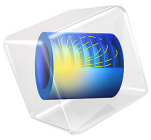
Created in COMSOL Multiphysics 6.2



# Heterojunction Tunneling

This benchmark model simulates a graded heterojunction using the thermionic emission formulation for the charge transfer over the junction. It shows the additional contribution to the current density from the quantum tunneling effect across the potential barrier, using the WKB approximation. Even though the simulated system is 1D in nature, a 2D model is created to illustrate the procedure for simulating a more general configuration. Also demonstrated is the setup of user-defined ternary material properties. The computed I–V curves, their temperature dependence, and energy band diagrams all agree well with results from the literature.

## *Introduction*

At a Schottky contact or a heterojunction where a thin layer of potential barrier forms due to the band bending, if the barrier width and/or barrier height are small, significant contribution to the current density can result from the quantum tunneling of the charge carriers across the barrier.

Within the drift–diffusion formulation of the semiconductor physics, the effect of tunneling can be incorporated as an extra current contribution scaling factor $\delta$, with the current density scaled by the factor $(1+\delta)$. Using the WKB approximation, the scaling factor can be computed as a double integral (Ref. 1). See the Semiconductor Module User's Guide for more details on the **WKB Tunneling Model** implemented in the **Semiconductor** physics interface.

## *Model Definition*

This model compares the simulated current density of a graded heterojunction with and without tunneling at different temperatures. All material properties and the device configuration are taken from the reference paper Ref. 1, in particular section 3.3, in order to compare the simulation results.

The device is an MBE grown $Al_xGa_{1-x}As$ graded heterojunction that forms a triangular shaped potential barrier for the electrons. To obtain the best fit to the experimental data, the authors of the paper have run each of their simulations with a selected set of material and device parameters that are not necessarily the same as the nominal experimental parameters. To compare the simulation results, we use the same set of simulation parameters selected by the authors, without any further justification other than the arguments already made by the authors in the paper.

The triangular barrier is formed by spatially varying the Al mole fraction of the $Al_xGa_{1-x}As$ layer. The Modeling Instructions section shows how to create a material with properties

depending on local variables such as the mole fraction, as well as depending on parameters and variables such as the reference temperature, lattice temperature, and doping concentrations. The mole fraction is in turn defined by a spatially varying variable. A variable can be made spatially varying by using explicit expressions, or using different definitions in different domains. See the Modeling Instructions section for both techniques.

Even though the simulated system is 1D in nature, we use a 2D model to illustrate the procedure for simulating a more general device configuration. In particular, we show how to use the Curvilinear Coordinates mathematics interface to create coordinates (approximately) along the electric field lines and the tunneling boundary. The solutions of two Curvilinear Coordinates interfaces are shown in the graph below. The coordinates along the electric field line are the vertical contours, parallel to the equipotential contours. The coordinates along the tunneling boundary are the horizontal contours, parallel to the electric field lines.

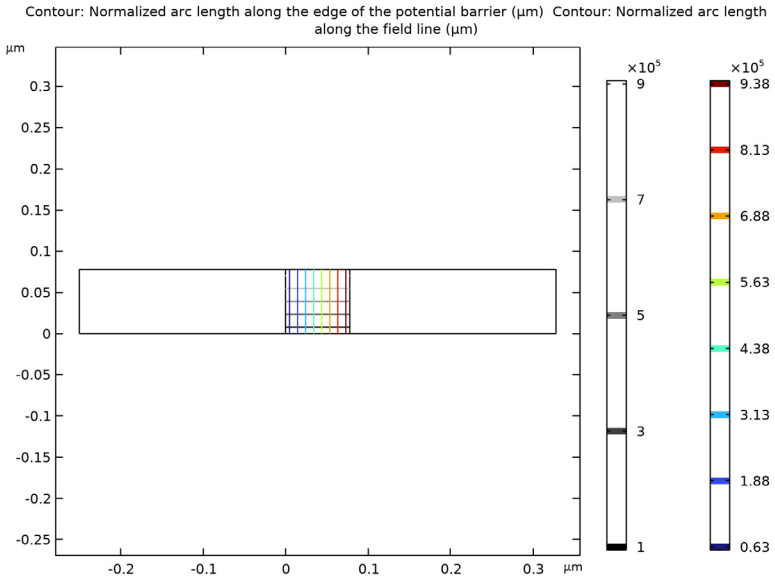



*Figure 1: The solutions of two Curvilinear Coordinates interfaces. The vertical contours are the coordinates for the electric field line and the horizontal contours are the coordinates for the tunneling boundary.*

Since the tunneling effect is highly sensitive to the shape of the potential barrier, we switch to the finite element quasi-Fermi level formulation. The default finite volume formulation would require much finer mesh, due to its discontinuous nature. Incomplete ionization,

mobility model, and Shockley–Read–Hall recombination are included with parameters given by the reference paper, which also assumes Maxwell–Boltzmann statistics.

| | |
|---|---|
|  | The equation system for heterojunctions is highly nonlinear and numerically challenging. In this tutorial we use the no tunneling result to provide a good initial condition for the study that includes tunneling. See the Modeling Instructions section for details. |

## *Results and Discussion*

Figure 2 shows a comparison of the current density vs. voltage (J–V) curves at 300 K between the cases with and without tunneling. The figure is in good agreement with the reference paper (Fig. 12 in Ref. 1).

