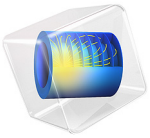


Model created in COMSOL Multiphysics 6.4

Surface-Trap-Induced Hysteresis in an InAs Nanowire FET — a Density-Gradient Analysis

This tutorial analyzes the hysteresis of the conductance–gate-voltage (G–Vg) curves of an InAs nanowire FET, using the density-gradient theory to add the effect of quantum confinement to the conventional drift–diffusion formulation, without a large increase of computational costs. The hysteresis is caused by the dynamic charging effects of fast and slow semiconductor–oxide interface traps of continuous energy distributions and of both donor and acceptor types. The capture probability is modeled as thermally activated with a barrier height that varies with the trap energy level. The qualitative behavior and the order of magnitude of the computed G–Vg curves under various voltage ramping conditions agree well with simulation and experiment results found in the literature.

Introduction

The effect of surface states plays an important role on the electronic behavior of nanowires. This tutorial follows the approach described in the reference paper (Ref. 1) to compute the conductance as a function of the gate voltage history of an InAs nanowire FET. Instead of solving Schrödinger–Poisson equations, the density-gradient theory (as reviewed in Ref. 2) is used to add the effect of quantum confinement in a computationally efficient manner.

Model Definition

The model computes the conductance and the Fermi level relative to the conduction band edge, to be compared with Fig. 3 in Ref. 1.

The Semiconductor interface is used to describe the governing physics. This approach is not exactly the same but is in close correspondence with the one described in Ref. 1 (more details later). Some parameters for our approach have to be guessed. In particular, the bulk material properties of InAs are taken from Ref. 3 and the density-gradient oxide barrier parameters from Ref. 4. The section Modeling Instructions lists all the parameters used in the model. The density-gradient parameters are directly entered in the physics features.

In the experiment reported in Ref. 1, the gate voltage is held at an initial voltage for a long time for the system to reach equilibrium. Then the gate voltage (Vg) is ramped to a peak or valley voltage and then immediately ramped back to the initial voltage. During this voltage ramp, the conductance (G) is measured and recorded. Different voltage ramp rates are used. The G–Vg curves show different degrees of hysteresis, with slower ramps showing larger hysteresis.

Three representative gate voltage ramping conditions are simulated in this model, as shown in the table below, to be compared with Fig. 3 in Ref. 1.

TABLE 1: GATE VOLTAGE RAMPING CONDITIONS SIMULATED IN THE MODEL

CONDITION	1	2	3
Ramp rate (dVdt)	44 uV/s	27 mV/s	27 mV/s
Initial voltage (V0)	6 V	-4 V	6 V
Peak/Valley voltage (V1)	-4 V	6 V	-4 V

In Ref. 1, the hexagonal InAs nanowire is approximated as an infinitely long cylinder to be modeled in 1D axial symmetric geometry. Comparing to the time scales of the voltage ramps, the carriers in the bulk are assumed to be instantaneously equilibrated, while the dynamics of the surface traps is simulated using time-dependent equations. In the tutorial model, on the other hand, everything is treated as time dependent and a grounded metal contact is placed at the center axis of the cylinder. This achieves the same instantaneous equilibrium for the carriers in the bulk.

In Ref. 1, the conductance is computed from the electron density divided by a weighted sum of the ionized surface trap densities to account for their scattering effects. The electron density is computed by summing quantized 1D subbands and the hole density using the bulk 3D formula. In the tutorial model, both carrier types are treated as bulk 3D, and the density-gradient formulation is used to include the quantum confinement effect. In addition, the zero-density-gradient boundary condition of the density-gradient formulation at metal contacts helps maintaining a reasonable carrier density profile at the center axis of the cylinder.

The gate contact boundary condition in the model incorporates the effective oxide relative permittivity and effective oxide thickness using the formulas given in Ref. 1. The properties of the four different types of surface traps are all provided by the reference paper and entered into the model accordingly.

See the comments in the section Modeling Instructions for more detailed discussions on the model construction, solution processes, and result visualization.

