

# PN-Junction ID

This model sets up a simple 1D benchmark of a pn-junction, or semiconductor diode, based on an example given in Ref. 1.

### Introduction

A semiconductor diode consists of two regions with different doping: a p-type region with a dominant concentration of holes, and an n-type region with a dominant concentration of electrons. The anode contact is adjacent to the p-type region, and the cathode connects to the n-type region. Impurities that the manufacturing process adds to the semiconductor material determine each region's doping type. Donor impurities add additional electrons to the material conduction band and create n-type material. Acceptor impurities remove electrons from the valence band and create p-type material.

It is possible to derive a semiconductor model from Maxwell's equations and the Boltzmann equation for carrier transport. The three basic semiconductor equations (for a stationary problem) are given below:

$$\begin{split} \nabla \cdot (\varepsilon \nabla V) &= -q(p-n+N_D^+ - N_A^-) \\ \nabla \cdot \mathbf{J}_n &= -q R_{SRH} \\ \nabla \cdot \mathbf{J}_p &= q R_{SRH} \end{split}$$

where  $\varepsilon$  is the dielectric permittivity of the semiconductor, V is the electric potential, p and n are the electron and hole concentrations respectively,  $N_D^+$  and  $N_A^-$  are the concentrations of ionized donors and acceptors respectively,  $J_n$  and  $J_p$  are the electron and hole currents, respectively, and  $R_{SRH}$  is the Shockley-Read-Hall recombination rate (see below for a description, in this case this term is assumed to be the only source of electron and hole recombination).

The electron and hole currents can be expressed in terms of V, n, and p in the following manner (assuming an isothermal, non-degenerate semiconductor with a constant band structure):

$$\begin{aligned} \mathbf{J}_n &= -nq\mu_n \nabla V + \mu_n k_B T \nabla n \\ \mathbf{J}_p &= -pq\mu_p \nabla V - \mu_p k_B T \nabla n \end{aligned}$$

where  $\mu_n$  and  $\mu_p$  are the carrier mobilities,  $k_B$  is Boltzmann's constant, and T is the absolute temperature. In this model, the mobility is a complex function of the temperature and the donor and acceptor concentrations, as defined in Ref. 1.

The term  $R_{SRH}$  gives the rate at which electrons recombine (by a mechanism known as Shockley-Read-Hall recombination—which is often dominant in silicon). This recombination process involves traps in the forbidden band gap of the semiconductor. The recombination rate due to this mechanism is given by:

$$R_{SRH} = \frac{np-n_i^2}{\tau_p(n+n_1)+\tau_n(p+p_1)}$$

where  $n_i$  is the intrinsic carrier concentration (that is the carrier concentration in an undoped semiconductor),  $\tau_n$  and  $\tau_p$  are the carrier lifetimes, and  $n_1$  and  $p_1$  are parameters related to the trap energy level. If the trap level is located at the middle of the band gap (which is assumed in this model), then  $n_1$  and  $p_1$  equal  $n_i$ .

# Model Definition

This model simulates the behavior of a pn-junction under reverse, equilibrium, and forward bias. The modeled junction has a length of 5  $\mu m$  and a net doping concentration of  $1\times10^{15}~cm^{-3}$  for both the p and n-doped side. A Shockley-Read-Hall recombination feature is also added to the model in order to simulate recombination usually observed in indirect band-gap semiconductor such as silicon, which is the material used in this model. The model uses the material parameters used in Ref. 1 and compares the carrier concentration profiles obtained from the computation with those obtained in the reference under different biasing conditions (–4 V, 0 V, and 0.5 V). Two different discretization methods are used to solve the model: the Finite Element Log Formation discretization; and the Finite Volume discretization. The results of these two computation methods are found to be in good agreement.

## Results and Discussion

Figure 1shows the electric potential in the junction for different biasing conditions. A good agreement is shown between the finite element, finite volume and reference for all biasing conditions. Figure 2, Figure 4, and Figure 6 show the energy diagrams for each biasing conditions. On these figures, one can notice a perfect agreement between the finite element (using streamline diffusion stabilization) and finite volume. Comparing the carrier concentrations also shows a very good agreement between the reference, finite element and finite volume computations - See Figure 3, Figure 5, and Figure 7

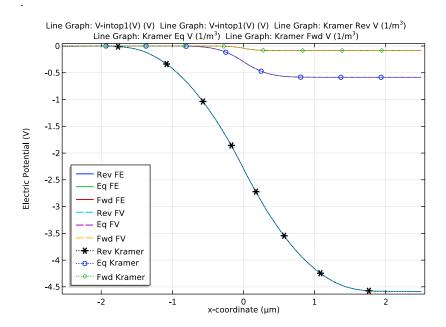


Figure 1: Electric potential obtained using the finite element (FE) and finite volume (FV) methods under different bias, that is, reverse (Rev), equilibrium (Eq), and forward (Fwd) bias. The results are compared to those calculated in Ref. 1 (Kramer)

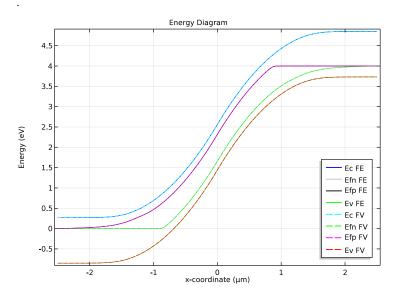


Figure 2: Energy diagram obtained using the finite element (FE) and finite volume (FV) methods under reverse bias  $(-4\ V)$ .

