (Junction Field Effect Transistor) A field effect transistor in which the electric field is applied to the semiconductor by a biased p-n junction.

k-space The space in which the wave vectors of the electron wave function (usually denoted **k**), are defined.

lattice A set of points in space that are all identical due to the periodicity of the structure represented.

Maxwell-Boltzmann distribution The limit of the Fermi-Dirac distribution when the Fermi energy is several times the thermal energy within the band gap.

Maxwell-Boltzmann statistics Electron or hole statistics that are described by the Maxwell-Boltzmann distribution.

metal A solid with good electrical conductivity. A metal has one or more partially filled bands.

MESFET (Metal Semiconductor Field Effect Transistor) A field effect transistor in which the electric field is applied to the semiconductor by a Schottky contact.

mobility A quantity (strictly a tensor) relating the velocity of electrons or holes to the applied electric field.

MOSFET (Metal Oxide Semiconductor Field Effect Transistor) A field effect transistor in which the electric field is applied to the semiconductor by a metal contact (or in some cases a heavily doped polysilicon) separated from the semiconductor by an insulator (often silicon oxide).

nearly free electron model A quantum mechanical model for the behavior of electrons moving in a weakly periodic potential.

nondegenerate semiconductor A semiconductor in which it is sufficient to use Maxwell-Boltzmann statistics to describe the carrier distribution functions.

n-type A region of semiconductor where the number of donors exceeds the number of acceptors.

ohmic contact A contact between a metal and a semiconductor that has a linear IV characteristic.

p-type A region of semiconductor where the number of acceptors exceeds the number of donors.

p-n junction A junction between p- and n- type regions of a semiconductor.

Pauli exclusion principle   The Pauli exclusion principle states that two Fermions (such as electrons) cannot occupy the same quantum mechanical state. A consequence of the principle is that each state in a crystal can be occupied only by two electrons, one spin up and another spin down.

quasi-Fermi level   Net current flows and/or thermal gradients in a semiconductor represent nonequilibrium conditions and consequently the concept of the Fermi level (derived from equilibrium thermodynamics) does not apply to these processes. However, in many devices it is possible to assume a collective (and different) quasi-equilibrium for electrons and holes, since the relaxation time for scattering within the band is much less than that for recombination processes. The electron and hole quasi-Fermi levels are the Fermi levels associated with these two quasi-equilibrium populations.

recombination   A process by which electrons and holes recombine, resulting in a return of the system to equilibrium.

rectifier   A device with much lower resistance when current flows in one direction (the forward direction) than when it flows in the other direction (the reverse direction).

reciprocal lattice   The lattice obtained by taking the Fourier transform of the lattice in real space. The reciprocal lattice is a set of vectors in k-space.

Schottky contact   A metal semiconductor contact where the barrier height and width is sufficient to result in rectifying behavior.

Schrödinger equation   A partial differential equation that describes the evolution of the wave function.

semiclassical model   A model that describes the dynamics of electrons moving in periodic solids in between collisions.

semiconductor   A solid that is an insulator at zero temperature but that has observable conductivity at temperatures below its melting point. The conductivity results from a significant number of electrons that are thermally excited across the band gap; consequently the gap energy must be of the same order as the thermal energy (most important semiconductors have a gap energy of less than 2 eV).

Shockley-Read-Hall recombination   This recombination mechanism is important in indirect band gap semiconductors, such as silicon and germanium (for these materials

direct recombination is not possible). A defect (usually with an energy close to the mid-gap) is involved in the process. An electron or hole is first trapped by the defect and then emitted into the valence/conduction band, resulting in a reduction in the number of available carriers. The carrier energy is typically converted to heat.

source (transistor) See *field effect transistor*.

spin An intrinsic form of angular momentum carried by elementary particles. The electron spin can take two values, +1/2 and -1/2, frequently referred to as *up* and *down*, respectively.

transistor A device used to amplify or switch electrical signals.

valence band A band with a range of energies that lie just below the band gap in which the Fermi-level lies.

wave function A complex-valued function that describes the quantum state of a particle. The modulus squared of the wave function represents the probability density of finding a given particle in a given region of space at a particular time.

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