Created in COMSOL Multiphysics 6.2

Surface Trapping in a Silicon Nanowire Gate-All-Around Device

Introduction

This example demonstrates the use of various traps. In particular the effect of gate field screening by surface trap charges is studied. A nanoscale gate-all-around MOSFET is modeled and the shift of turn-on voltage due to the screening effect is computed.

Surface traps can have important effects on the operation of many semiconductor devices. These traps are associated with donor and acceptor atoms, with other impurity atoms, 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 shown in Figure 1. There are four processes that occur, corresponding to the emission and capture of both electrons and holes between states in the bands

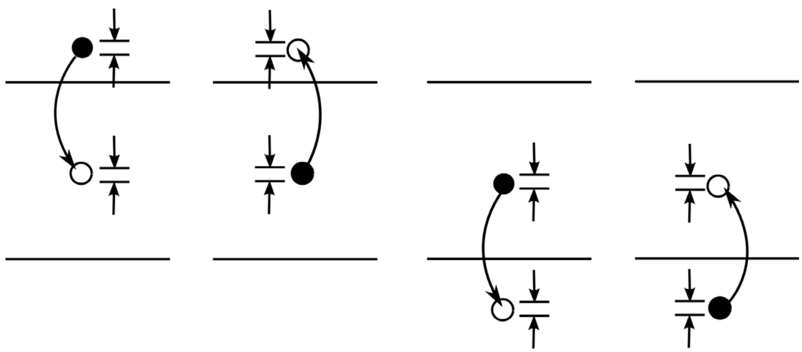


Figure 1: The four processes that contribute to SRH recombination. Left: An electron in the conduction band with energy E is captured by a trap with energy E_t (ec). Center left: An electron in a trap at energy E_t is emitted to an empty state with energy E in the conduction band (ee). Center right: 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 one 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 are possible in the Semiconductor Module, but in this model a discrete set of traps is considered, with trap density per unit area N_t at a trap energy, E_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 area for each process:

$$
\begin{aligned}
dr_{ec} &= f(E)g_c(E)(1-f_t)N_t c_{ec}(E)dE \\
dg_{ee} &= (1-f(E))g_c(E)f_t N_t c_{ee}(E)dE \\
dr_{hc} &= (1-f(E))g_v(E)f_t N_t c_{hc}(E)dE \\
dg_{he} &= f(E)g_v(E)(1-f_t)N_t c_{he}(E)dE
\end{aligned}
$$

where N_t is the number of traps per area 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:

$$
\begin{aligned}
dr_e &= [f(E)(1-f_t)c_{ec}(E)-(1-f(E))f_t c_{ee}(E)]g_c(E)N_t dE \\
dr_h &= [(1-f(E))c_{hc}(E)f_t - f(E)(1-f_t)c_{he}(E)]g_v(E)N_t dE
\end{aligned}
\tag{1}
$$

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:

$$
\begin{aligned}
c_{ee}(E) &= \frac{f(E)}{1-f(E)}\frac{1-f_t}{f_t}c_{ec}(E) \\
c_{he}(E) &= \frac{1-f(E)}{f(E)}\frac{f_t}{1-f_t}c_{hc}(E)
\end{aligned}
$$

In thermal equilibrium the occupancy of the electron traps f_{te} are determined by Fermi Dirac statistics, f_{te}=1/[1 + $\exp(E_t - E_f)/g_D$] (where g_D is the degeneracy factor). The above equations can therefore be simplified to yield:

$$
\begin{aligned}
c_{ee}(E) &= \frac{1}{g_D}\exp\left(-\frac{E-E_t}{k_B T}\right)c_{ec}(E) \\
c_{he}(E) &= g_D\exp\left(-\frac{E_t-E}{k_B T}\right)c_{hc}(E)
\end{aligned}
\tag{2}
$$

Equation 2 applies even away from equilibrium. Substituting this equation back into Equation 1, rearranging and integrating, gives the total rate of electron (r_e) or hole (r_h) capture to traps at the specified energy, E_t:

$$
\begin{aligned}
r_e &= N_t\left[1-f_t\left(1+\frac{1}{g_D}\exp\left(-\frac{E_{fn}-E_t}{k_B T}\right)\right)\right]\int_{E_c}^{\infty} f(E)c_{ec}(E)g_c(E)dE \\
r_h &= N_t\left[f_t-(1-f_t)g_D\exp\left(-\frac{E_t-E_{fp}}{k_B T}\right)\right]\int_{-\infty}^{E_v}(1-f(E))c_{hc}(E)g_v(E)dE
\end{aligned}
$$

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:

$$
C_n = \frac{\int_{E_c} f(E)c_{ec}(E)g_c(E)dE}{\int_{E_c}^{\infty} f(E)g_c(E)dE}
$$

$$
C_p = \frac{\int_{-\infty}^{E_v}(1-f(E))c_{hc}(E)g_v(E)dE}{\int_{-\infty}^{E_v}(1-f(E))g_v(E)dE}
$$

and noting that:

$$
\begin{aligned}
n &= \int_{E_c}^{\infty} f(E)g_c(E)dE = N_c\gamma_n\exp\left(-\frac{E_c-E_{fn}}{k_B T}\right) = \gamma_n n_{i,eff}\exp\left(\frac{E_{fn}-E_i}{k_b T}\right) \\
p &= \int_{-\infty}^{E_v}(1-f(E))g_v(E)dE = N_v\gamma_p\exp\left(-\frac{E_{fp}-E_v}{k_B T}\right) = \gamma_p n_{i,eff}\exp\left(\frac{E_i-E_{fp}}{k_b T}\right)
\end{aligned}
$$

the following equations are obtained:

$$
\begin{aligned}
r_e &= nC_nN_t\left[1-f_t\left(1+\frac{1}{g_D}\exp\left(-\frac{E_{fn}-E_t}{k_B T}\right)\right)\right] = C_nN_t\left[n-nf_t-\frac{n_1}{g_D}f_t\right] \\
r_h &= pC_pN_t\left[f_t-(1-f_t)g_D\exp\left(-\frac{E_t-E_{fp}}{k_B T}\right)\right] = C_pN_t[pf_t+g_D(p_1f_t-p_1)]
\end{aligned}
\tag{3}
$$

where:

$$
\begin{gathered}
n_1 = \gamma_n n_{i,eff}e^{\Delta E_t/(k_B T)} \qquad p_1 = \gamma_p n_{i,eff}e^{-\Delta E_t/(k_B T)} \\
\Delta E_t = E_i - E_t
\end{gathered}
\tag{4}
$$