Results and Discussion

Figure 1 shows the simulated conductance as a function of the gate voltage, to be compared with Fig. 3(a) and (b) in Ref. 1. The hysteresis and order of magnitude match reasonably well with the experiment and model results shown in the reference paper.

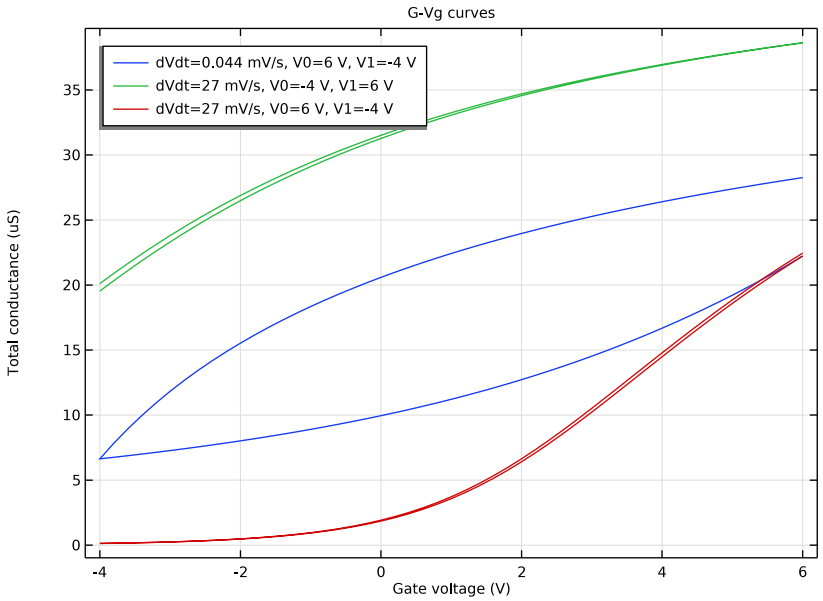


Figure 1: Conductance versus gate voltage curves.

Figure 2 plots the Fermi level relative to the conduction band edge versus the gate voltage, to be compared with Fig. 3(c) in the reference paper. The general trend and order of magnitude match reasonably well.

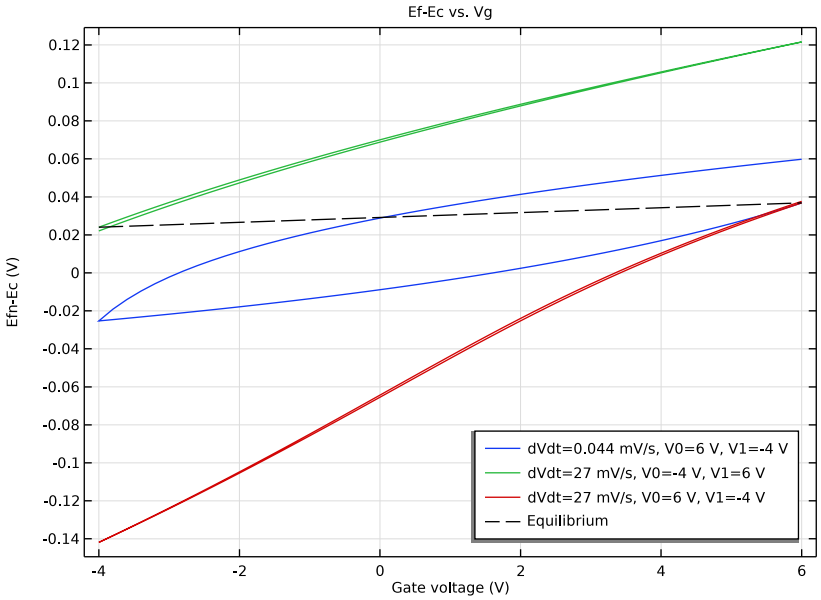


Figure 2: Fermi level versus gate voltage.

References

1. D. Lynall and others, "Surface state dynamics dictating transport in InAs nanowires," *Nano Letters*, vol. 18, no. 2, p. 1387, 2018.

2. M.G. Ancona, "Density-gradient theory: a macroscopic approach to quantum confinement and tunneling in semiconductor devices," *J. Comput. Electron.*, vol. 10, p. 65, 2011.