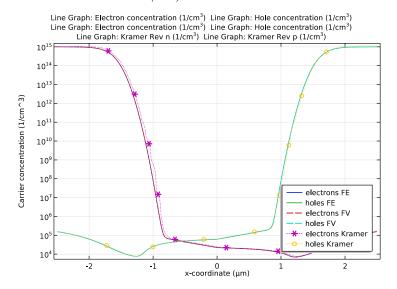


Figure 3: Electron and hole concentrations obtained using the finite element (FE) and finite volume (FV) methods under reverse bias (-4 V). The profiles are compared to those calculated in Ref.  $1\,(Kramer)$ 

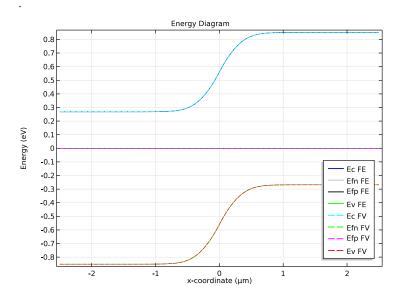


Figure 4: Energy diagram obtained using the finite element (FE) and finite volume (FV) methods at equilibrium (0 V).

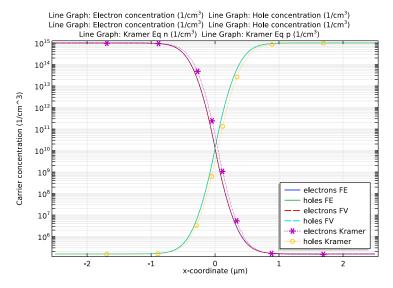


Figure 5: Electron and hole concentrations obtained using the finite element (FE) and finite volume (FV) methods at equilibrium (0 V). The profiles are compared to those calculated in Ref. 1 (Kramer)

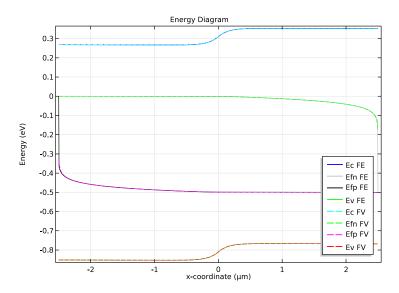


Figure 6: Energy diagram obtained using the finite element (FE) and finite volume (FV) methods under forward bias  $(0.5\ V)$ .

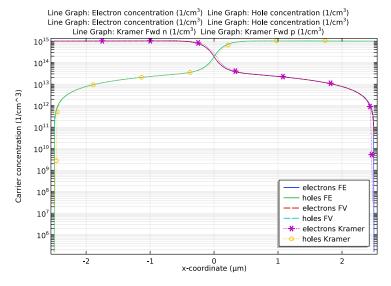


Figure 7: Electron and hole concentrations obtained using the finite element (FE) and finite volume (FV) methods under forward bias (0.5 V). The profiles are compared to those calculated in Ref.  $1\,(Kramer)$ 

# Reference

1. K.M. Kramer and W.N.G. Hitchon, *Semiconductor Devices a Simulation Approach*, Prentice Hall, Upper Saddle River, NJ, 1997.

**Application Library path:** Semiconductor\_Module/Verification\_Examples/pn\_junction\_1d

# Modeling Instructions

From the File menu, choose New.

#### NFW

In the New window, click Model Wizard.

#### MODEL WIZARD

- I In the Model Wizard window, click ID.
- 2 In the Select Physics tree, select Semiconductor>Semiconductor (semi).
- 3 Click Add.
- 4 Click Study.
- 5 In the Select Study tree, select Preset Studies>Stationary.
- 6 Click Done.

# GEOMETRY I

In the **Model Builder** window's toolbar, click the **Show** button and select **Discretization** in the menu.

## SEMICONDUCTOR (SEMI)

- I In the Model Builder window, under Component I (compl) click Semiconductor (semi).
- **2** In the **Settings** window for **Semiconductor**, click to expand the **Discretization** section.
- 3 From the Formulation list, choose Finite element, log formulation (linear shape function).

## GEOMETRY I

- I In the Model Builder window, under Component I (compl) click Geometry I.
- 2 In the Settings window for Geometry, locate the Units section.

3 From the Length unit list, choose  $\mu m$ .

Interval I (i1)

- I On the Geometry toolbar, click Interval.
- 2 In the Settings window for Interval, locate the Interval section.
- 3 In the Left endpoint text field, type -2.5.
- 4 In the Right endpoint text field, type 2.5.

Point I (ptl)

- I On the Geometry toolbar, click Point.
- 2 In the Settings window for Point, click Build All Objects.