Equation 3 and Equation 4 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:

$$N_t\frac{\partial f_t}{\partial t} = r_e - r_h = C_n N_t\left[n - nf_t - \frac{n_1}{g_D}f_t\right] - C_p N_t[pf_t + g_D p_1 f_t - p_1] \qquad (5)$$

Equation 5 determines the occupancy of the traps at the level E_t.

The total surface recombination rate for electrons and holes is given by summing over the distinct discrete traps (denoted by the superscript i), giving the following result:

$$R_e = \sum_i C_n^i N_t^i\left[n - nf_t^i - \frac{n_1^i}{g_D}f_t^i\right]$$

$$R_h = \sum_i C_p^i N_t^i[pf_t^i + g_D(p_1^i f_t^i - p_1^i)]$$

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 1 summarizes the different trap types currently included in the Semiconductor Module.

TABLE 1: CHARGE DUE TO DIFFERENT TYPES OF TRAP.

Trap type	**Species trapped**	**Charge occupied**	**Charge unoccupied**	**Number density**
Donor trap	Electron	0	+	N_t^D
Acceptor trap	Hole	0	-	N_t^A
Neutral electron trap	Electron	-	0	N_t^e
Neutral hole trap	Hole	+	0	N_t^h

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:

$$Q = q\sum_i (1 - f_t^i)N_t^{D,i} - f_t^i N_t^{A,i} - f_t^i N_t^{e,i} + (1 - f_t^i)N_t^{h,i} \qquad (6)$$

Equation 6 can be rewritten in the form:

$$Q = q\sum_i [N_t^{D,i} + N_t^{h,i}] - q\sum_i f_t^i N_t^i$$

$$Q = q\sum_i [N_t^{D,i} + N_t^{h,i}] - q\sum_{E_i \geq E_0} f_t^i N_t^i + q\sum_{E_i < E_0} (1 - f_t^i) N_t^i - q\sum_{E_i < E_0} N_t^i$$

where E_0 is an energy within the band gap referred to as the neutral level. E_0 is chosen such that:

$$\sum_i [N_t^{D,i} + N_t^{h,i}] = \sum_{E_i < E_0} N_t^i$$

So if a neutral energy is employed the following equation applies for the charge on the traps:

$$Q = -q\sum_{E_i \geq E_0} f_t^i N_t^i + q\sum_{E_i < E_0} (1 - f_t^i) N_t^i \tag{7}$$

A neutral level is often a convenient way of characterizing a set of traps at a boundary, because the details of the types of trapping sites are frequently not known. However, it is possible to assign a neutral level to the boundary using experimental techniques such as capacitance measurements. In this model the neutral level is assumed to be below the midgap, whilst the traps are assumed to be at the midgap. This means that only the first term on the right-hand side of Equation 7 applies.

Model Definition

The nanoscale gate-all-around MOSFET is modeled as a simple cylinder of 10 nm radius in 2D axisymmetric geometry (see Figure 2). The 100 nm long silicon channel is p-doped at a concentration level of $1 \cdot 10^{17}$ cm^{-3}. The 10 nm long drain and source regions are n-doped at a concentration level of $1 \cdot 10^{20}$ cm^{-3}. Figure 3 shows the overall signed doping profile. The gate with a 2 nm thick oxide layer and surface traps is modeled using the thin insulator gate boundary condition around the perimeter of the channel. The source boundary is grounded and the drain is set at 0.5 V; both with ideal ohmic contacts. The gate voltage is swept from –0.5 to 1.5 V at 0.1 V intervals, for three different surface trap densities: $0.1 \cdot 10^{12}$, and $5 \cdot 10^{12}$ cm^{-2}.

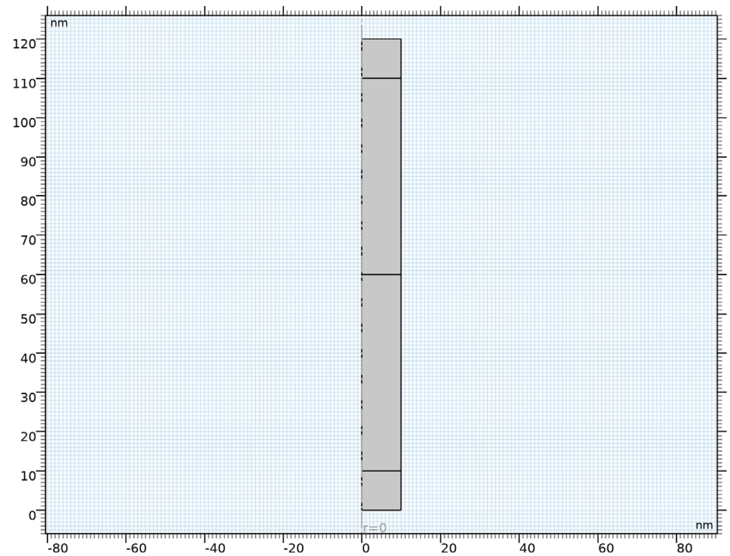


Figure 2: Geometry.