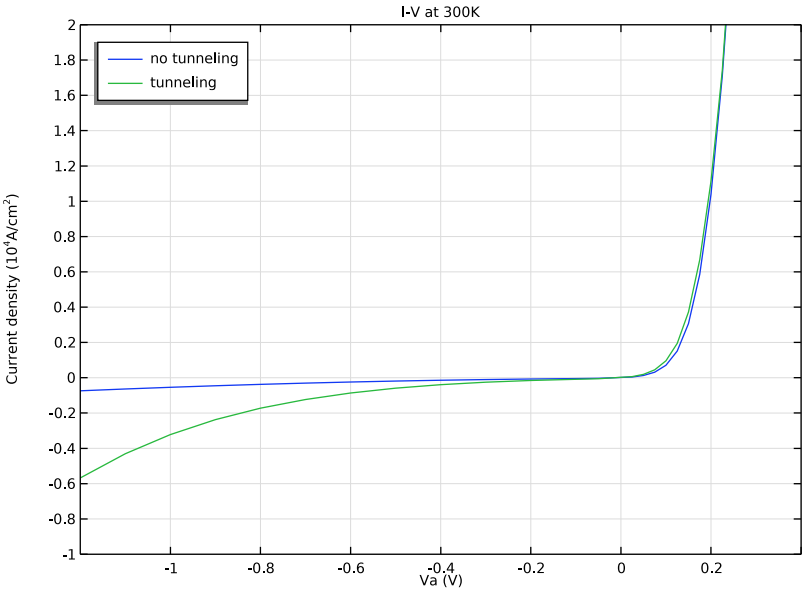



*Figure 2: Comparison of the current density vs. voltage (J–V) curves obtained with and without tunneling.*

Figure 3 shows the conduction band diagram and the electron quasi-Fermi level at two bias voltages. The figure agrees well with Fig. 13 in Ref. 1.

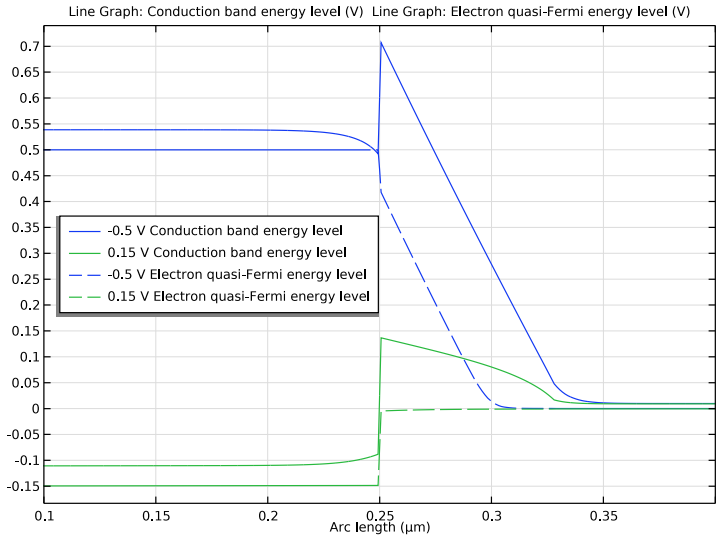



*Figure 3: Band diagram and quasi-Fermi level under forward and reverse bias.*

Figure 4 shows good agreement of the J–V curves at different temperatures.

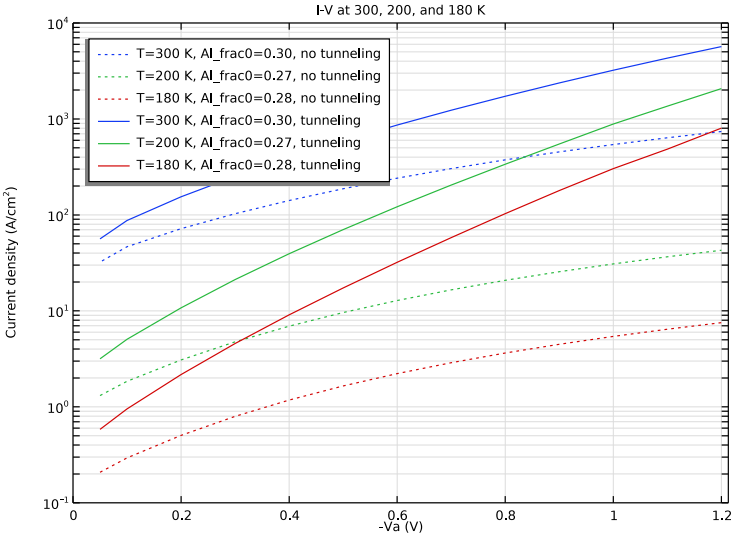



*Figure 4: J–V curves at different temperatures agree well with Fig. 14 in Ref. 1.*

## *Reference*

1. K. Yang, J.R. East, and G.I. Haddad, "Numerical Modeling of Abrupt Heterojunctions using a Thermionic-Field Emission Boundary Condition," *Solid State Electronics*, vol. 36, no. 3, pp. 321–330, 1993.

**Application Library path:** `Semiconductor_Module/Verification_Examples/heterojunction_tunneling`

## *Modeling Instructions*

From the **File** menu, choose **New**.

### NEW

In the **New** window, click **Model Wizard**.

### MODEL WIZARD

1. In the **Model Wizard** window, The model is 1D in nature. However to demonstrate the general procedure for setting up 2D and 3D models, we will build an equivalent 2D model.
2. click **2D**.
3. In the **Select Physics** tree, select **Semiconductor>Semiconductor (semi)**.
4. Click **Add**.

   In addition to the Semiconductor interface, we will use two **Curvilinear Coordinates** mathematical interfaces to set up the coordinate system for the tunneling effect. This procedure is not necessary for this simple example which is 1D in nature, however it will be required for true 2D models.
5. In the **Select Physics** tree, select **Mathematics>Curvilinear Coordinates (cc)**.
6. Click **Add**.
7. Click **Add**.
8. Click **Study**.
9. In the **Select Study** tree, select **General Studies>Stationary**.
10. Click **Done**.

## GEOMETRY 1

The model wizard brings us to the **Geometry** node in the Model Builder tree structure. We can use this opportunity to set the length unit to µm.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **µm**.

Load some global parameters from a text file. These parameters are independent of space and time in a model.