#### **GLOBAL DEFINITIONS**

**Parameters** 

- I In the Model Builder window, under Global Definitions click Parameters.
- 2 In the Settings window for Parameters, locate the Parameters section.
- 3 Click Load from File.
- **4** Browse to the model's Application Libraries folder and double-click the file pn\_junction\_1d\_parameters.txt.

# DEFINITIONS

Variables 1

- I On the Home toolbar, click Variables and choose Local Variables.
- 2 In the Settings window for Variables, locate the Variables section.
- 3 Click Load from File.
- **4** Browse to the model's Application Libraries folder and double-click the file pn\_junction\_1d\_variables.txt.

Interpolation I (int I)

- I On the Home toolbar, click Functions and choose Local>Interpolation.
- 2 In the Settings window for Interpolation, locate the Definition section.
- 3 In the Function name text field, type kramer\_eq\_V.
- 4 Click Load from File.
- **5** Browse to the model's Application Libraries folder and double-click the file pn\_junction\_1d\_Kramer\_eq\_V.txt.

- 6 Locate the Units section. In the Arguments text field, type m.
- 7 In the Function text field, type 1/m<sup>3</sup>.
- 8 Right-click Interpolation I (intl) and choose Rename.
- $\textbf{9} \ \ In the \ \textbf{Rename Interpolation} \ \ dialog \ box, type \ \ \textbf{Kramer} \ \ \textbf{Eq} \ \ \textbf{V} \ in the \ \textbf{New label} \ text \ field.$

IO Click OK.

- Interpolation 2 (int2)
- I On the Home toolbar, click Functions and choose Local>Interpolation.
- 2 In the Settings window for Interpolation, locate the Definition section.
- 3 In the Function name text field, type kramer\_fwd\_V.
- 4 Click Load from File.
- **5** Browse to the model's Application Libraries folder and double-click the file pn\_junction\_1d\_Kramer\_fwd\_V.txt.
- 6 Locate the Units section. In the Arguments text field, type m.
- 7 In the Function text field, type 1/m<sup>3</sup>.
- 8 Right-click Interpolation 2 (int2) and choose Rename.
- 9 In the Rename Interpolation dialog box, type Kramer Fwd V in the New label text field.
- IO Click OK.

Interpolation 3 (int3)

- I On the Home toolbar, click Functions and choose Local>Interpolation.
- 2 In the Settings window for Interpolation, locate the Definition section.
- 3 In the Function name text field, type kramer\_rev\_V.
- 4 Click Load from File.
- **5** Browse to the model's Application Libraries folder and double-click the file pn\_junction\_1d\_Kramer\_rev\_V.txt.
- **6** Locate the **Units** section. In the **Arguments** text field, type m.
- 7 In the Function text field, type 1/m<sup>3</sup>.
- 8 Right-click Interpolation 3 (int3) and choose Rename.
- 9 In the Rename Interpolation dialog box, type Kramer Rev V in the New label text field.
- IO Click OK.

Interpolation 4 (int4)

I On the Home toolbar, click Functions and choose Local>Interpolation.

- 2 In the Settings window for Interpolation, locate the Definition section.
- 3 Click Load from File.
- **4** Browse to the model's Application Libraries folder and double-click the file pn\_junction\_1d\_Kramer\_eq\_n.txt.
- 5 In the Function name text field, type kramer\_eq\_n.
- f 6 Locate the **Units** section. In the **Arguments** text field, type f m.
- 7 In the Function text field, type 1/m<sup>3</sup>.
- 8 Right-click Interpolation 4 (int4) and choose Rename.
- 9 In the Rename Interpolation dialog box, type Kramer Eq n in the New label text field.

  10 Click OK.

## Interpolation 5 (int5)

- I On the Home toolbar, click Functions and choose Local>Interpolation.
- 2 In the Settings window for Interpolation, locate the Definition section.
- 3 Click Load from File.
- **4** Browse to the model's Application Libraries folder and double-click the file pn\_junction\_1d\_Kramer\_eq\_p.txt.
- 5 In the Function name text field, type kramer\_eq\_p.
- 6 Locate the Units section. In the Arguments text field, type m.
- 7 In the Function text field, type 1/m<sup>3</sup>.
- 8 Right-click Interpolation 5 (int5) and choose Rename.
- 9 In the Rename Interpolation dialog box, type Kramer Eq p in the New label text field.
- IO Click OK.

## Interpolation 6 (int6)

- I On the Home toolbar, click Functions and choose Local>Interpolation.
- 2 In the Settings window for Interpolation, locate the Definition section.
- 3 In the Function name text field, type kramer\_fwd\_n.
- 4 Click Load from File.
- **5** Browse to the model's Application Libraries folder and double-click the file pn\_junction\_1d\_Kramer\_fwd\_n.txt.
- $\pmb{6}$  Locate the  $\pmb{Units}$  section. In the  $\pmb{Arguments}$  text field, type m.
- 7 In the Function text field, type 1/m^3.
- 8 Right-click Interpolation 6 (int6) and choose Rename.

**9** In the **Rename Interpolation** dialog box, type Kramer Fwd n in the **New label** text field. **10** Click **OK**.