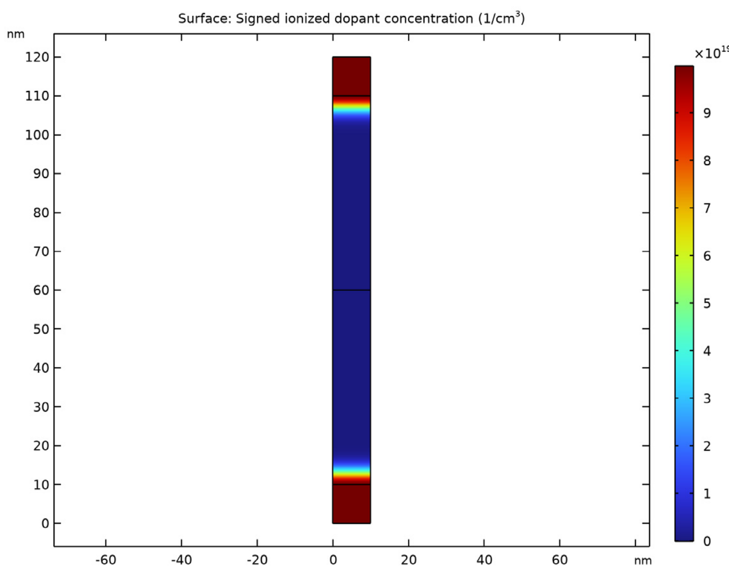


Figure 3: Doping profile.

Results and Discussion

The computed current–voltage curves for the three trap densities are shown in Figure 4 in semi-log scale. The higher turn-on voltages for higher densities of surface traps is a direct result of the screening effect of the surface trap charges, as discussed in the next few paragraphs.

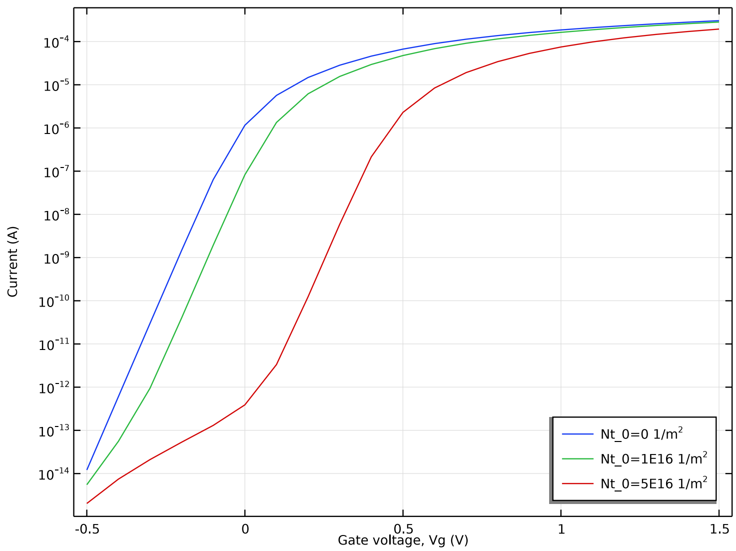


Figure 4: Current vs gate voltage.

Figure 5 shows the relevant energy levels along the radius at the central cross section of the silicon channel when the MOSFET is in the ON state, for the case of trap density of $5 \cdot 10^{12}$ cm^{-2} and gate voltage of 1.5 V. The main effect of the gate voltage is to pull the conduction band (blue curve) below the electron quasi-Fermi level (red curve), leading to an increase in the electron density (and thus the current density) underneath the gate.

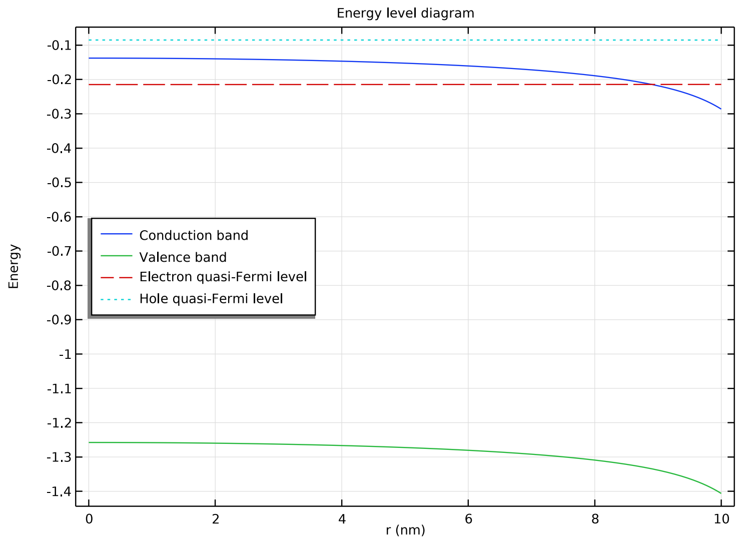


Figure 5: Conduction band (blue), valence band (green), electron quasi-Fermi level (red) and hole quasi-Fermi level (cyan) along the radius at the central cross section of the silicon channel when the MOSFET is in the on state, for the case of a trap density of $5{\cdot}10^{12}$ cm^{-2} and a gate voltage of 1.5 V.

Figure 6 shows, from left to right, the current density, the hole concentration (log scale), the electron concentration (log scale), and the electric field, when the MOSFET is in the on state, for the case of trap density of $5{\cdot}10^{12}$ cm^{-2} and gate voltage of 1.5 V. The hole concentration is much lower than the electron concentration. Thus it does not contribute to the conduction current. The increase in the electron concentration and current density beneath the gate surface is clearly seen.