3. M. Levinshtein, S. Rumyantsev, and M. Shur, *Handbook Series on Semiconductor Parameters*, vol. 1, World Scientific, 1996, reprinted 2000.

4. S. Jin, Y.J. Park, and H.S. Min, "Simulation of Quantum Effects in the Nano-scale Semiconductor Device," *J. Semicond. Tech. Sci.*, vol. 4, no. 1, p. 32, 2004.

Application Library path: `Semiconductor_Module/Transistors/inas_nanowire_traps_hysteresis_density_gradient`

Modeling Instructions

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

NEW

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

MODEL WIZARD

1. In the **Model Wizard** window, Approximate the nanowire as an infinitely long cylinder using the 1D axial symmetric geometry.
2. click **1D Axisymmetric**.
3. In the **Select Physics** tree, select **Semiconductor** > **Semiconductor (semi)**.
4. Click **Add**.

   Use the Semiconductor Equilibrium study step to simulate the initial condition of the experiment after the sample has been biased at a fixed gate voltage for a long time.
5. Click **Study**.
6. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces** > **Semiconductor Equilibrium**.
7. Click **Done**.

GEOMETRY 1

The Model Wizard exits and opens the Model Builder desktop environment at the Geometry node. Set the length scale here right away.

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

Next, enter model parameters. Use separate Parameters nodes to organize the parameters in different categories, beginning with the nanowire parameters: the radius, length, temperature, and gate oxide parameters are from Ref. 1. The semiconductor material

parameters are guess values using bulk material properties. The series conductance is also a guess value which in the paper was a fitting parameter to account for other effects such as the contact resistances.

Parameters 1 - Nanowire FET

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

2 In the **Settings** window for **Parameters**, type `Parameters 1 - Nanowire FET` in the **Label** text field.

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

Name	Expression	Value	Description
R0	23[nm]	2.3E-8 m	Radius of nanowire
L0	1.6[um]	1.6E-6 m	Length of nanowire FET channel
mun0	4e4[cm^2/V/s]	4 m²/(V·s)	Electron mobility
mup0	5e2[cm^2/V/s]	0.05 m²/(V·s)	Hole mobility
epsr0	15.15	15.15	Relative permittivity
Eg00	0.354[V]	0.354 V	Band gap
chi00	4.9[V]	4.9 V	Electron affinity
Nc0	8.7e16[cm^-3]	8.7E22 1/m³	Conduction band effective density of state
Nv0	6.6e18[cm^-3]	6.6E24 1/m³	Valence band effective density of state
T0	300[K]	300 K	Temperature
d_ox0	100[nm]	1E-7 m	Thickness of gate oxide
d_ox	d_ox0*acosh((d_ox0+R0)/R0)	2.361E-7 m	Effective thickness of gate oxide
epsr_ox	2.12	2.12	Effective relative permittivity of gate oxide
G_s	50[uS]	5E-5 S	Series conductance

Hide these parameters from parameter selections, such as for parametric sweeps, to make it easier to set up the studies later with a smaller number of parameters to choose from.

4 Click to expand the **Visibility** section. Clear the **Show in parameter selections** checkbox.

Next, enter the trap parameters from Ref. 1 in a new Parameters node and hide also these ones from study settings.

Parameters 2 - Surface Traps

1 In the **Home** toolbar, click **Parameters** and choose **Add** > **Parameters**.

2 In the **Settings** window for **Parameters**, type `Parameters 2 - Surface Traps` in the **Label** text field.

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

Name	Expression	Value	Description
Ds_tot	4e13[cm^-2]	4E17 1/m²	Total trap density
Ds_f	1.6e12[cm^-2]	1.6E16 1/m²	Fast trap density
Ds_s	Ds_tot-Ds_f	3.84E17 1/m²	Slow trap density
Ea0_f	0[mV]	0 V	Emission barrier parameter of fast trap
Ea0_s	700[mV]	0.7 V	Emission barrier parameter of slow trap
gamma0	1e6[1/s]	1E6 1/s	Capture rate constant
Et0_a	-400[mV]	-0.4 V	Center of acceptor trap energy level distribution below Ec (negative value means above Ec, that is, inside the conduction band)
Et0_d	300[mV]	0.3 V	Center of donor trap energy level distribution below Ec
sig0	200[mV]	0.2 V	Width of trap energy level distribution
gD0	2	2	Degeneracy factor

4 Locate the **Visibility** section. Clear the **Show in parameter selections** checkbox.

Before entering the remaining parameters, define a triangle function to be used in the subsequent parameter definition for the ramping of the gate voltage.