Interpolation 7 (int7)

- I On the Home toolbar, click Functions and choose Local>Interpolation.
- 2 In the Settings window for Interpolation, locate the Definition section.
- 3 In the Function name text field, type kramer\_fwd\_p.
- 4 Click Load from File.
- **5** Browse to the model's Application Libraries folder and double-click the file pn\_junction\_1d\_Kramer\_fwd\_p.txt.
- 6 Locate the Units section. In the Arguments text field, type m.
- 7 In the Function text field, type 1/m<sup>3</sup>.
- 8 Right-click Interpolation 7 (int7) and choose Rename.
- 9 In the Rename Interpolation dialog box, type Kramer Fwd p in the New label text field.
- IO Click OK.

Interpolation 8 (int8)

- I On the Home toolbar, click Functions and choose Local>Interpolation.
- 2 In the Settings window for Interpolation, locate the Definition section.
- 3 In the Function name text field, type kramer\_rev\_n.
- 4 Click Load from File.
- **5** Browse to the model's Application Libraries folder and double-click the file pn\_junction\_1d\_Kramer\_rev\_n.txt.
- **6** Locate the **Units** section. In the **Arguments** text field, type m.
- 7 In the Function text field, type 1/m<sup>3</sup>.
- 8 Right-click Interpolation 8 (int8) and choose Rename.
- 9 In the Rename Interpolation dialog box, type Kramer Rev n in the New label text field.
- IO Click OK.

Interpolation 9 (int9)

- I On the Home toolbar, click Functions and choose Local>Interpolation.
- 2 In the Settings window for Interpolation, locate the Definition section.
- 3 Click Load from File.
- **4** Browse to the model's Application Libraries folder and double-click the file pn\_junction\_1d\_Kramer\_rev\_p.txt.

- 5 In the Function name text field, type kramer\_rev\_p.
- 6 Locate the Units section. In the Arguments text field, type m.
- 7 In the Function text field, type 1/m<sup>3</sup>.
- 8 Right-click Interpolation 9 (int9) and choose Rename.
- 9 In the Rename Interpolation dialog box, type Kramer Rev p in the New label text field.

#### IO Click OK.

Integration | (intop |)

- I On the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.
- 2 In the Settings window for Integration, locate the Source Selection section.
- 3 From the Geometric entity level list, choose Boundary.
- 4 Select Boundary 1 only.

## SEMICONDUCTOR (SEMI)

Semiconductor Material Model I

- I In the Model Builder window, expand the Component I (compl)>Semiconductor (semi) node, then click Semiconductor Material Model I.
- 2 In the Settings window for Semiconductor Material Model, locate the Model Inputs section.
- **3** In the T text field, type T1.
- **4** Locate the **Mobility Model** section. From the  $\mu_n$  list, choose **User defined**. In the associated text field, type mu\_n.
- **5** From the  $\mu_p$  list, choose **User defined**. In the associated text field, type mu\_p.

Trap-Assisted Recombination 1

- I On the Physics toolbar, click Domains and choose Trap-Assisted Recombination.
- 2 In the Settings window for Trap-Assisted Recombination, locate the Domain Selection section.
- 3 From the Selection list, choose All domains.

Analytic Doping Model I

- I On the Physics toolbar, click Domains and choose Analytic Doping Model.
- **2** Select Domain 1 only.
- 3 In the Settings window for Analytic Doping Model, locate the Impurity section.
- 4 From the Impurity type list, choose Donor doping (n-type).

**5** In the  $N_{D0}$  text field, type Nd.

Analytic Doping Model 2

- I On the Physics toolbar, click Domains and choose Analytic Doping Model.
- 2 Select Domain 2 only.
- ${\bf 3}\ \ {\bf In\ the\ Settings\ window\ for\ Analytic\ Doping\ Model}, locate\ the\ Impurity\ section.$
- **4** In the  $N_{A0}$  text field, type Na.

Metal Contact I

- I On the Physics toolbar, click Boundaries and choose Metal Contact.
- 2 Select Boundary 1 only.

Metal Contact 2

- I On the Physics toolbar, click Boundaries and choose Metal Contact.
- 2 In the Settings window for Metal Contact, locate the Terminal section.
- **3** In the  $V_0$  text field, type Va.
- 4 Select Boundary 3 only.

## MATERIALS

Material I (mat I)

- I In the Model Builder window, under Component I (compl) right-click Materials and choose Blank Material.
- 2 In the Settings window for Material, locate the Material Contents section.
- **3** In the table, enter the following settings:

| Property                                     | Variable | Value          | Unit | Property group            |
|--|----------|----------------|------|---------------------------|
| Relative permittivity                        | epsilonr | epsilonr_param | 1    | Basic                     |
| Band gap                                     | Eg0      | Eg0_param      | ٧    | Semiconductor material    |
| Electron affinity                            | chi0     | chi0_param     | ٧    | Semiconductor<br>material |
| Effective density of states, conduction band | Nc       | Nc_param       | I/m³ | Semiconductor<br>material |
| Effective density of states, valence band    | Nv       | Nv_param       | I/m³ | Semiconductor<br>material |

| Property                  | Variable | Value      | Unit | Property group                   |
|---------------------------|----------|------------|------|----------------------------------|
| Electron lifetime,<br>SRH | taun     | taun_param | s    | Shockley-Read-Hall recombination |
| Hole lifetime, SRH        | taup     | taup_param | s    | Shockley-Read-Hall recombination |

#### MESH I

#### Distribution I

- I In the Model Builder window, under Component I (compl) right-click Mesh I and choose
- 2 Right-click Edge I and choose Distribution.
- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 In the Number of elements text field, type 500.