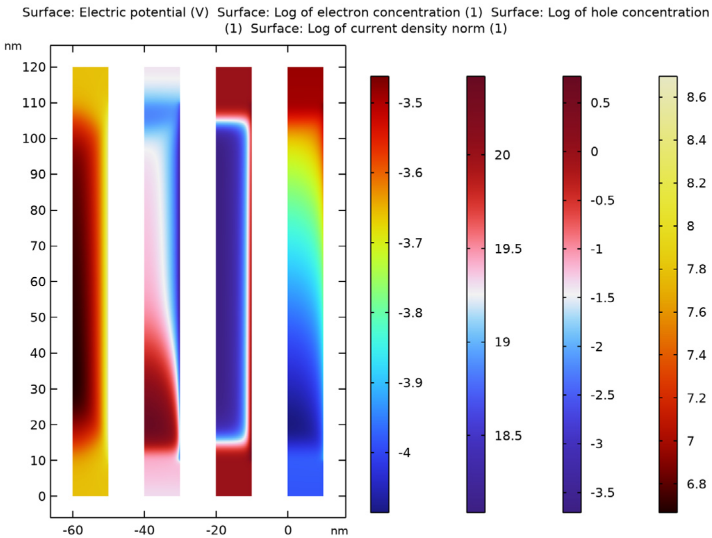


Figure 6: From left to right, the current density, the hole concentration (log scale), the electron concentration (log scale), and the electric field, when the MOSFET is in the ON state, for the case of trap density of $5 \cdot 10^{12}$ cm^{-2} and gate voltage of 1.5 V.

Figure 7 illustrates the screening effect by plotting the electric potential along the radius at the central cross section of the channel, for the gate voltage of 1.5V. The blue, green, and red curves are for the trap densities of $0.1 \cdot 10^{12}$, and $5 \cdot 10^{12}$ cm^{-2}, respectively. The electric potential is pulled down further by higher concentrations of surface traps, leading to less pileup and higher turn-on voltage.

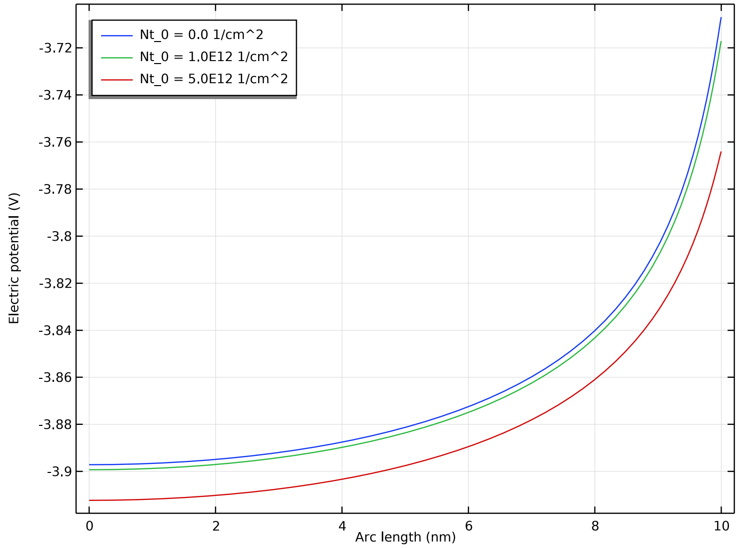


Figure 7: Electric potential along the radius at the central cross section of the channel, for the gate voltage of 1.5V. The blue, green, and red curves are for the trap concentrations of 0, $1 \cdot 10^{12}$, and $5 \cdot 10^{12}$ cm^{-2}, respectively.

Figure 8 shows the trap occupancy fraction along the length of the channel, at three gate voltages for the trap density of $5 \cdot 10^{12}$ cm^{-2}. At the gate voltage of -0.5 V, the occupancy is less than 10% in the central portion of the channel. At 0 V (still below turn-on), it is about 90%, and quickly rises to 100% in the ON state.

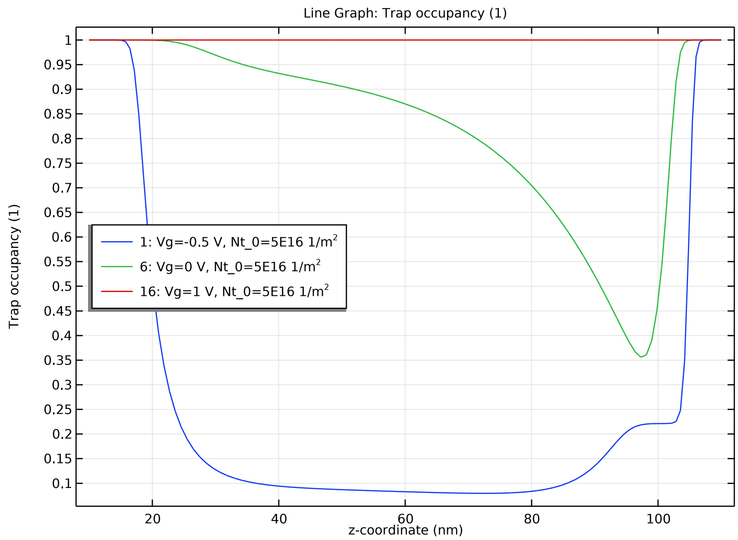


Figure 8: Trap occupancy fraction along the length of the channel, at three gate voltages for the trap density of $5 \cdot 10^{12}\ cm^{-2}$.

Application Library path: `Semiconductor_Module/Transistors/nanowire_traps`

Modeling Instructions

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **2D Axisymmetric**.

2 In the **Select Physics** tree, select **Semiconductor>Semiconductor (semi)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies>Stationary**.

6 Click **Done**.

GEOMETRY 1

The Model Wizard exits and starts the COMSOL Desktop at the Geometry node. We can set the length scale here right away. Then enter some model parameters.