Triangle 1 (tri1)

1 In the **Home** toolbar, click **Functions** and choose **Global** > **Triangle**.

2 In the **Settings** window for **Triangle**, locate the **Parameters** section.

3 In the **Lower limit** text field, type `0`.

4 In the **Upper limit** text field, type `1`.

5 Click to expand the **Smoothing** section. Clear the **Size of transition zone** checkbox.

Now define the parameters for the gate voltage bias conditions of the experiment. Use the triangle function to define the voltage sweep as a function of time: the gate voltage `Vg` is swept from `V0` to `V1` and then back to `V0` at the ramp rate of `dVdt`. Leave this set of parameters visible for study settings.

Parameters 3 - Bias Conditions

1 In the **Home** toolbar, click **Parameters** and choose **Add** > **Parameters**.

2 In the **Settings** window for **Parameters**, type `Parameters 3 - Bias Conditions` in the **Label** text field.

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

Name	Expression	Value	Description
dVdt	44[uV/s]	4.4E-5 V/s	Voltage ramp rate
V0	6[V]	6 V	Initial and final voltage of triangular voltage ramp
V1	-4[V]	-4 V	Peak (or valley) voltage of triangular voltage ramp
t	0[s]	0 s	Time parameter
t_max	2*abs(V1-V0)/dVdt	4.5455E5 s	Duration of voltage ramp
Vg	V0+(V1-V0)*tri1(t/t_max)	6 V	Gate voltage

To approximate the nanowire as an infinitely long cylinder using the 1D axial symmetric geometry, simply add a line interval with the length set to the radius of the cylinder `R0`.

GEOMETRY 1

Interval 1 (i1)

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

2 In the **Settings** window for **Interval**, locate the **Interval** section.

3 In the table, enter the following settings:

Coordinates (nm)
0
R0

4 Click **Build All Objects**.

Add a blank material and enter the parameters for the semiconductor material properties defined earlier.

MATERIALS

Material 1 (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

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

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Electron mobility	mun	mun0	m²/(V·s)	Semiconductor material
Hole mobility	mup	mup0	m²/(V·s)	Semiconductor material
Relative permittivity	epsilonr_iso ; epsilonrii = epsilonr_iso, epsilonrij = 0	epsr0	1	Basic
Band gap	Eg0	Eg00	V	Semiconductor material
Electron affinity	chi0	chi00	V	Semiconductor material
Effective density of states, conduction band	Nc	Nc0	1/m³	Semiconductor material
Effective density of states, valence band	Nv	Nv0	1/m³	Semiconductor material

SEMICONDUCTOR (SEMI)

Now set up the physics. Enter the channel length parameter as the out-of-plane thickness. Choose Fermi–Dirac statistics and use the density-gradient formulation to add quantum-confinement effect to the drift–diffusion equation system.

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Semiconductor (semi)**.
2. In the **Settings** window for **Semiconductor**, locate the **Vertical Height** section.
3. In the d text field, type `L0`.
4. Locate the **Model Properties** section. From the **Carrier statistics** list, choose **Fermi–Dirac**.
5. Click to expand the **Discretization** section. From the **Formulation** list, choose **Finite element density-gradient (quadratic shape function)**.

Enter the temperature and some guess values for the density-gradient effective masses.

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 `T0`.
4. Locate the **Material Properties, Density-Gradient** section. In the $\mathbf{m}_e^{DG}$ text field, type `me_const*0.03`.
5. In the $\mathbf{m}_h^{DG}$ text field, type `me_const*0.4`.