Configure the first study. The finite element log formulation discretization requires the voltage applied to the device to be ramped on. This is achieved using the 'sweep' variable, which is ramped from 0 to 1 using the solver's continuation functionality. The voltage applied to the device, Va, is calculated using Va=bias\*sweep, as can be seen in the parameters table within the Definitions node. The first study will be configured to apply three different biases, with each bias being ramped from 0 V to the intended value as 'sweep' increases from 0 to 1.

### STUDY I

- I In the Model Builder window, click Study I.
- 2 In the **Settings** window for **Study**, type **Study** 1 Finite Element Log Formulation in the **Label** text field.

# STUDY I - FINITE ELEMENT LOG FORMULATION

## Step 1: Stationary

- I In the Model Builder window, expand the Study I Finite Element Log Formulation node, then click Step I: Stationary.
- 2 In the Settings window for Stationary, click to expand the Study extensions section.
- 3 Locate the Study Extensions section. Select the Auxiliary sweep check box.
- 4 From the Sweep type list, choose All combinations.
- 5 Click Add.

**6** In the table, enter the following settings:

| Parameter name     | Parameter value list | Parameter unit |
|--------------------|----------------------|----------------|
| bias (Device bias) | -4 0 0.5             |                |

- 7 Click Add.
- **8** In the table, enter the following settings:

| Parameter name  | Parameter value list | Parameter unit |
|---|----------------------|----------------|
| sweep (Sweep parameter for gradually turning on bias) | 0 1                  |                |

9 On the Home toolbar, click Compute.

## RESULTS

Energy Levels (semi)

- I In the Model Builder window, under Results click Energy Levels (semi).
- 2 In the Settings window for ID Plot Group, locate the Data section.
- 3 From the Parameter selection (bias) list, choose First.
- 4 From the Parameter selection (sweep) list, choose Last.

Conduction Band Energy Level

- I In the Model Builder window, expand the Energy Levels (semi) node, then click Conduction Band Energy Level.
- 2 In the Settings window for Line Graph, locate the x-Axis Data section.
- 3 From the Parameter list, choose Expression.
- 4 In the Expression text field, type x.
- 5 Click to expand the **Legends** section. In the table, enter the following settings:

# Legends Ec FE

Electron\_quasi-Fermi\_energy\_level

- I In the Model Builder window, under Results>Energy Levels (semi) click Electron\_quasi-Fermi\_energy\_level.
- 2 In the Settings window for Line Graph, locate the x-Axis Data section.
- 3 From the Parameter list, choose Expression.
- **4** In the **Expression** text field, type x.

# Legends Efn FE

- **6** Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Solid**.
- 7 From the Color list, choose Gray.

Hole\_quasi-Fermi\_energy\_level

- I In the Model Builder window, under Results>Energy Levels (semi) click Hole\_quasi-Fermi\_energy\_level.
- 2 In the Settings window for Line Graph, locate the x-Axis Data section.
- 3 From the Parameter list, choose Expression.
- **4** In the **Expression** text field, type x.
- 5 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose Solid.
- **6** Locate the **Legends** section. In the table, enter the following settings:

# Legends Efp FE

Valence Band Energy Level

- I In the Model Builder window, under Results>Energy Levels (semi) click Valence Band Energy Level.
- 2 In the Settings window for Line Graph, locate the x-Axis Data section.
- 3 From the Parameter list, choose Expression.
- 4 In the Expression text field, type x.
- **5** Locate the **Legends** section. In the table, enter the following settings:

# Legends Ev FE

Energy Levels (semi)

- I In the Model Builder window, under Results click Energy Levels (semi).
- 2 In the Settings window for ID Plot Group, click to expand the Legend section.
- 3 From the Position list, choose Lower right.

- 4 Right-click Results>Energy Levels (semi) and choose Rename.
- 5 In the Rename ID Plot Group dialog box, type Energy Levels Reverse Bias in the New label text field.
- 6 Click OK.

Carrier Concentrations (semi)

- I In the Settings window for ID Plot Group, locate the Legend section.
- 2 From the Position list, choose Lower right.
- 3 Right-click Results>Carrier Concentrations (semi) and choose Rename.
- 4 In the Rename ID Plot Group dialog box, type Carrier Concentrations Reverse Bias in the New label text field.
- 5 Click OK.

Carrier Concentrations Reverse Bias

- I In the Settings window for ID Plot Group, locate the Data section.
- 2 From the Parameter selection (bias) list, choose First.
- 3 From the Parameter selection (sweep) list, choose Last.