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 **nm**.

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 In the table, enter the following settings:

Name	Expression	Value	Description
Rw	10[nm]	1E-8 m	Nanowire radius
L	100[nm]	1E-7 m	Gate length
t_ox	2[nm]	2E-9 m	Oxide thickness
t_np	Rw	1E-8 m	Additional length
Na_0	1e17[1/cm^3]	1E23 $1/m^3$	Background acceptor concentration
Nd_0	1e20[1/cm^3]	1E26 $1/m^3$	Maximum donor concentration
Nt_0	1e10[1/cm^2]	1E14 $1/m^2$	Trap density
Vd	500[mV]	0.5 V	Drain voltage
Vg	-500[mV]	-0.5 V	Gate voltage
ramp	1	1	Ramp parameter

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 `Rw`.

4 In the **Height** text field, type `L+2*t_np`.

Rectangle 2 (r2)

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 `Rw`.

4 In the **Height** text field, type `L/2+t_np`.

5 Click **Build All Objects**.

Rectangle 3 (r3)

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 `Rw`.

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

5 Locate the **Position** section. In the **z** text field, type `t_np`.

6 Click **Build Selected**.

ADD MATERIAL

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

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

3 In the tree, select **Semiconductors>Si - Silicon**.

4 Right-click and choose **Add to Component 1 (comp1)**.

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

MATERIALS

Si - Silicon (mat1)

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

2 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Electron mobility	mun	500[cm^2/(V*s)]	$m^2/(V\cdot s)$	Semiconductor material

SEMICONDUCTOR (SEMI)

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

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

3 From the **Carrier statistics** list, choose **Fermi–Dirac**.

4 Click to expand the **Continuation Settings** section. From the **Doping and trap density continuation parameter** list, choose **User defined**.

5 In the C_p^{dop} text field, type `ramp`.

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. In the N_{A0} text field, type `Na_0`.

Analytic Doping Model 2

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 **Distribution** section. From the list, choose **Box**.

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

6 In the N_{D0} text field, type `Nd_0`.

7 Locate the **Uniform Region** section. In the W text field, type `Rw`.

8 In the H text field, type `t_np`.

9 Locate the **Profile** section. In the d_j text field, type `t_np`.

10 From the N_b list, choose **Acceptor concentration (semi/adm1)**.

Analytic Doping Model 3

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 **Distribution** section. From the list, choose **Box**.

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

6 In the N_{D0} text field, type `Nd_0`.

7 Locate the **Uniform Region** section. Specify the r_0 vector as

`0[um]`	R
`L+t_np`	Z

8 In the W text field, type `Rw`.

9 In the H text field, type `t_np`.

10 Locate the **Profile** section. In the d_j text field, type `t_np`.

11 From the N_b list, choose **Acceptor concentration (semi/adm1)**.

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**.

Metal Contact 1

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

2 Select Boundary 2 only.

Metal Contact 2

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

2 Select Boundary 9 only.

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

4 In the V_0 text field, type `Vd`.

Thin Insulator Gate 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Thin Insulator Gate**.

2 Select Boundaries 11 and 12 only.

3 In the **Settings** window for **Thin Insulator Gate**, locate the **Terminal** section.

4 In the V_0 text field, type `Vg`.

5 Locate the **Gate Contact** section. In the ε_{ins} text field, type `3.9`.

6 In the d_{ins} text field, type `t_ox`.

Define a selection for the boundaries occupied by the gate, to provide easier setup for the next step (adding surface traps).

7 Locate the **Boundary Selection** section. Click **Create Selection**.

8 In the **Create Selection** dialog box, type `Gate` in the **Selection name** text field.

9 Click **OK**.

Create a Trap-Assisted Surface Recombination boundary condition to add surface traps.

Trap-Assisted Surface Recombination 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Trap-Assisted Surface Recombination**.

2 In the **Settings** window for **Trap-Assisted Surface Recombination**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Gate**.

Define traps at a discrete energy level using the neutral energy level formulation to determine the trapped charge. The default energy level for discrete traps is set to the midbandgap energy, which coincides with the default neutral level. By convention, traps with energy levels equal to or greater than the neutral level are treated as contributing a negative charge when occupied. Traps with energy level below the neutral level are treated as contributing a positive charge when occupied. Thus, in this case where the default levels are used, the traps will behave as if they capture electrons and accumulate a negative charge.

4 Locate the **Trap-Assisted Recombination** section. From the **Trapping model** list, choose **Explicit trap distribution**.

Discrete Energy Level 1

1 In the **Physics** toolbar, click **Attributes** and choose **Discrete Energy Level**.

2 In the **Settings** window for **Discrete Energy Level**, locate the **Traps** section.

3 In the N_t text field, type `Nt_0`.

Since the mosfet base is floating, the doping will need to be ramped on and the initial values should be set to start from an intrinsic semiconductor.

Initial Values 1

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

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 From the **Specify initial values** list, choose **Intrinsic (carriers and potential)**.

MESH 1

Mapped 1

In the **Mesh** toolbar, click **Mapped**.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 2, 4, 6, 8, and 9 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 50.

6 In the **Element ratio** text field, type 40.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 3 and 11 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 50.

6 In the **Element ratio** text field, type 5.

Distribution 3

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 5 and 12 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 In the **Number of elements** text field, type 50.

5 From the **Distribution type** list, choose **Predefined**.

6 In the **Number of elements** text field, type 50.

7 In the **Element ratio** text field, type 5.

8 Select the **Reverse direction** check box.

Distribution 4

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 1 and 10 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 10.