Use a metal contact boundary condition at the center of the cylinder to capture the effect of the source and drain contacts used in the experiment, which are located out-of-plane in the 1D axisymmetric geometry for this model. The zero-gradient boundary condition for the carrier concentrations at the metal contact as given by the density-gradient formulation is particularly suitable in the case to approximate the carrier density profile near the origin.

Metal Contact 1

1. In the **Physics** toolbar, click **Boundaries** and choose **Metal Contact**.
2. Select Boundary 1 only.

Add a gate contact boundary condition at the circumference of the cylinder, using the nanowire gate parameters defined earlier and some guess values for the density-gradient formulation of the potential barrier at the semiconductor–oxide interface.

Thin Insulator Gate 1

1. In the **Physics** toolbar, click **Boundaries** and choose **Thin Insulator Gate**.
2. Select Boundary 2 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 `epsr_ox`.

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

7 Locate the **Density-Gradient** section. From the **Formulation** list, choose **Potential barrier**.

8 In the $\mathbf{m}_e^{Ox}$ text field, type `me_const*0.5`.

9 In the $\mathbf{m}_e^{Ox*}$ text field, type `me_const*0.22`.

10 In the Φ_n^{Ox} text field, type `3[V]`.

11 In the Φ_p^{Ox} text field, type `3[V]`.

Ref. 1 used four kinds of continuous trap energy distributions to simulate the effect of traps at the semiconductor–oxide interface. This can be done in the model using a **Trap-Assisted Surface Recombination** physics node with four **Continuous Energy Levels** subnodes. First add the parent physics node. Use the **Trap occupancy** formulation which works better for time-dependent studies.

Trap-Assisted Surface Recombination 1

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

2 Select Boundary 2 only.

3 In the **Settings** window for **Trap-Assisted Surface Recombination**, locate the **Trap-Assisted Recombination** section.

4 From the **Trapping model** list, choose **Explicit trap distribution**.

5 Locate the **Trapping** section. From the list, choose **Specify continuous and/or discrete levels**.

6 Select the **Specify trap species** checkbox.

7 From the **Formulation** list, choose **Trap occupancy**.

Next, add the subnodes using the trap parameters for the fast acceptors defined earlier, except for the electron capture probability. Since the latter varies with the trap energy level, enter it later after having defined some relevant variables. In Ref. 1, the hole capture probability is assumed to be zero. Discretize the continuous trap energy distribution using 100 levels as was done in Ref. 1. In this model the 100 levels are distributed within three standard deviations of the Gaussian distribution to efficiently cover the majority of the traps.

Continuous Energy Levels - Fast Acceptor

1 In the **Physics** toolbar, click **Attributes** and choose **Continuous Energy Levels**.

2 In the **Settings** window for **Continuous Energy Levels**, type `Continuous Energy Levels - Fast Acceptor` in the **Label** text field.

3 Locate the **Trap Type** section. From the **Trap type** list, choose **Acceptor traps**.

4 Locate the **Traps** section. In the N_t text field, type `Ds_f`.

5 From the **Distribution center point** list, choose **From conduction band edge**.

6 In the $E_{t,0}$ text field, type `Et0_a`.

7 In the σ text field, type `sig0`.

8 In the g_D text field, type `gD0`.

9 In the $N^{\mathrm{xd}}_{\mathrm{elem}}$ text field, type `100`.

10 In the $E_{\mathrm{t,min}}$ text field, type `semi.tasr1.Ec0t-Et0_a-3*sig0`.

11 In the $E_{\mathrm{t,max}}$ text field, type `semi.tasr1.Ec0t-Et0_a+3*sig0`.

12 Locate the **Carrier Capture** section. From the **Probability of electron capture** list, choose **User defined**. From the **Probability of hole capture** list, choose **User defined**. In the C_p text field, type `0[cm^3/s]`.

Duplicate the subnode to reuse most settings for the fast donors. Enter the settings that are different for the fast donors: the trap type and the parameter for the center of the trap distribution.

Continuous Energy Levels - Fast Donor

1 Right-click **Continuous Energy Levels - Fast Acceptor** and choose **Duplicate**.

2 In the **Settings** window for **Continuous Energy Levels**, type `Continuous Energy Levels - Fast Donor` in the **Label** text field.

