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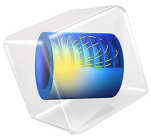


Surface-Trap-Induced Hysteresis in an InAs Nanowire FET — a Density-Gradient Analysis

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.

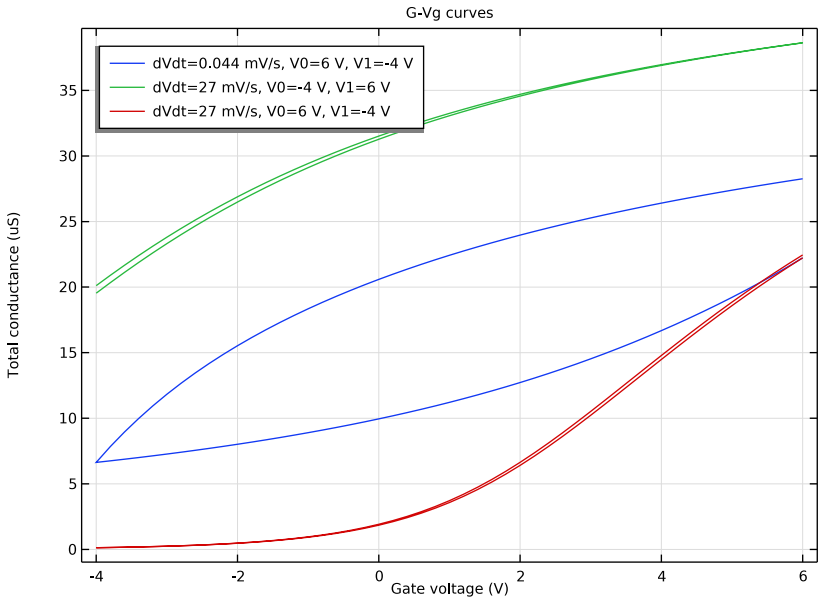


Figure 1: Conductance versus gate voltage curves.

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.

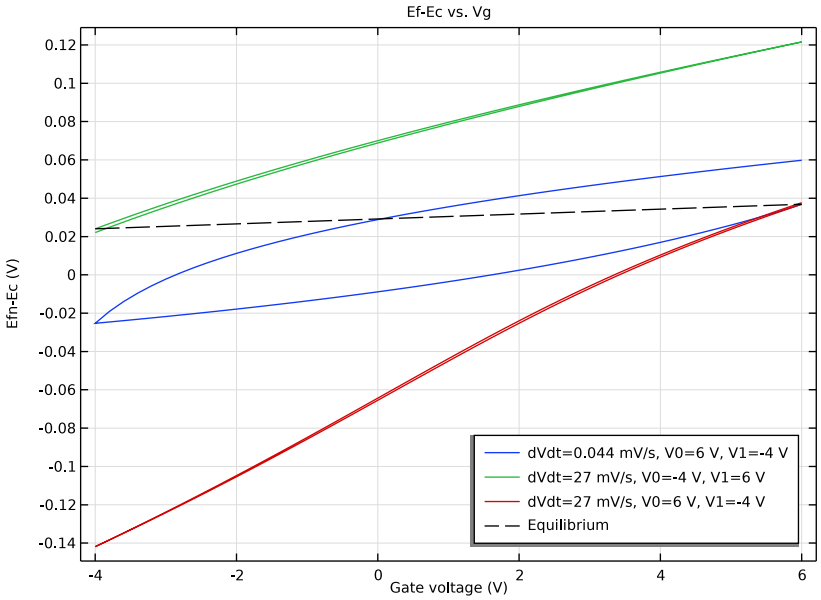


Figure 2: Fermi level versus gate voltage.

References

1. D. Lynall and others, "Surface State Dynamics Dictating Transport in InAs Nanowires", *Nano Letters*, vol. 18, 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 starts the COMSOL Desktop at the Geometry node. We can 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**.

Enter model parameters. Use a few Parameters nodes to organize the parameters into different categories. First the nanowire parameters. The radius, length, temperature and gate oxide parameters are from the reference paper. 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.

GLOBAL DEFINITIONS

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 study settings such as for parametric sweeps, so that it will be easier to set up the studies later with a smaller number of parameters in the drop-down menu to choose from.

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

Next, enter the trap parameters from the reference paper in a new Parameters node and also hide them 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** check box.

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 f(x) **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** check box.

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 Pi **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`	$m^2/(V \cdot s)$	Semiconductor material
Hole mobility	mup	`mup0`	$m^2/(V \cdot s)$	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`	$1/m^3$	Semiconductor material
Effective density of states, valence band	Nv	`Nv0`	$1/m^3$	Semiconductor material

Set up 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.

SEMICONDUCTOR (SEMI)

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 axial symmetric 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]`.