## GLOBAL DEFINITIONS

### *Parameters 1*

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

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 `heterojunction_tunneling_parameters.txt`.

Create the geometry of three rectangular domains according to Fig. 2(b) in the reference paper.

## GEOMETRY 1

### *Rectangle 1 (r1)*

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `d1+d2+d3`.

4 In the **Height** text field, type `d2`.

5 Locate the **Position** section. In the **x** text field, type `-d1`.

6 Click to expand the **Layers** section. Clear the **Layers on bottom** check box.

7 Select the **Layers to the left** check box.

8 In the table, enter the following settings:

| Layer name | Thickness (µm) |
|---|---|
| Layer 1 | d1 |
| Layer 2 | d2 |

9 Click **Build All Objects**.

Define local variables and operators. The variables can be spatially varying and can be grouped into different nodes for convenience.

First, use three separate **Variables** nodes for the n doping and mole fraction of Al in each of the three domains.

### DEFINITIONS

*Variables for Domain 1*

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables for Domain 1` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 1 only.

5 Locate the **Variables** section. In the table, enter the following settings:

| Name | Expression | Unit | Description |
|---|---|---|---|
| N_D | N_D1 | 1/m³ | n doping |
| Al_frac | 0 | | Mole fraction of Al |

6 Right-click **Variables for Domain 1** and choose **Duplicate**.

*Variables for Domain 2*

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** click **Variables for Domain 1.1**.

2 In the **Settings** window for **Variables**, type `Variables for Domain 2` in the **Label** text field.

3 Select Domain 2 only.

4 Locate the **Variables** section. In the table, enter the following settings:

| Name | Expression | Unit | Description |
|---|---|---|---|
| N_D | N_D2 | 1/m³ | n doping |
| Al_frac | Al_frac0*(1-x/d2) | | Mole fraction of Al |

*Variables for Domain 1*

In the **Model Builder** window, right-click **Variables for Domain 1** and choose **Duplicate**.

*Variables for Domain 3*

1. In the **Model Builder** window, under **Component 1 (comp1)>Definitions** click **Variables for Domain 1.1**.
2. In the **Settings** window for **Variables**, type `Variables for Domain 3` in the **Label** text field.
3. Select Domain 3 only.
4. Locate the **Variables** section. In the table, enter the following settings:

| Name | Expression | Unit | Description |
|---|---|---|---|
| N_D | N_D3 | 1/m³ | n doping |

Define material properties according to the reference paper. The electron effective mass will be needed when we define variables for the tunneling effect later.

## MATERIALS

*Al(x)Ga(1-x)As (Yang et al 1993)*

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.
2. In the **Settings** window for **Material**, type `Al(x)Ga(1-x)As (Yang et al 1993)` in the **Label** text field.

   First define local material variables for the mole fraction and the effective masses.
3. In the **Model Builder** window, expand the **Component 1 (comp1)>Materials>Al(x)Ga(1-x)As (Yang et al 1993) (mat1)** node, then click **Basic (def)**.
4. In the **Settings** window for **Basic**, locate the **Local Properties** section.

5 In the **Local properties** table, enter the following settings:

| Name | Expression | Unit | Description |
|---|---|---|---|
| x | Al_frac | | Mole fraction of Al |
| me | (0.067+0.083*def.x)* me_const | kg | Electron DOS effective mass |
| mh | (0.48+0.31*def.x)* me_const | kg | Hole DOS effective mass |

Note that these variables are accessed with the scope name `def`, for example `def.x`, because the tag of the **Basic** node is `def`.

Then enter the material properties using formulas and descriptions given in the reference paper.

6 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Al(x)Ga(1-x)As (Yang et al 1993) (mat1)**.

7 In the **Settings** window for **Material**, locate the **Material Contents** section.

8 In the table, enter the following settings:

| Property | Variable | Value | Unit | Property group |
|---|---|---|---|---|
| Electron mobility | mun | 7200[cm^2/V/s]/(1+5.51e-17[cm^3]*(N_D+N_A))^0.233*(T0/T)^2.3*(1-0.127*def.x/0.1) | $m^2/(V·s)$ | Semiconductor material |
| Hole mobility | mup | 380[cm^2/V/s]/(1+3.17e-17[cm^3]*(N_D+N_A))^0.266*(T0/T)^2.7*(1-0.067*def.x/0.1) | $m^2/(V·s)$ | Semiconductor material |
| Relative permittivity | epsilonr_iso ; epsilonrii = epsilonr_iso, epsilonrij = 0 | 13.1-3*def.x | 1 | Basic |

| Property | Variable | Value | Unit | Property group |
|---|---|---|---|---|
| Band gap | Eg0 | `1.519[V]+ 1.247[V]* def.x- 5.405e-4[V/ K]*T^2/(T+ 204[K])` | V | Semiconductor material |
| Electron affinity | chi0 | `4.07[V]-0.6* 1.247[V]* def.x` | V | Semiconductor material |
| Effective density of states, conduction band | Nc | `2*((def.me* k_B_const* T)/(2*pi* hbar_const^2 ))^1.5` | 1/m³ | Semiconductor material |
| Effective density of states, valence band | Nv | `2*((def.mh* k_B_const* T)/(2*pi* hbar_const^2 ))^1.5` | 1/m³ | Semiconductor material |

Before defining the variables for the tunneling effect, we need to prepare the coordinate systems.

In this example, domain 2 happens to cover the region of interest for the line integration across the potential barrier. In general, the region of interest can be defined by different boundaries drawn in the geometry, which may or may not coincide with the material boundaries.

First, set up the coordinate along the heterojunction using the first **Curvilinear Coordinates** mathematical interface.

### CURVILINEAR COORDINATES (CC)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Curvilinear Coordinates (cc)**.

2 Select Domain 2 only.

*Diffusion Method 1*

In the **Physics** toolbar, click **Domains** and choose **Diffusion Method**.