3 Locate the **Trap Type** section. From the **Trap type** list, choose **Donor traps**.

4 Locate the **Traps** section. In the $E_{t,0}$ text field, type `Et0_d`.

5 In the $E_{\mathrm{t,min}}$ text field, type `semi.tasr1.Ec0t-Et0_d-3*sig0`.

6 In the $E_{\mathrm{t,max}}$ text field, type `semi.tasr1.Ec0t-Et0_d+3*sig0`.

Similarly, duplicate the subnodes to reuse most settings and enter the setting that is different between the fast and slow traps: trap number density.

Continuous Energy Levels - Slow Acceptor

1 In the **Model Builder** window, right-click **Continuous Energy Levels - Fast Acceptor** and choose **Duplicate**.

2 In the **Settings** window for **Continuous Energy Levels**, type `Continuous Energy Levels - Slow Acceptor` in the **Label** text field.

3 Locate the **Traps** section. In the N_t text field, type `Ds_s`.

Continuous Energy Levels - Slow Donor

1 In the **Model Builder** window, right-click **Continuous Energy Levels - Fast Donor** and choose **Duplicate**.

2 In the **Settings** window for **Continuous Energy Levels**, type `Continuous Energy Levels - Slow Donor` in the **Label** text field.

3 Locate the **Traps** section. In the N_t text field, type `Ds_s`.

DEFINITIONS (COMP1)

Now define variables for the electron capture probability, which depends on the trap energy level. The dependence is based on an energy barrier between the trap level and the conduction band edge as formulated in Ref. 1. Since the density-gradient formulation reduces the electron density at the semiconductor–oxide interface as the result of quantum confinement, but the actual electron flux should not be reduced by the same factor, a factor `Nfac` with a guess value of 10 is introduced to compensate for the reduced electron density.

Variables 1 - Capture Probabilities

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 1 - Capture Probabilities` in the **Label** text field.

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

Name	Expression	Unit	Description
`dE_fa`	`semi.tasr1.ctb1.Vxd-semi.tasr1.EcOt`	V	`Fast acceptor trap energy level relative to conduction band edge`
`dE_fd`	`semi.tasr1.ctb2.Vxd-semi.tasr1.EcOt`	V	`Fast donor trap energy level relative to conduction band edge`
`dE_sa`	`semi.tasr1.ctb3.Vxd-semi.tasr1.EcOt`	V	`Slow acceptor trap energy level relative to conduction band edge`
`dE_sd`	`semi.tasr1.ctb4.Vxd-semi.tasr1.EcOt`	V	`Slow donor trap energy level relative to conduction band edge`

Name	Expression	Unit	Description
Eb_fa	dE_fa+max(-dE_fa, EaO_f)	V	Fast acceptor trap capture barrier
Eb_fd	dE_fd+max(-dE_fd, EaO_f)	V	Fast donor trap capture barrier
Eb_sa	dE_sa+max(-dE_sa, EaO_s)	V	Slow acceptor trap capture barrier
Eb_sd	dE_sd+max(-dE_sd, EaO_s)	V	Slow donor trap capture barrier
Nfac	10		Compensation factor for electron flux
Cn_fa	gammaO/NcO*exp(-Eb_fa*e_const/k_B_const/TO)*Nfac	m^3/s	Fast acceptor trap electron capture probability
Cn_fd	gammaO/NcO*exp(-Eb_fd*e_const/k_B_const/TO)*Nfac	m^3/s	Fast donor trap electron capture probability
Cn_sa	gammaO/NcO*exp(-Eb_sa*e_const/k_B_const/TO)*Nfac	m^3/s	Slow acceptor trap electron capture probability
Cn_sd	gammaO/NcO*exp(-Eb_sd*e_const/k_B_const/TO)*Nfac	m^3/s	Slow donor trap electron capture probability

SEMICONDUCTOR (SEMI)

Enter the electron capture probabilities defined above into the physics settings.

Continuous Energy Levels - Fast Acceptor

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Semiconductor (semi)** > **Trap-Assisted Surface Recombination 1** click **Continuous Energy Levels - Fast Acceptor**.