**Electron Concentration** 

- I In the Model Builder window, expand the Results>Carrier Concentrations Reverse Bias node, then click **Electron Concentration**.
- 2 In the Settings window for Line Graph, locate the x-Axis Data section.
- 3 From the Parameter list, choose Expression.
- **4** In the **Expression** text field, type x.
- **5** Locate the **Legends** section. In the table, enter the following settings:

# Legends

electrons FE

Hole Concentration

- I In the Model Builder window, under Results>Carrier Concentrations Reverse Bias click Hole Concentration.
- 2 In the Settings window for Line Graph, locate the x-Axis Data section.
- 3 From the Parameter list, choose Expression.
- 4 In the Expression text field, type x.

# Legends holes FE

### Line Graph 1

- I In the Model Builder window, expand the Results>Electric Potential (semi) node, then click Line Graph 1.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- **3** In the **Expression** text field, type V-intop1(V).
- 4 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- **5** In the **Expression** text field, type x.
- 6 Click to expand the **Legends** section. Select the **Show legends** check box.
- 7 From the Legends list, choose Manual.
- **8** In the table, enter the following settings:

# Legends Rev FE Eq FE Fwd FE

# Electric Potential (semi)

- I In the Model Builder window, under Results click Electric Potential (semi).
- 2 In the Settings window for ID Plot Group, locate the Legend section.
- 3 From the Position list, choose Lower left.
- 4 Locate the Data section. From the Parameter selection (sweep) list, choose Last.

In order to compare the finite element log formulation discretization with finite volume discretization, change the discretization and add a second study to re-solve the model with the new selection.

# SEMICONDUCTOR (SEMI)

- I In the Model Builder window, under Component I (compl) click Semiconductor (semi).
- 2 In the Settings window for Semiconductor, locate the Discretization section.
- 3 From the Formulation list, choose Finite volume (constant shape function).

#### ADD STUDY

- I On the Home toolbar, click Add Study to open the Add Study window.
- 2 Go to the Add Study window.
- 3 Find the Studies subsection. In the Select Study tree, select Preset Studies>Stationary.
- 4 Click Add Study in the window toolbar.
- 5 On the Home toolbar, click Add Study to close the Add Study window.

### STUDY 2

- I In the Settings window for Study, type Study 2 Finite Volume in the Label text field.
- 2 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

  Unlike in the previous study, the finite volume discretization does not require that the voltage be ramped up gradually. Therefore the desired values of 'Va' can be set directly in the auxiliary sweep.

#### STUDY 2 - FINITE VOLUME

Step 1: Stationary

- I In the Model Builder window, under Study 2 Finite Volume click Step 1: Stationary.
- 2 In the Settings window for Stationary, click to expand the Study extensions section.
- 3 Locate the Study Extensions section. Select the Auxiliary sweep check box.
- 4 Click Add
- **5** In the table, enter the following settings:

| Parameter name | Parameter value list | Parameter unit |
|----------------|----------------------|----------------|
| Va             | -4 0 0.5             |                |

6 On the Home toolbar, click Compute.

### RESULTS

Line Graph 2

- I In the Model Builder window, under Results>Electric Potential (semi) right-click
  Line Graph I and choose Duplicate.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Data set list, choose Study 2 Finite Volume/Solution 2 (sol2).
- 4 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose Dashed.

# Rev FV Eq FV Fwd FV

#### Line Graph 3

- I Right-click Line Graph I and choose Duplicate.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- 3 In the Expression text field, type kramer\_rev\_V(x).
- 4 Locate the Data section. From the Data set list, choose Study I Finite Element Log Formulation/Solution I (sol1).
- 5 From the Parameter selection (bias) list, choose First.
- **6** From the Parameter selection (sweep) list, choose Last.
- 7 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose Dotted.
- 8 Find the Line markers subsection. From the Marker list, choose Cycle.
- **9** Locate the **Legends** section. In the table, enter the following settings:

# Legends Rev Kramer

## Line Graph 4

- I Right-click Results>Electric Potential (semi)>Line Graph 3 and choose Duplicate.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- 3 In the Expression text field, type  $kramer_eq_V(x)$ .
- **4** Locate the **Legends** section. In the table, enter the following settings:

# **Legends** Eq Kramer

# Line Graph 5

- I Right-click Results>Electric Potential (semi)>Line Graph 4 and choose Duplicate.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- 3 In the Expression text field, type kramer\_fwd\_V(x).

**Legends**Fwd Kramer

- 5 On the Electric Potential (semi) toolbar, click Plot.
- 6 In the Model Builder window, under Results>Energy Levels Reverse Bias right-click Conduction Band Energy Level, hold the 'shift' key and left click Valence Band Energy Level to select all four Line Graphs. Right click the selection and choose Duplicate.