*Inlet 1*

1 In the **Physics** toolbar, click **Attributes** and choose **Inlet**.

2 Select Boundary 6 only.

*Diffusion Method 1*

In the **Model Builder** window, click **Diffusion Method 1**.

*Outlet 1*

1 In the **Physics** toolbar, click **Attributes** and choose **Outlet**.

2 Select Boundary 5 only.

Next, set up the coordinate along the field lines using the second **Curvilinear Coordinates** mathematical interface. Here we assume the field lines are perpendicular to the heterojunction, which should be a good approximation when the tunneling effect is significant.

### CURVILINEAR COORDINATES 2 (CC2)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Curvilinear Coordinates 2 (cc2)**.

2 Select Domain 2 only.

*Diffusion Method 1*

In the **Physics** toolbar, click **Domains** and choose **Diffusion Method**.

*Inlet 1*

1 In the **Physics** toolbar, click **Attributes** and choose **Inlet**.

2 Select Boundary 7 only.

*Diffusion Method 1*

In the **Model Builder** window, click **Diffusion Method 1**.

*Outlet 1*

1 In the **Physics** toolbar, click **Attributes** and choose **Outlet**.

2 Select Boundary 4 only.

Give the coordinates convenient names for subsequent definitions.

### DEFINITIONS

*Variables for tunneling*

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables for tunneling` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 2 only.

5 Locate the **Variables** section. In the table, enter the following settings:

| Name | Expression | Unit | Description |
|---|---|---|---|
| pbcc | cc.diff1.U | m | Normalized arc length along the edge of the potential barrier |
| flcc | cc2.diff1.U | m | Normalized arc length along the field line |

Set up the device physics. Since the tunneling effect is highly sensitive to the shape of the potential barrier, we switch to the finite element quasi-Fermi level formulation. The default finite volume formulation would require much finer mesh, due to its discontinuous nature.

### SEMICONDUCTOR (SEMI)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Semiconductor (semi)**.

2 In the **Settings** window for **Semiconductor**, locate the **Thickness** section.

3 In the $d$ text field, type `thickness`.

4 Click to expand the **Discretization** section. From the **Formulation** list, choose **Finite element quasi Fermi level (quadratic shape function)**.

Enable **Advanced Physics Options** to unhide and set the reference temperature.

5 Click the **Show More Options** button in the **Model Builder** toolbar.

6 In the **Show More Options** dialog box, in the tree, select the check box for the node **Physics>Advanced Physics Options**.

7 Click **OK**.

8 In the **Settings** window for **Semiconductor**, click to expand the **Reference Temperature** section.

9 In the $T_0$ text field, type `T0`.

Set up the lattice temperature and incomplete ionization according to the reference paper. Note that the paper does not use a consistent formula for the donor activation energy for all examples, and here we take the values for the example in section 3.3 of the paper which we reproduce in this tutorial.

*Semiconductor Material Model 1*

1 In the **Model Builder** window, under **Component 1 (comp1)>Semiconductor (semi)** click **Semiconductor Material Model 1**.

2 In the **Settings** window for **Semiconductor Material Model**, locate the **Model Input** section.

3 In the $T$ text field, type `T`.

4 Click to expand the **Dopant Ionization** section. From the **Dopant ionization** list, choose **Incomplete ionization**.

5 In the $\Delta E_d \equiv E_c - E_d$ text field, type `0.005[V]+0.03[V]*material.def.x/Al_frac0`.

Note the use of the prefix `material` in the expression so that the software will use the material properties assigned to each domain, in the same way that the option of **From material** works in many drop-down menus for material properties in the user interface.

6 In the $\Delta E_a \equiv E_a - E_v$ text field, type `0.026[V]`.

Set the model of the heterojunction to thermionic emission. This heterojunction boundary condition will be used to compute the case of no tunneling, to be compared with the case that includes tunneling.

*Continuity/Heterojunction 1*

1 In the **Model Builder** window, click **Continuity/Heterojunction 1**.

2 In the **Settings** window for **Continuity/Heterojunction**, locate the **Heterojunction** section.

3 From the **Continuity model** list, choose **Thermionic emission**.

Duplicate the heterojunction boundary condition to add extra current contribution from the tunneling effect at the abrupt junction (the left heterojunction). In this example, only electron tunneling is significant.

4 Right-click **Continuity/Heterojunction 1** and choose **Duplicate**.

*Continuity/Heterojunction 2*

1 In the **Model Builder** window, click **Continuity/Heterojunction 2**.

2 In the **Settings** window for **Continuity/Heterojunction**, locate the **Boundary Selection** section.

3 Click  **Clear Selection**.

4 Select Boundary 4 only.

5 Click to expand the **Extra Current Contribution** section. From the **Extra electron current** list, choose **WKB tunneling model**.

Add a **WKB Tunneling Model** subnode to set up the tunneling effect.

*WKB Tunneling Model, Electrons 1*

1 In the **Physics** toolbar, click **Attributes** and choose **WKB Tunneling Model, Electrons**.

As mentioned earlier, domain 2 covers the region of interest for the line integration across the potential barrier.

2 In the **Settings** window for **WKB Tunneling Model, Electrons**, locate the **Potential Barrier Domain Selection** section.

3 Click to select the **Activate Selection** toggle button.

4 Select Domain 2 only.

Select the boundary that is on the other side of domain 2 from the tunneling boundary.

5 Locate the **Opposite Boundary Selection** section. Click to select the **Activate Selection** toggle button.

6 Select Boundary 7 only.

The electron effective mass is defined in the material properties.

7 Locate the **WKB Tunneling Model, Electrons** section. In the *m* text field, type `material.def.me`.

The field line and tunneling boundary coordinates have been defined earlier as variables in terms of the curvilinear coordinates.