2 In the **Settings** window for **Continuous Energy Levels**, locate the **Carrier Capture** section.

3 In the C_n text field, type `Cn_fa`.

Continuous Energy Levels - Fast Donor

1 In the **Model Builder** window, click **Continuous Energy Levels - Fast Donor**.

2 In the **Settings** window for **Continuous Energy Levels**, locate the **Carrier Capture** section.

3 In the C_n text field, type `Cn_fd`.

Continuous Energy Levels - Slow Acceptor

1 In the **Model Builder** window, click **Continuous Energy Levels - Slow Acceptor**.

2 In the **Settings** window for **Continuous Energy Levels**, locate the **Carrier Capture** section.

3 In the C_n text field, type `Cn_sa`.

Continuous Energy Levels - Slow Donor

1 In the **Model Builder** window, click **Continuous Energy Levels - Slow Donor**.

2 In the **Settings** window for **Continuous Energy Levels**, locate the **Carrier Capture** section.

3 In the C_n text field, type `Cn_sd`.

DEFINITIONS (COMPI)

Define variables for the conductance using the formula given in Ref. 1 to account for the ionized impurity scattering effect. First define coupling operators to access the trap variables at the gate and to integrate the computed conductance over the modeling domain. Then define the variables.

Integration 1 - Access Trap Variables at the Gate

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, type `Integration 1 - Access Trap Variables at the Gate` in the **Label** text field.

3 Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 2 only.

5 Locate the **Advanced** section. Clear the **Compute integral in revolved geometry** checkbox.

Integration 2 - Integrate Over the Cylinder

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, type `Integration 2 - Integrate Over the Cylinder` in the **Label** text field.

3 Locate the **Source Selection** section. From the **Selection** list, choose **All domains**.

Variables 2 - Conductance

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

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

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

Name	Expression	Unit	Description
NAm	`-intop1(semi.tasr1.ctb1.rho_tr+semi.tasr1.ctb3.rho_tr)/e_const`	1/m²	`NA- : Ionized acceptor trap density`
NDp	`intop1(semi.tasr1.ctb2.rho_tr+semi.tasr1.ctb4.rho_tr)/e_const`	1/m²	`ND+ : Ionized donor trap density`
G_0	`intop2(mun0*semi.N)*e_const*Ds_tot/(NDp+30*NAm)/L0`	S	`Channel conductance`
G	`1/(1/G_0+1/G_s)`	S	`Total conductance`

STUDY 1 - TWO FAST AND ONE SLOW GATE VOLTAGE RAMPS

The default mesh works fine for this model so you can proceed directly to setting up the studies. Use an outer Parametric Sweep to run two fast and one slow gate voltage ramps as in the abstract panel of Ref. 1.

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

2 In the **Settings** window for **Study**, type `Study 1 - Two Fast and One Slow Gate Voltage Ramps` in the **Label** text field.

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** three times.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
dVdt (Voltage ramp rate)	`44[uV/s] 27[mV/s] 27[mV/s]`	`mV/s`
V0 (Initial and final voltage of triangular voltage ramp)	`6 -4 6`	`V`
V1 (Peak (or valley) voltage of triangular voltage ramp)	`-4 6 -4`	`V`

Note that the list in the **Parameter name** column is populated only with the last set of parameters, as set up earlier.

Add a time-dependent step to run the transient study.

Step 2: Time Dependent

1 In the **Study** toolbar, click **Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `range(0,0.01,1)*t_max`.

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

RESULTS

Net Dopant Concentration (semi)

Because the model has no doping profiles defined, the default plot of net dopant concentration is not needed.

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

Create a G–Vg plot to compare with the simulation and experimental results of Ref. 1. We find a good match of both the qualitative hysteresis behavior and the order of the magnitude of the conductance. Use the model-tree node label as the plot title.

G-Vg curves

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

2 In the **Settings** window for **1D Plot Group**, type `G-Vg curves` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1 - Two Fast and One Slow Gate Voltage Ramps/Parametric Solutions 1 (sol3)**.