Conduction Band Energy Level I

- I In the Model Builder window, under Results>Energy Levels Reverse Bias click Conduction Band Energy Level I.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Data set list, choose Study 2 Finite Volume/Solution 2 (sol2).
- 4 From the Parameter selection (Va) list, choose First.
- 5 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose Dashed.
- 6 From the Color list, choose Cyan.
- 7 Locate the Legends section. In the table, enter the following settings:

# Legends Ec FV

Electron\_quasi-Fermi\_energy\_level | I

- I In the Model Builder window, under Results>Energy Levels Reverse Bias click Electron\_quasi-Fermi\_energy\_level I.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Data set list, choose Study 2 Finite Volume/Solution 2 (sol2).
- 4 From the Parameter selection (Va) list, choose First.
- 5 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose Dashed.
- 6 From the Color list, choose Green.
- 7 Locate the **Legends** section. In the table, enter the following settings:

**Legends** Efn FV Hole\_quasi-Fermi\_energy\_level | I

- I In the Model Builder window, under Results>Energy Levels Reverse Bias click Hole\_quasi-Fermi\_energy\_level I.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Data set list, choose Study 2 Finite Volume/Solution 2 (sol2).
- 4 From the Parameter selection (Va) list, choose First.
- 5 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose Dashed.
- 6 From the Color list, choose Magenta.
- 7 Locate the **Legends** section. In the table, enter the following settings:

# Legends Efp FV

Valence Band Energy Level 1

- I In the Model Builder window, under Results>Energy Levels Reverse Bias click Valence Band Energy Level 1.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Data set list, choose Study 2 Finite Volume/Solution 2 (sol2).
- 4 From the Parameter selection (Va) list, choose First.
- 5 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose Dashed.
- 6 From the Color list, choose Red.
- 7 Locate the **Legends** section. In the table, enter the following settings:

# Legends Ev FV

8 On the Energy Levels Reverse Bias toolbar, click Plot.

Carrier Concentrations Reverse Bias

Left click Electron Concentration, hold the 'shift' key and left click Hole Concentration to select both Line Graphs. Right-click the selection and choose Duplicate.

Electron Concentration I

I In the Model Builder window, expand the Carrier Concentrations Reverse Bias node, then click Electron Concentration 1.

- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Data set list, choose Study 2 Finite Volume/Solution 2 (sol2).
- 4 From the Parameter selection (Va) list, choose First.
- 5 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose Dashed.
- **6** Locate the **Legends** section. In the table, enter the following settings:

| Legends   |    |  |
|-----------|----|--|
| electrons | FV |  |

Hole Concentration I

- I In the Model Builder window, under Results>Carrier Concentrations Reverse Bias click Hole Concentration I.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Data set list, choose Study 2 Finite Volume/Solution 2 (sol2).
- 4 From the Parameter selection (Va) list, choose First.
- 5 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose Dashed.
- **6** Locate the **Legends** section. In the table, enter the following settings:

# Legends holes FV

7 In the Model Builder window, under Results>Carrier Concentrations Reverse Bias left click Electron Concentration I, hold the 'shift' key and left-click Hole Concentration I. Rightclick the selection and choose **Duplicate**.

Electron Concentration 1.1

- I In the Model Builder window, under Results>Carrier Concentrations Reverse Bias click Electron Concentration 1.1.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- 3 In the Expression text field, type kramer\_rev\_n(x).
- 4 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose Dotted.
- 5 Find the Line markers subsection. From the Marker list, choose Cycle.

| Legends   |        |
|-----------|--------|
| electrons | Kramer |

Hole Concentration 1.1

- I In the Model Builder window, under Results>Carrier Concentrations Reverse Bias click Hole Concentration 1.1.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- 3 In the Expression text field, type  $kramer_rev_p(x)$ .
- 4 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose **Dotted**.
- 5 Find the Line markers subsection. From the Marker list, choose Cycle.
- **6** Locate the **Legends** section. In the table, enter the following settings:

| Legends |        |  |
|---------|--------|--|
| holes   | Kramer |  |

- 7 On the Carrier Concentrations Reverse Bias toolbar, click Plot.
- 8 In the Model Builder window, under Results, click Energy Levels Reverse Bias, hold the 'shift' key and click Carrier Concentrations Reverse Bias. Right-click the selection and choose **Duplicate**.
- 9 In the Model Builder window, under Results, click Energy Levels Reverse Bias I, hold the 'shift' key and left-click Carrier Concentrations Reverse Bias 1. Right-click the selection and choose **Duplicate**.

Energy Levels Reverse Bias I

- I In the Model Builder window, under Results right-click Energy Levels Reverse Bias I and choose Rename.
- 2 In the Rename ID Plot Group dialog box, type Energy Levels Equilibrium in the New label text field.
- 3 Click OK.
- 4 In the Settings window for ID Plot Group, locate the Data section.
- 5 From the Parameter selection (sweep) list, choose From list.
- 6 In the Parameter values (sweep) list, select 0.

Conduction Band Energy Level 1

- I In the Model Builder window, expand the Results>Energy Levels Equilibrium node, then click Conduction Band Energy Level I.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Parameter selection (Va) list, choose From list.
- 4 In the Parameter values (Va) list, select 0.