8 In the *flc* text field, type `flcc`.

9 In the *bndc* text field, type `pbcc`.

Add doping and SRH recombination. The latter requires more material parameters.

*Analytic Doping Model 1*

1 In the **Physics** toolbar, click **Domains** and choose **Analytic Doping Model**.

2 In the **Settings** window for **Analytic Doping Model**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Impurity** section. From the **Impurity type** list, choose **Donor doping (n-type)**.

5 In the $N_{D0}$ text field, type `N_D`.

*Trap-Assisted Recombination 1*

1 In 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**.

## MATERIALS

*Al(x)Ga(1-x)As (Yang et al 1993) (mat1)*

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Al(x)Ga(1-x)As (Yang et al 1993) (mat1)**.

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 |
|---|---|---|---|---|
| Electron lifetime, SRH | taun | 1[ns] | s | Shockley-Read-Hall recombination |
| Hole lifetime, SRH | taup | 1[ns] | s | Shockley-Read-Hall recombination |

Add metal contacts.

## SEMICONDUCTOR (SEMI)

*Metal Contact 1*

1 In the **Physics** toolbar, click **Boundaries** and choose **Metal Contact**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Metal Contact**, locate the **Terminal** section.

4 In the $V_0$ text field, type Va.

*Metal Contact 2*

1 In the **Physics** toolbar, click **Boundaries** and choose **Metal Contact**.

2 Select Boundary 10 only.

Adjust mesh to save computation time. Mesh refinement studies are always recommended.

## MESH 1

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Edit Physics-Induced Sequence**.

*Size 1*

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size 1**.

2 Select Boundary 4 only.

First solve the case of no tunneling effects. Sweep the applied voltage to obtain the I-V curve.

## STUDY 1: NO TUNNELING

1 In the **Model Builder** window, click **Study 1**.

2 In the **Settings** window for **Study**, type `Study 1: no tunneling` in the **Label** text field.

### *Step 1: Stationary*

For this study we only solve for the **Semiconductor** physics, so leave it enabled and disable the two **Curvilinear Coordinates** interfaces.

1 In the **Model Builder** window, under **Study 1: no tunneling** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check boxes for **Curvilinear Coordinates (cc)** and **Curvilinear Coordinates 2 (cc2)**.

4 Select the **Modify model configuration for study step** check box.

5 In the tree, select **Component 1 (comp1)>Semiconductor (semi)>Continuity/ Heterojunction 2**.

6 Click **Disable**.

7 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

8 Click **Add**.

9 In the table, enter the following settings:

| Parameter name | Parameter value list | Parameter unit |
|---|---|---|
| Va (Applied voltage) | `range(-1.2,0.1,-0.01) -0.05 range(0.025,0.025, 0.25)` | V |

10 In the table, click to select the cell at row number 1 and column number 3.

11 In the **Home** toolbar, click **Compute**.

## RESULTS

### *P-type*

The model has only n-type dopant therefore, the p-type part of the default generated plot is not needed.

1 In the **Model Builder** window, expand the **Net Dopant Concentration (semi)** node.

2 Right-click **P-type** and choose **Delete**.

Plot the I-V curve for the no tunneling case. Set the scale and range to be the same as Fig. 12 in the reference paper for ease of comparison.

*I-V at 300 K*

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `I-V at 300 K` in the **Label** text field.

3 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `I-V at 300K`.

5 Locate the **Plot Settings** section.

6 Select the **y-axis label** check box. In the associated text field, type `Current density (10<sup>4</sup>A/cm<sup>2</sup>)`.

7 Locate the **Axis** section. Select the **Manual axis limits** check box.

8 In the **x minimum** text field, type `-1.2`.

9 In the **x maximum** text field, type `0.4`.

10 In the **y maximum** text field, type `2`.

11 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

*Global 1*

1 Right-click **I-V at 300 K** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `semi.IO_1/d2/thickness/1e4[A/cm^2]` | 1 | `no tunneling` |

4 In the **I-V at 300 K** toolbar, click **Plot**.

Solve the equations for the curvilinear systems before solving the case with the tunneling effect. In general, the curvilinear coordinates provide a good approximation to the field lines and equipotential contours where the tunneling effect is significant.

### ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

For this study we only solve for the two **Curvilinear Coordinates** interfaces, so leave them enabled and disable the **Semiconductor** physics.

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Semiconductor (semi)**.

4 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.

5 Click **Add Study** in the window toolbar.

6 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

### STUDY 2: CURVILINEAR COORDINATES

1 In the **Model Builder** window, click **Study 2**.

2 In the **Settings** window for **Study**, type `Study 2: curvilinear coordinates` in the **Label** text field.

3 In the **Home** toolbar, click **Compute**.

Plot the curvilinear coordinates, which in general provide a good approximation to the field lines and equipotential contours where the tunneling effect is significant.

### RESULTS

*Curvilinear coordinates*

1 In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Curvilinear coordinates` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: curvilinear coordinates/ Solution 2 (sol2)**.