6 In the **Element ratio** text field, type 5.

7 Select the **Reverse direction** check box.

Distribution 5

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 7 and 13 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

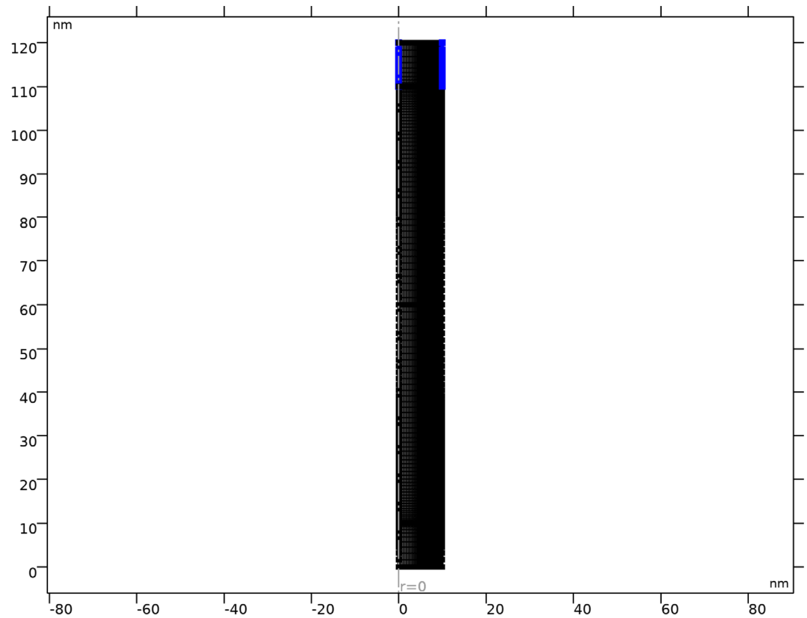
4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 10.

6 In the **Element ratio** text field, type 5.

7 Click **Build All**.

The mesh is shown in the image below.



The first study will find initial solutions for each of the trap densities.

STUDY 1

Step 2: Stationary 2

In the **Study** toolbar, click **Study Steps** and choose **Stationary>Stationary**.

Step 1: Stationary

1 In the **Model Builder** window, click **Step 1: Stationary**.

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

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

4 In the tree, select **Component 1 (comp1)>Semiconductor (semi)>Trap-Assisted Surface Recombination 1**.

5 Click **Disable**.

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

7 Click **Add**.

8 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Nt_0 (Trap density)	`0`	`1/m^2`

9 Click **Add**.

10 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
ramp (Ramp parameter)	`1e-6 1e-4 1e-3 1e-2 1`	

11 From the **Sweep type** list, choose **All combinations**.

Step 2: Stationary 2

1 In the **Model Builder** window, click **Step 2: Stationary 2**.

2 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.

3 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
Vg (Gate voltage)	`-0.49`	`V`

7 Click **Add**.

8 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Nt_0 (Trap density)	`0 100e14 500e14`	`1/m^2`

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

10 In the **Settings** window for **Study**, locate the **Study Settings** section.

11 Clear the **Generate default plots** check box.

12 In the **Label** text field, type `Study 1: Ramp doping and traps`.

13 In the **Study** toolbar, click **Compute**.

Check the doping has the correct form.

RESULTS

2D Plot Group 1

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

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

3 From the **Parameter value (Nt_0 (1/m^2))** list, choose **0**.

Surface 1

1 Right-click **2D Plot Group 1** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Semiconductor>Carriers and dopants>semi.Ndoping - Signed ionized dopant concentration - 1/m³**.

3 Locate the **Expression** section. In the **Unit** field, type `1/cm^3`.

4 Click to expand the **Quality** section. From the **Resolution** list, choose **No refinement**.

5 From the **Smoothing** list, choose **Everywhere**.

6 In the **2D Plot Group 1** toolbar, click **Plot**.

7 Click the **Zoom Extents** button in the **Graphics** toolbar.

Doping

1 In the **Model Builder** window, under **Results** click **2D Plot Group 1**.

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

Add studies to sweep the gate voltage at different trap densities.

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 **General Studies>Stationary**.

4 Right-click and choose **Add Study**.

5 In the **Select Study** tree, select **General Studies>Stationary**.

6 Right-click and choose **Add Study**.

7 In the **Select Study** tree, select **General Studies>Stationary**.

8 Right-click and choose **Add Study**.

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

STUDY 2

Step 1: Stationary

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

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

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

4 From the **Study** list, choose **Study 1: Ramp doping and traps, Stationary 2**.

5 From the **Parameter value (Nt_0 (1/m^2),Vg (V))** list, choose **1: Nt_0=0 1/m^2, Vg=-0.49 V**.

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

7 From the **Sweep type** list, choose **All combinations**.

8 Click **Add**.

9 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Nt_0 (Trap density)	0	1/m^2

10 Click **Add**.

11 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vg (Gate voltage)	`range(-0.5,0.1,1.5)`	V

For assistance in entering ranges of different kinds in the **Parameter value list** column, click the **Range** button to launch the **Range** dialog.

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

13 In the **Settings** window for **Study**, locate the **Study Settings** section.

14 Clear the **Generate default plots** check box.

15 In the **Label** text field, type `Study 2: Vg sweep no traps`.

STUDY 3: VG SWEEP NT=1E12[1/CM^2]

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

2 In the **Settings** window for **Stationary**, locate 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: Ramp doping and traps, Stationary 2**.

6 From the **Parameter value (Nt_0 (1/m^2),Vg (V))** list, choose **2: Nt_0=1E16 1/m^2, Vg=-0.49 V**.

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

8 From the **Sweep type** list, choose **All combinations**.

9 Click **+ Add**.

10 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Nt_0 (Trap density)	`1e16`	`1/m^2`

11 Click **+ Add**.

12 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vg (Gate voltage)	`range(-0.5,0.1,1.5)`	`V`

For assistance in entering ranges of different kinds in the **Parameter value list** column, click the **Range** button to launch the **Range** dialog.