Electron\_quasi-Fermi\_energy\_level | I

- I In the Model Builder window, under Results>Energy Levels Equilibrium click Electron\_quasi-Fermi\_energy\_level I.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Parameter selection (Va) list, choose From list.
- 4 In the Parameter values (Va) list, select 0.

Hole\_quasi-Fermi\_energy\_level |

- I In the Model Builder window, under Results>Energy Levels Equilibrium click Hole\_quasi-Fermi\_energy\_level I.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Parameter selection (Va) list, choose From list.
- 4 In the Parameter values (Va) list, select 0.

Valence Band Energy Level 1

- I In the Model Builder window, under Results>Energy Levels Equilibrium click Valence Band Energy Level 1.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Parameter selection (Va) list, choose From list.
- 4 In the Parameter values (Va) list, select 0.
- 5 On the Energy Levels Equilibrium toolbar, click Plot.

Carrier Concentrations Reverse Bias I

- I In the Model Builder window, under Results click Carrier Concentrations Reverse Bias I.
- 2 In the Settings window for ID Plot Group, locate the Data section.
- 3 From the Parameter selection (sweep) list, choose From list.
- 4 In the Parameter values (sweep) list, select 0.

Electron Concentration I

- I In the Model Builder window, expand the Carrier Concentrations Reverse Bias I node, then click Electron Concentration I.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Parameter selection (Va) list, choose From list.
- 4 In the Parameter values (Va) list, select 0.

Hole Concentration I

- I In the Model Builder window, under Results>Carrier Concentrations Reverse Bias I click Hole Concentration I.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Parameter selection (Va) list, choose From list.
- 4 In the Parameter values (Va) list, select 0.

Electron Concentration 1.1

- I In the Model Builder window, under Results>Carrier Concentrations Reverse Bias I click Electron Concentration 1.1.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- 3 In the Expression text field, type  $kramer_eq_n(x)$ .

Hole Concentration 1.1

- I In the Model Builder window, under Results>Carrier Concentrations Reverse Bias I click Hole Concentration 1.1.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- 3 In the Expression text field, type  $kramer_eq_p(x)$ .
- 4 On the Carrier Concentrations Reverse Bias I toolbar, click Plot.

Carrier Concentrations Reverse Bias I

- I In the Model Builder window, under Results right-click
  Carrier Concentrations Reverse Bias I and choose Rename.
- 2 In the Rename ID Plot Group dialog box, type Carrier Concentrations Equilibrium in the New label text field.
- 3 Click OK.

Energy Levels Reverse Bias 1.1

- I In the Settings window for ID Plot Group, locate the Data section.
- 2 From the Parameter selection (bias) list, choose Last.

Conduction Band Energy Level 1

- I In the Model Builder window, expand the Energy Levels Reverse Bias I.I node, then click Conduction Band Energy Level I.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Parameter selection (Va) list, choose Last.

Electron\_quasi-Fermi\_energy\_level | I

- I In the Model Builder window, under Results>Energy Levels Reverse Bias 1.1 click Electron\_quasi-Fermi\_energy\_level 1.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Parameter selection (Va) list, choose Last.

Hole\_quasi-Fermi\_energy\_level |

- I In the Model Builder window, under Results>Energy Levels Reverse Bias 1.1 click Hole\_quasi-Fermi\_energy\_level 1.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Parameter selection (Va) list, choose Last.

Valence Band Energy Level 1

- I In the Model Builder window, under Results>Energy Levels Reverse Bias 1.1 click
  Valence Band Energy Level 1.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Parameter selection (Va) list, choose Last.
- 4 On the Energy Levels Reverse Bias I.I toolbar, click Plot.

Energy Levels Reverse Bias 1.1

- I In the Model Builder window, under Results right-click Energy Levels Reverse Bias 1.1 and choose Rename.
- 2 In the Rename ID Plot Group dialog box, type Energy Levels Forward Bias in the New label text field.
- 3 Click OK.

Carrier Concentrations Reverse Bias 1.1

- I In the Model Builder window, under Results right-click
  Carrier Concentrations Reverse Bias I.I and choose Rename.
- 2 In the Rename ID Plot Group dialog box, type Carrier Concentrations Forward Bias in the New label text field.
- 3 Click OK.

- 4 In the Settings window for ID Plot Group, locate the Data section.
- 5 From the Parameter selection (bias) list, choose Last.

Electron Concentration I

- I In the Model Builder window, expand the Results>Carrier Concentrations Forward Bias node, then click Electron Concentration I.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Parameter selection (Va) list, choose Last.

Hole Concentration I

- I In the Model Builder window, under Results>Carrier Concentrations Forward Bias click Hole Concentration 1.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Parameter selection (Va) list, choose Last.

Electron Concentration 1.1

- I In the Model Builder window, under Results>Carrier Concentrations Forward Bias click Electron Concentration 1.1.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- 3 In the Expression text field, type kramer\_fwd\_n(x).

Hole Concentration 1.1

- I In the Model Builder window, under Results>Carrier Concentrations Forward Bias click Hole Concentration 1.1.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- 3 In the Expression text field, type kramer\_fwd\_p(x).
- 4 On the Carrier Concentrations Forward Bias toolbar, click Plot.