*Contour 1*

1 Right-click **Curvilinear coordinates** and choose **Contour**.

2 In the **Settings** window for **Contour**, locate the **Expression** section.

3 In the **Expression** text field, type `pbcc`.

4 Locate the **Levels** section. In the **Total levels** text field, type `5`.

5 Right-click **Contour 1** and choose **Duplicate**.

*Contour 2*

1 In the **Model Builder** window, click **Contour 2**.

2 In the **Settings** window for **Contour**, locate the **Expression** section.

3 In the **Expression** text field, type `flcc`.

4 Locate the **Levels** section. In the **Total levels** text field, type `8`.

*Contour 1*

1 In the **Model Builder** window, click **Contour 1**.

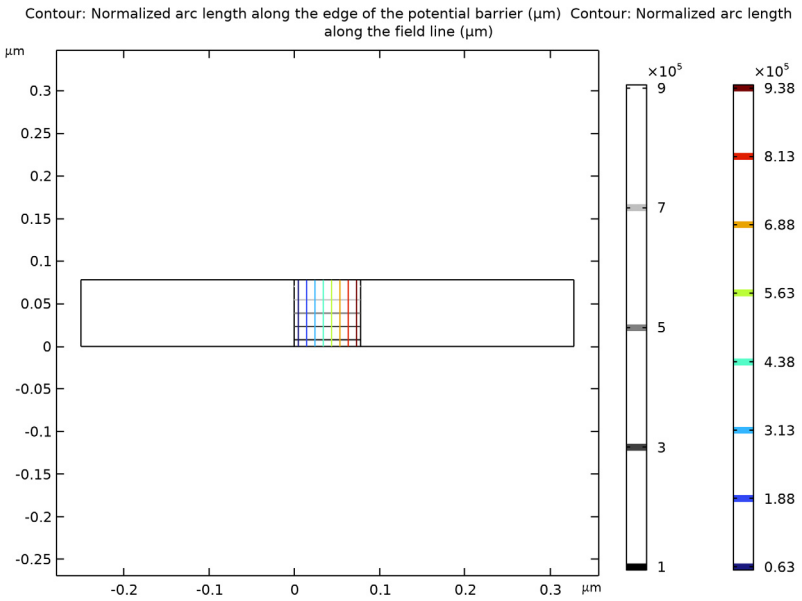
2 In the **Settings** window for **Contour**, locate the **Coloring and Style** section.

3 Click **Change Color Table**.

4 In the **Color Table** dialog box, select **Linear>GrayScale** in the tree.

5 Click **OK**.

6 In the **Curvilinear coordinates** toolbar, click **Plot**.




Now solve the case with tunneling effects. Since we will only solve the semiconductor physics, not the curvilinear systems, we use the **Initial values of variables solved for** settings to provide a good initial condition for the semiconductor physics from Study 1, but we use the **Values of variables not solved for** settings to provide the curvilinear coordinates from the solution of Study 2. Sweep the applied voltage to obtain the I-V curve.

### ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

For this study we only solve for the **Semiconductor** physics, so leave it enabled and disable the two **Curvilinear Coordinates** interfaces.

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check boxes for **Curvilinear Coordinates (cc)** and **Curvilinear Coordinates 2 (cc2)**.

4 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.

5 Click **Add Study** in the window toolbar.

6 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

### STUDY 3: TUNNELING

1 In the **Model Builder** window, click **Study 3**.

2 In the **Settings** window for **Study**, type `Study 3: tunneling` in the **Label** text field.

*Step 1: Stationary*

1 In the **Model Builder** window, under **Study 3: tunneling** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, click to expand the **Values of Dependent Variables** section.

3 Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

4 From the **Method** list, choose **Solution**.

5 From the **Study** list, choose **Study 1: no tunneling, Stationary**.

6 From the **Parameter value (Va (V))** list, choose **-1.2 V**.

7 Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

8 From the **Method** list, choose **Solution**.

9 From the **Study** list, choose **Study 2: curvilinear coordinates, Stationary**.

10 Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

11 Click **Add**.

12 In the table, enter the following settings:

| Parameter name | Parameter value list | Parameter unit |
|---|---|---|
| Va (Applied voltage) | `range(-1.2,0.1,-0.01) -0.05 range(0.025,0.025, 0.25)` | V |

13 In the table, click to select the cell at row number 1 and column number 3.

14 In the **Home** toolbar, click **Compute**.

### RESULTS

*Net Dopant Concentration (semi) 1*

In the **Model Builder** window, under **Results** right-click **Net Dopant Concentration (semi) 1** and choose **Delete**.

Add the tunneling result to the I-V curve plot. This matches well with Fig. 12 in the reference paper.

*Global 1*

In the **Model Builder** window, under **Results>I-V at 300 K** right-click **Global 1** and choose **Duplicate**.

*Global 2*

1 In the **Model Builder** window, click **Global 2**.

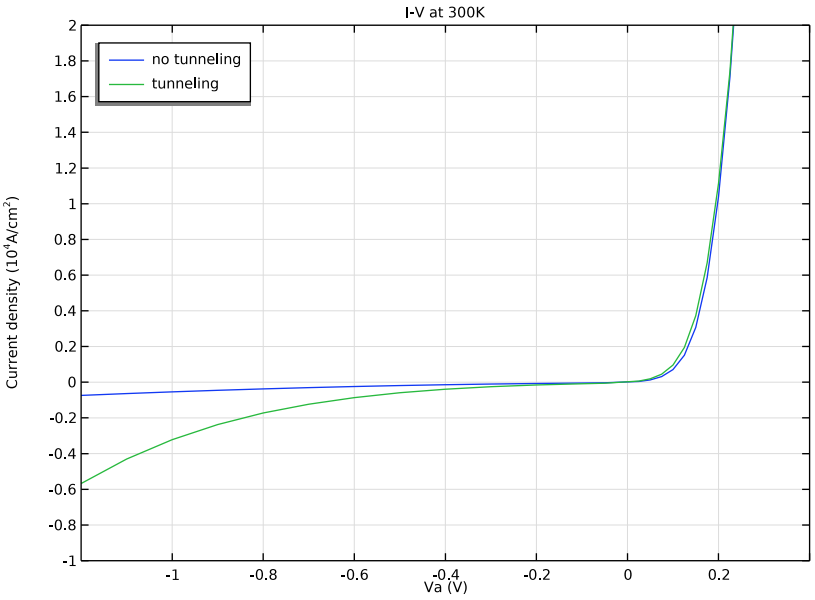
2 In the **Settings** window for **Global**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 3: tunneling/Solution 3 (sol3)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `semi.IO_1/d2/thickness/1e4[A/cm^2]` | 1 | `tunneling` |

5 In the **I-V at 300 K** toolbar, click **Plot**.




Add a 1D plot group to plot the band diagram at two bias points -0.5 V and 0.15 V. This compares well with Fig. 13 in the reference paper.