4 Click to expand the **Title** section. From the **Title type** list, choose **Label**.

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

Global 1

1 Right-click **G-Vg curves** and choose **Global**.

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

3 In the table, enter the following settings:

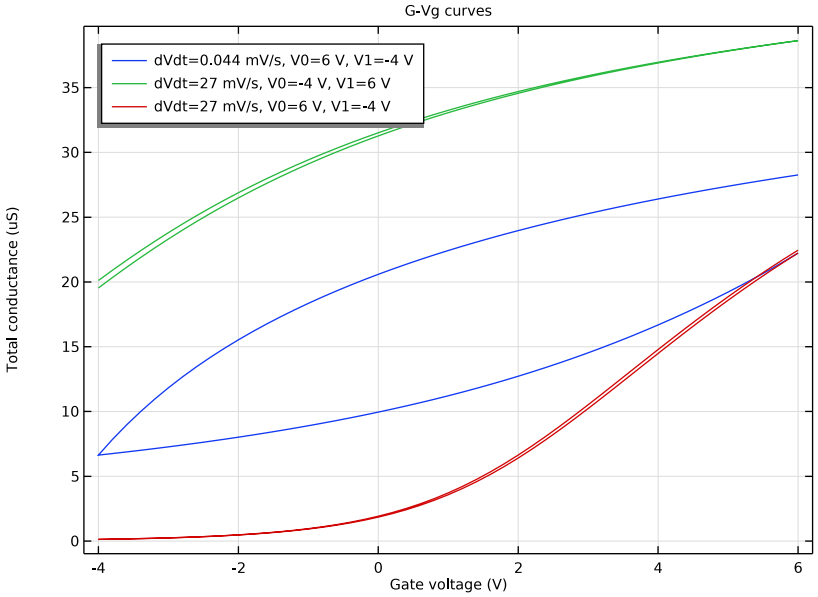
Expression	Unit	Description
G	uS	Total conductance

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

5 In the **Expression** text field, type Vg.

6 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Description** checkbox.

7 In the **G-Vg curves** toolbar, click **Plot**.



Create an Ef–Vg plot to compare with the simulation results of Ref. 1. We again find a good match of both the qualitative hysteresis behavior and the order of the magnitude of the nonequilibrium Fermi level relative to the conduction band edge.

Ef-Ec vs. Vg

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

2 In the **Settings** window for **1D Plot Group**, type Ef-Ec vs. Vg in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1 - Two Fast and One Slow Gate Voltage Ramps/Parametric Solutions 1 (sol3)**.

4 Locate the **Title** section. From the **Title type** list, choose **Label**.

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

Point Graph 1

1 Right-click **Ef-Ec vs. Vg** and choose **Point Graph**.

2 Select Boundary 2 only.

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

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

5 Select the **Description** checkbox. In the associated text field, type `Efn-Ec`.

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

7 In the **Expression** text field, type `Vg`.

8 Click to expand the **Legends** section. Select the **Show legends** checkbox.

9 Find the **Include** subsection. Clear the **Point** checkbox.

10 In the **Ef-Ec vs. Vg** toolbar, click **Plot**.

ADD STUDY

Add a study to compute the equilibrium Fermi level relative to the conduction band edge to add to the Ef–Vg plot to compare with the simulation results of Ref. 1.

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 **Preset Studies for Selected Physics Interfaces** > **Semiconductor Equilibrium**.

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

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

STUDY 2 - EQUILIBRIUM

1 In the **Settings** window for **Study**, type `Study 2 - Equilibrium` in the **Label** text field.

2 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

Step 1: Semiconductor Equilibrium

1 In the **Model Builder** window, under **Study 2 - Equilibrium** click **Step 1: Semiconductor Equilibrium**.

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

3 Select the **Auxiliary sweep** checkbox.

4 Click + **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vg (Gate voltage)	`range(-4,1,6)`	V

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

RESULTS

Point Graph 2

1 In the **Model Builder** window, under **Results** > **Ef-Ec vs. Vg** right-click **Point Graph 1** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Study 2 - Equilibrium/Solution 7 (sol7)**.

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 **Black**.

6 Locate the **Legends** section. Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `Equilibrium`.

7 In the **Ef-Ec vs. Vg** toolbar, click **Plot**.

The results are similar as expected.