The reference paper used 4 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 4 **Continuous Energy Levels** subnodes. First add the parent physics node. Use the **Trap occupancy** formulation which works better with 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** check box.

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

Then add the subnodes using the trap parameters for fast acceptors defined earlier, except for the electron capture probability which varies with the trap energy level. So we will define variables for that and enter it later. The hole capture probability is assumed to be zero by the reference paper. Discretize the continuous trap energy distribution using 100 levels as was done in the reference paper. In this model the 100 levels are distributed within 3 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.

13 Right-click **Continuous Energy Levels - fast acceptor** and choose **Duplicate**.

Continuous Energy Levels - fast donor

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

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 - fast acceptor

In the **Model Builder** window, right-click **Continuous Energy Levels - fast acceptor** and choose **Duplicate**.

Continuous Energy Levels - slow acceptor

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

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 - fast donor

In the **Model Builder** window, right-click **Continuous Energy Levels - fast donor** and choose **Duplicate**.

Continuous Energy Levels - slow donor

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

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`.

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 the reference paper. 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.

DEFINITIONS (COMP1)

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

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

SEMICONDUCTOR (SEMI)

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`.

Define variables for the conductance using the formula given in the reference paper 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.

DEFINITIONS (COMP1)

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** check box.

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`

The default mesh works fine for this model. Set up the studies. Use an outer Parametric Sweep to run two fast and one slow gate voltage ramps as in the abstract panel of the reference paper. Note how the parameter drop-down menu is populated only with the last set of parameters visible as we have set up earlier. Add the time dependent step to run the transient study.

STUDY 1 - TWO FAST AND ONE SLOW GATE VOLTAGE RAMPS

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**.

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`

5 Click **Add**.

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
V0 (Initial and final voltage of triangular voltage ramp)	6 -4 6	V

7 In the table, click to select the cell at row number 2 and column number 3.

8 Click + **Add**.

9 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
V1 (Peak (or valley) voltage of triangular voltage ramp)	-4 6 -4	V

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

Step 2: Time Dependent

1 In the **Study** toolbar, click **Study Steps** and choose **Time Dependent>** **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)

The model has a no doping profiles defined, therefore the default generated plot, 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 simulation and experiment results shown in the reference paper. We find a good match of both the qualitative hysteresis behavior and the order of the magnitude of the conductance. Use the Model Builder tree node label as the plot title.

G-Vg curves

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

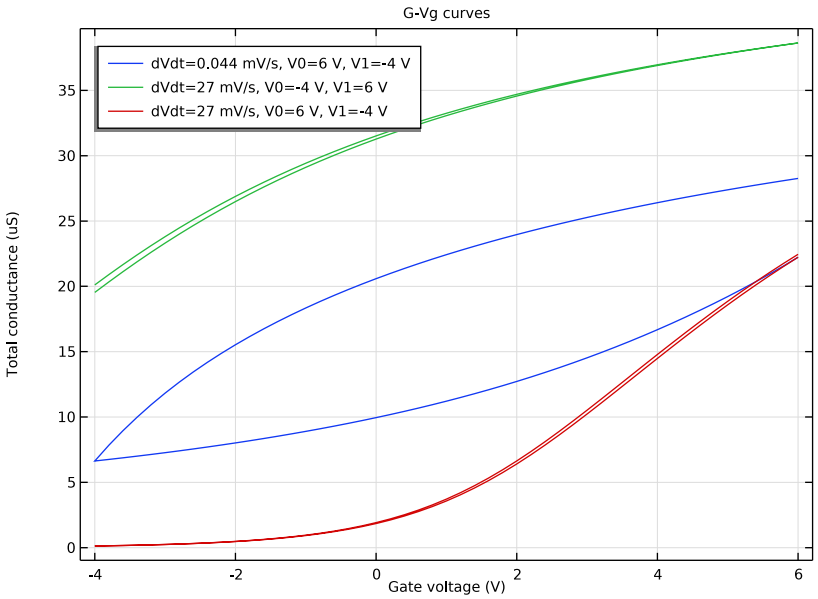
Expression	Unit	Description
G	uS	Total conductance

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** check box.

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



Create an Ef-Vg plot to compare with simulation results shown in the reference paper. 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 **Home** toolbar, click **Add Plot Group** and choose **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** check box. 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** check box.

9 Find the **Include** subsection. Clear the **Point** check box.

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

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 simulation results shown in the reference paper - the results are similar as expected. Disable default plots for this study to keep the Results branch of the Model Builder tree simple.

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

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

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

STUDY 2 - EQUILIBRIUM

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

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

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

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** check box.

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

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

RESULTS

Point Graph 1

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

Point Graph 2

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

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**.