*Conduction band profiles*

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Conduction band profiles` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3: tunneling/ Solution 3 (sol3)**.

4 From the **Parameter selection (Va)** list, choose **From list**.

To select the two bias points -0.5 V and 0.15 V, hold down the Control key to enable multiple selection by mouse clicking.

5 In the **Parameter values (Va (V))** list, choose **-0.5** and **0.15**.

*Line Graph 1*

1 Right-click **Conduction band profiles** and choose **Line Graph**.

2 Select Boundaries 2, 5, and 8 only.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `semi.Ec`.

5 Click to expand the **Quality** section. From the **Smoothing** list, choose **Everywhere**.

6 Click to expand the **Legends** section. Select the **Show legends** check box.

7 Find the **Include** subsection. Select the **Description** check box.

8 Right-click **Line Graph 1** and choose **Duplicate**.

*Line Graph 2*

1 In the **Model Builder** window, click **Line Graph 2**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `semi.Efn`.

4 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

5 From the **Color** list, choose **Cycle (reset)**.

*Conduction band profiles*

1 In the **Model Builder** window, click **Conduction band profiles**.

2 In the **Settings** window for **1D Plot Group**, locate the **Axis** section.

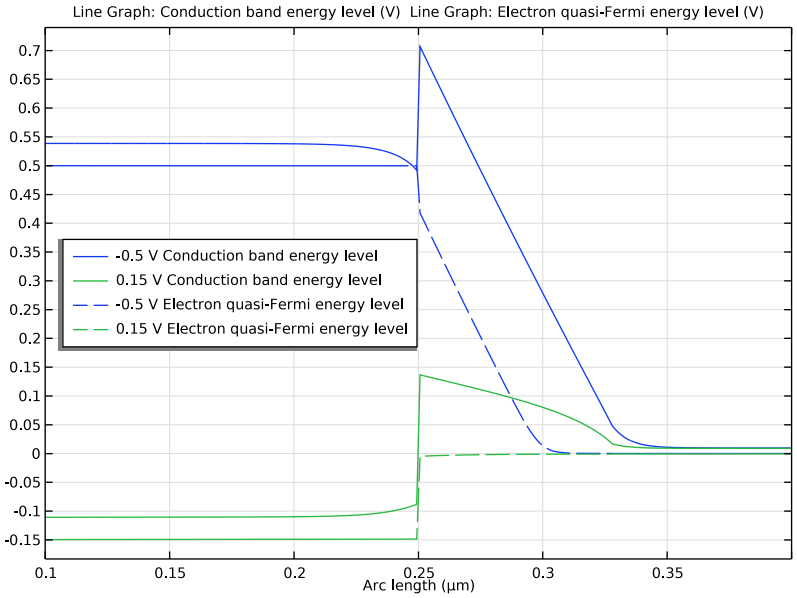
3 Select the **Manual axis limits** check box.

4 In the **x minimum** text field, type `0.1`.

5 In the **x maximum** text field, type `0.4`.

6 Locate the **Legend** section. From the **Position** list, choose **Middle left**.

7 In the **Conduction band profiles** toolbar, click **Plot**.




Now add two studies for the low-temperature cases, to compare with Fig. 14 in the reference paper. First create an empty study and copy over the study step for the nontunneling case from **Study 1**.

### ADD STUDY

1 In 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 **Empty Study**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

### STUDY 4: NO TUNNELING, LOWER TS

In the **Settings** window for **Study**, type `Study 4: no tunneling, lower Ts` in the **Label** text field.

## STUDY 1: NO TUNNELING

*Step 1: Stationary*

In the **Model Builder** window, under **Study 1: no tunneling** right-click **Step 1: Stationary** and choose **Copy**.

## STUDY 4: NO TUNNELING, LOWER TS

In the **Model Builder** window, right-click **Study 4: no tunneling, lower Ts** and choose **Paste Stationary**.

The very nonlinear equation system often needs to be parametrically swept from a favorable initial condition. In this case, we found it easier for convergence to start the sweep from the other end of the parameter range, with the corresponding solution from **Study 1** as the initial condition.

1. In the **Model Builder** window, under **Study 4: no tunneling, lower Ts** click **Step 1: Stationary**.
2. In the **Settings** window for **Stationary**, locate the **Study Extensions** section.
3. In the table, enter the following settings:

| Parameter name | Parameter value list | Parameter unit |
|---|---|---|
| Va (Applied voltage) | `-0.05 range(-0.1,-0.1,-1.2)` | V |

4. In the table, click to select the cell at row number 1 and column number 3.
5. Click to expand the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.
6. From the **Method** list, choose **Solution**.
7. From the **Study** list, choose **Study 1: no tunneling, Stationary**.
8. From the **Parameter value (Va (V))** list, choose **-0.05 V**.

Add a parametric sweep node for the two low-temperature cases, with the Al fraction adjusted for each case according to the reference paper.

*Parametric Sweep*

1. In the **Study** toolbar, click **Parametric Sweep**.
2. In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.
3. Click **Add**.

4 In the table, enter the following settings:

| Parameter name | Parameter value list | Parameter unit |
|---|---|---|
| T (Lattice temperature) | 200 180 | K |

5 Click + **Add**.

6 In the table, enter the following settings:

| Parameter name | Parameter value list | Parameter unit |
|---|---|---|
| Al_frac0 (Mole fraction of Al at heterojunction) | 0.27 0.28 | |

7 In the **Study** toolbar, click = **Compute**.

## RESULTS

### *Net Dopant Concentration (semi) 1*

In the **Model Builder** window, under **Results** right-click **Net Dopant Concentration (semi) 1** and choose **Delete**.