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

14 In the **Settings** window for **Study**, locate the **Study Settings** section.

15 Clear the **Generate default plots** check box.

16 In the **Label** text field, type `Study 3: Vg sweep Nt=1e12[1/cm^2]`.

STUDY 4: VG SWEEP NT=5E12[1/CM^3]

1 In the **Model Builder** window, under **Study 4** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate 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: Ramp doping and traps, Stationary 2**.

6 From the **Parameter value (Nt_0 (1/m^2),Vg (V))** list, choose **3: Nt_0=5E16 1/m^2, Vg=-0.49 V**.

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

8 From the **Sweep type** list, choose **All combinations**.

9 Click **Add**.

10 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Nt_0 (Trap density)	`5e16`	`1/m^2`

11 Click **Add**.

12 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vg (Gate voltage)	`range(-0.5,0.1,1.5)`	`V`

For assistance in entering ranges of different kinds in the **Parameter value list** column, click the **Range** button to launch the **Range** dialog.

13 In the **Model Builder** window, click **Study 4**.

14 In the **Settings** window for **Study**, locate the **Study Settings** section.

15 Clear the **Generate default plots** check box.

16 In the **Label** text field, type `Study 4: Vg sweep Nt=5e12[1/cm^3]`.

STUDY 2: VG SWEEP NO TRAPS

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

STUDY 3: VG SWEEP NT=1E12[1/CM^2]

Click **Compute**.

STUDY 4: VG SWEEP NT=5E12[1/CM^3]

Click **Compute**.

RESULTS

1D Plot Group 2

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

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** check box. In the associated text field, type `Gate voltage, Vg (V)`.

6 Select the **y-axis label** check box. In the associated text field, type `Current (A)`.

7 Locate the **Axis** section. Select the **y-axis log scale** check box.

8 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Global 1

1 Right-click **1D Plot Group 2** and choose **Global**.

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

3 From the **Dataset** list, choose **Study 2: Vg sweep no traps/Solution 3 (sol3)**.

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

Expression	Unit	Description
`abs(semi.I0_1)`	`A`	`Nt_0 = 0 1/cm^2`

5 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Description** check box.

6 In the **1D Plot Group 2** toolbar, click **Plot**.

7 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: Vg sweep Nt=1e12[1/cm^2]/Solution 4 (sol4)**.

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

Expression	Unit	Description
`abs(semi.I0_1)`	`A`	`Nt_0 = 1e-12 1/cm^2`

5 In the **1D Plot Group 2** toolbar, click **Plot**.

6 Right-click **Global 2** 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 4: Vg sweep Nt=5e12[1/cm^3]/Solution 5 (sol5)**.

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

Expression	Unit	Description
abs(semi.I0_1)	A	Nt_0 = 5e-12 1/cm^2

5 In the **1D Plot Group 2** toolbar, click **Plot**.

Current vs. gate voltage

1 In the **Model Builder** window, under **Results** click **1D Plot Group 2**.

2 In the **Settings** window for **1D Plot Group**, type `Current vs. gate voltage` in the **Label** text field.

Add a plot to show the current density, carrier concentrations and potential in the nanowire.

2D Plot Group 3

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

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

3 From the **Dataset** list, choose **Study 4: Vg sweep Nt=5e12[1/cm^3]/Solution 5 (sol5)**.

4 From the **Parameter value (Vg (V))** list, choose **1.5**.

5 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

Surface 1

1 Right-click **2D Plot Group 3** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Semiconductor>Electric>V - Electric potential - V**.

3 Locate the **Quality** section. From the **Resolution** list, choose **No refinement**.

4 From the **Smoothing** list, choose **Everywhere**.

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

Surface 2

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

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

3 Click **Change Color Table**.

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

5 Click **OK**.

6 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Semiconductor>Carriers and dopants>Electrons>semi.log10N - Log of electron concentration - 1**.

Deformation 1

1. Right-click **Surface 2** and choose **Deformation**.
2. In the **Settings** window for **Deformation**, locate the **Expression** section.
3. In the **R-component** text field, type `-20`.
4. Locate the **Scale** section.
5. Select the **Scale factor** check box. In the associated text field, type `1`.

Surface 2

Right-click **Surface 2** and choose **Duplicate**.

Surface 3

1. In the **Model Builder** window, click **Surface 3**.
2. In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Semiconductor>Carriers and dopants>Holes>semi.log10P - Log of hole concentration - 1**.

Deformation 1

1. In the **Model Builder** window, expand the **Surface 3** node, then click **Deformation 1**.
2. In the **Settings** window for **Deformation**, locate the **Expression** section.
3. In the **R-component** text field, type `-40`.
4. In the **2D Plot Group 3** toolbar, click **Plot**.

Surface 3

In the **Model Builder** window, right-click **Surface 3** and choose **Duplicate**.

Surface 4

1. In the **Model Builder** window, click **Surface 4**.
2. In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Semiconductor>Currents and charge>semi.log10normJ - Log of current density norm - 1**.
3. Locate the **Coloring and Style** section. Click **Change Color Table**.
4. In the **Color Table** dialog box, select **Thermal>ThermalDark** in the tree.
5. Click **OK**.

Deformation 1

1 In the **Model Builder** window, expand the **Surface 4** node, then click **Deformation 1**.

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

3 In the **R-component** text field, type `-60`.

4 In the **2D Plot Group 3** toolbar, click **Plot**.

5 Click the **Zoom Extents** button in the **Graphics** toolbar.

J, P, N, V

1 In the **Model Builder** window, under **Results** click **2D Plot Group 3**.

2 In the **Settings** window for **2D Plot Group**, type `J, P, N, V` in the **Label** text field.

Add a plot to show the current along the mid line.