Add a 1D plot group to plot the I-V curves at the three temperatures for the nontunneling cases computed so far.

### *I-V at different Ts*

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `I-V at different Ts` in the **Label** text field.

### *Global 1*

1 Right-click **I-V at different Ts** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `-semi.IO_1/d2/thickness` | `A/cm^2` | `T=300 K, Al_frac0=0.30, no tunneling` |

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 In the **Expression** text field, type `-Va`.

6 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dotted**.

*I-V at different Ts*

1 In the **Model Builder** window, click **I-V at different Ts**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Parameter selection (Va)** list, choose **From list**.

4 In the **Parameter values (Va (V))** list, choose **-1.2**, **-1.1**, **-1**, **-0.9**, **-0.8**, **-0.7**, **-0.6**, **-0.5**, **-0.4**, **-0.3**, **-0.2**, **-0.1**, and **-0.05**.

5 Locate the **Title** section. From the **Title type** list, choose **Manual**.

6 In the **Title** text area, type `I-V at 300, 200, and 180 K`.

7 Locate the **Plot Settings** section.

8 Select the **y-axis label** check box. In the associated text field, type `Current density (A/cm<sup>2</sup>)`.

*Global 1*

In the **Model Builder** window, right-click **Global 1** and choose **Duplicate**.

*Global 2*

1 In the **Model Builder** window, click **Global 2**.

2 In the **Settings** window for **Global**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 4: no tunneling, lower Ts/ Parametric Solutions 1 (sol5)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `-semi.IO_1/d2/thickness` | `A/cm^2` | `no tunneling` |

5 Click the  **y-Axis Log Scale** button in the **Graphics** toolbar.

6 In the **I-V at different Ts** toolbar, click  **Plot**.

Create another empty study and copy the study steps from **Study 4** to modify for the tunneling case. Similar to Study 3, here we use the **Initial values of variables solved for** settings to provide a good initial condition for the semiconductor physics from Study 4, but we use the **Values of variables not solved for** settings to provide the curvilinear coordinates from the solution of Study 2.

### ADD STUDY

1 In 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 **Empty Study**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

### STUDY 5: TUNNELING, LOWER TS

In the **Settings** window for **Study**, type `Study 5: tunneling, lower Ts` in the **Label** text field.

### STUDY 4: NO TUNNELING, LOWER TS

*Parametric Sweep*

In the **Model Builder** window, under **Study 4: no tunneling, lower Ts** right-click **Parametric Sweep** and choose **Copy**.

### STUDY 5: TUNNELING, LOWER TS

In the **Model Builder** window, right-click **Study 5: tunneling, lower Ts** and choose **Paste Parametric Sweep**.

### STUDY 4: NO TUNNELING, LOWER TS

*Step 1: Stationary*

In the **Model Builder** window, under **Study 4: no tunneling, lower Ts** right-click **Step 1: Stationary** and choose **Copy**.

### STUDY 5: TUNNELING, LOWER TS

In the **Model Builder** window, right-click **Study 5: tunneling, lower Ts** and choose **Paste Stationary**.

1 In the **Model Builder** window, under **Study 5: tunneling, lower Ts** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 Clear the **Modify model configuration for study step** check box.

4 Locate the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Study** list, choose **Study 4: no tunneling, lower Ts, Stationary**.

5 From the **Solution** list, choose **Parametric Solutions 1 (sol5)**.

6 From the **Use** list, choose **T=200, Al_frac0=0.27 (sol6)**.

7 From the **Parameter value (Va (V))** list, choose **First**.

8 Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

9 From the **Method** list, choose **Solution**.

10 From the **Study** list, choose **Study 2: curvilinear coordinates, Stationary**.

11 In the **Home** toolbar, click **Compute**.

## RESULTS

*Net Dopant Concentration (semi) 1*

In the **Model Builder** window, under **Results** right-click **Net Dopant Concentration (semi) 1** and choose **Delete**.

Add the tunneling result to the I-V curve plot. This matches well with Fig. 14 in the reference paper.

*Global 1*

In the **Model Builder** window, under **Results>I-V at different Ts** right-click **Global 1** and choose **Duplicate**.

*Global 3*

1 In the **Model Builder** window, click **Global 3**.

2 In the **Settings** window for **Global**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 3: tunneling/Solution 3 (sol3)**.

4 From the **Parameter selection (Va)** list, choose **From list**.

5 In the **Parameter values (Va (V))** list, choose **-1.2**, **-1.1**, **-1**, **-0.9**, **-0.8**, **-0.7**, **-0.6**, **-0.5**, **-0.4**, **-0.3**, **-0.2**, **-0.1**, and **-0.05**.

6 Locate the **y-Axis Data** section. In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `-semi.IO_1/d2/thickness` | `A/cm^2` | `T=300 K, Al_frac0=0.30, tunneling` |

7 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Solid**.

8 From the **Color** list, choose **Cycle (reset)**.

9 Right-click **Global 3** and choose **Duplicate**.

*Global 4*

1 In the **Model Builder** window, click **Global 4**.

2 In the **Settings** window for **Global**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 5: tunneling, lower Ts/Parametric Solutions 2 (sol9)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `-semi.IO_1/d2/thickness` | `A/cm^2` | `tunneling` |

5 Locate the **Coloring and Style** section. From the **Color** list, choose **Cycle**.

*I-V at different Ts*

1 In the **Model Builder** window, click **I-V at different Ts**.

2 In the **Settings** window for **1D Plot Group**, locate the **Axis** section.

3 Select the **Manual axis limits** check box.

4 In the **x minimum** text field, type `0`.

5 In the **y minimum** text field, type `0.1`.

6 In the **y maximum** text field, type `1e4`.

7 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

8 In the **I-V at different Ts** toolbar, click **Plot**.