1D Plot Group 4

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

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

3 From the **Dataset** list, choose **Study 3: Vg sweep Nt=1e12[1/cm^2]/Solution 4 (sol4)**.

Line Graph 1

1 Right-click **1D Plot Group 4** and choose **Line Graph**.

2 Select Boundary 6 only.

3 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Semiconductor>Currents and charge>semi.normJ - Total current density norm, nodal value - A/m²**.

4 Click to expand the **Quality** section. From the **Resolution** list, choose **No refinement**.

5 From the **Smoothing** list, choose **Everywhere**.

6 In the **1D Plot Group 4** toolbar, click **Plot**.

Current along mid line

1 In the **Model Builder** window, under **Results** click **1D Plot Group 4**.

2 In the **Settings** window for **1D Plot Group**, type `Current along mid line` in the **Label** text field.

Add a plot to show the voltage along the mid line.

1D Plot Group 5

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

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

3 From the **Dataset** list, choose **Study 2: Vg sweep no traps/Solution 3 (sol3)**.

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

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

Line Graph 1

1 Right-click **1D Plot Group 5** and choose **Line Graph**.

2 Select Boundary 6 only.

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

4 In the **Expression** text field, type `V`.

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

6 From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
`Nt_0 = 0.0 1/cm^2`

8 Locate the **Quality** section. From the **Resolution** list, choose **No refinement**.

9 From the **Smoothing** list, choose **Everywhere**.

10 In the **1D Plot Group 5** toolbar, click **Plot**.

11 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 **Data** section.

3 From the **Dataset** list, choose **Study 3: Vg sweep Nt=1e12[1/cm^2]/Solution 4 (sol4)**.

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

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

Legends
`Nt_0 = 1.0E12 1/cm^2`

6 Right-click **Line Graph 2** and choose **Duplicate**.

Line Graph 3

1 In the **Model Builder** window, click **Line Graph 3**.

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

3 From the **Dataset** list, choose **Study 4: Vg sweep Nt=5e12[1/cm^3]/Solution 5 (sol5)**.

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

Legends
`Nt_0 = 5.0E12 1/cm^2`

5 In the **1D Plot Group 5** toolbar, click **Plot**.

Voltage along mid line

1 In the **Model Builder** window, click **1D Plot Group 5**.

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

3 From the **Title type** list, choose **None**.

4 In the **1D Plot Group 5** toolbar, click **Plot**.

5 In the **Label** text field, type `Voltage along mid line`.

Add a plot to show the band diagram along the mid line.

1D Plot Group 6

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

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

3 From the **Dataset** list, choose **Study 4: Vg sweep Nt=5e12[1/cm^3]/Solution 5 (sol5)**.

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

Line Graph 1

1 Right-click **1D Plot Group 6** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Semiconductor>Fermi levels and band edges>Energies>semi.Ec_e - Conduction band energy level - J**.

3 Locate the **y-Axis Data** section. From the **Unit** list, choose **eV**.

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

5 In the **Expression** text field, type `r`.

6 Locate 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
`Conduction band`

9 Locate the **Quality** section. From the **Resolution** list, choose **No refinement**.

10 From the **Smoothing** list, choose **Everywhere**.

11 Select Boundary 6 only.

12 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**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Semiconductor>Fermi levels and band edges>Energies>semi.Ev_e - Valence band energy level - J**.

3 Locate the **Legends** section. In the table, enter the following settings:

Legends
`Valence band`

4 In the **1D Plot Group 6** toolbar, click **Plot**.

5 Right-click **Line Graph 2** and choose **Duplicate**.

Line Graph 3

1 In the **Model Builder** window, click **Line Graph 3**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Semiconductor>Fermi levels and band edges>Energies>semi.Efn_e - Electron quasi-Fermi energy level - J**.

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

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

Legends
`Electron quasi-Fermi level`

5 Right-click **Line Graph 3** and choose **Duplicate**.

Line Graph 4

1 In the **Model Builder** window, click **Line Graph 4**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>**

Semiconductor>Fermi levels and band edges>Energies>semi.Efp_e - Hole quasi-Fermi energy level - J.

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

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

Legends
`Hole quasi-Fermi level`

Band diagram along mid line

1 In the **Model Builder** window, click **1D Plot Group 6**.

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

3 From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Energy level diagram`.

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** check box. In the associated text field, type `r (nm)`.

7 Select the **y-axis label** check box. In the associated text field, type `Energy`.

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

9 In the **1D Plot Group 6** toolbar, click **Plot**.

10 In the **Label** text field, type `Band diagram along mid line`.

Finally, plot the trap occupancy along the surface of the gate.

1D Plot Group 7

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

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

3 From the **Dataset** list, choose **Study 4: Vg sweep Nt=5e12[1/cm^3]/Solution 5 (sol5)**.

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

5 In the **Parameter values (Vg (V))** list, choose **-0.5**, **0**, and **1**.

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

Line Graph 1

1 Right-click **1D Plot Group 7** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

3 From the **Selection** list, choose **Gate**.

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Semiconductor>Trapping>semi.tasr1.dtb1.ft - Trap occupancy - 1**.

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

6 In the **Expression** text field, type `z`.

7 Locate the **Quality** section. From the **Resolution** list, choose **No refinement**.

8 From the **Smoothing** list, choose **Everywhere**.

9 Locate the **Legends** section. Select the **Show legends** check box.

10 In the **1D Plot Group 7** toolbar, click  **Plot**.

Trap occupancy

1 In the **Model Builder** window, right-click **1D Plot Group 7** and choose **Rename**.

2 In the **Rename 1D Plot Group** dialog box, type `Trap occupancy` in the **New label** text field.

3 Click **OK**.