



Model created in COMSOL Multiphysics 6.4

# Interface Trapping Effects of a MOSCAP



This tutorial compares experimental data from the literature with a COMSOL model of a MOSCAP with interface traps (surface states). The Trap-Assisted Surface Recombination feature is used to simulate the effects of the trap charges and the processes of carrier capturing and emitting by the traps. The effect of the fixed charges in the gate oxide is also included. The computed values of the capacitance and conductance as functions of the gate voltage and frequency reproduce the qualitative behavior of the experimental data with comparable magnitudes. The model uses the quasi-Fermi level formulation and shows how to plot quantities such as the trap occupancy as a function of the energy.

### *Introduction*

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The metal–silicon–oxide (MOS) structure is the fundamental building block for many silicon planar devices. In a practical interface between the silicon and the oxide, defects and dangling bonds form interface traps (surface states) that can affect the charge transport by capturing and emitting carriers, and can affect the electrostatics via the net surface charge density of the traps. In addition, fixed charges in the oxide also affect the electrostatics. This tutorial constructs a simple 1D model of a MOS capacitor (MOSCAP) to explore these effects and compare with experimental observations.

### *Model Definition*

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The 1D MOSCAP model is based on the experimental device (the n-type sample) described in Fig. 14 of Ref. 1. The simulation parameters are taken from the nominal experimental values whenever possible, as detailed below.

The experimental samples were prepared with a 10  $\mu\text{m}$  thick epitaxial layer grown on low-resistivity substrates to minimize the effect of the bulk series resistance. In the model the epilayer is assumed to be the same thickness (10  $\mu\text{m}$ ), and the substrate is 2  $\mu\text{m}$  thick, assuming the bulk series resistance can be ignored. The oxide thickness is assumed to be 60 nm, in the middle of the experimental range of 50–70 nm. The diameter of the gate is  $3.8 \cdot 10^{-2}$  cm as given in the figure caption.

The electron mobility is assumed to be constant  $1450 \text{ cm}^2/\text{V}\cdot\text{s}$ . The n-doping concentrations in the epilayer and the substrate are then computed from the experimental values of resistivity of 0.75 and 0.005 ohm-cm, respectively.

The oxide dielectric constant is assumed to be 3.9. The oxide capacitance is then computed from its dielectric constant, thickness, and the gate diameter.

The fixed oxide charge density is  $9 \cdot 10^{11} \text{ cm}^{-2}$  as given by the reference paper.

The trap energy distribution is assumed to be rectangular, with a range of 0.2 eV, centered around the mid-gap. The height of the rectangle is assumed to be  $2 \cdot 10^{11} \text{ cm}^{-2} \text{ eV}^{-1}$ , as suggested by Fig. 15 of the reference paper. For the capture process, the thermal velocity is assumed to be  $10^7 \text{ cm/s}$ , and the cross sections are  $1 \cdot 10^{-15} \text{ cm}^2$  and  $2 \cdot 2 \cdot 10^{-16} \text{ cm}^2$  for the electrons and holes, respectively, as given on the same page as Fig. 15 of the paper.

The metal work function of the gate is assumed to be 4.5 eV.

### Results and Discussion

Figure 1 shows the computed terminal capacitance and the equivalent parallel conductance as functions of the gate voltage to compare with Fig. 23 in Ref. 1. The curves show the same qualitative behavior with comparable magnitudes.

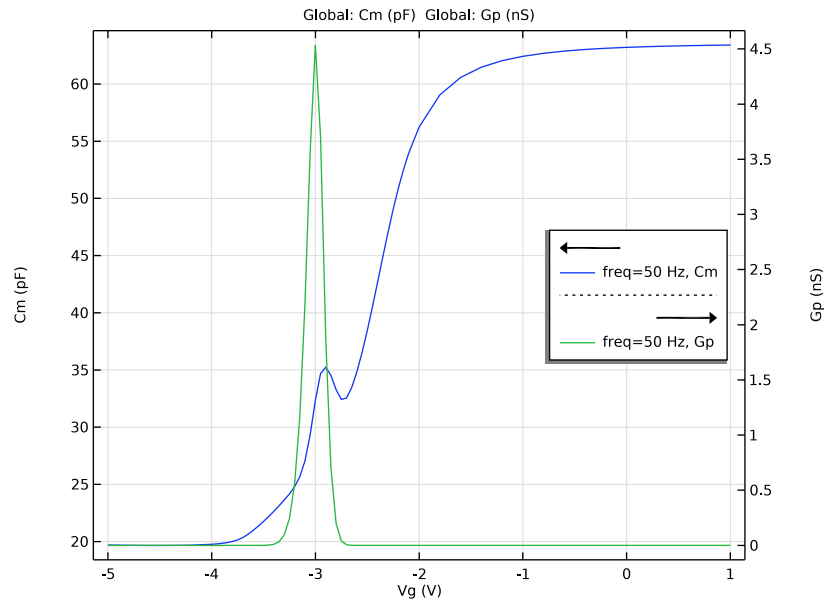


Figure 1:  $C_m$ - $V$  and  $G_p$ - $V$  curves.

Figure 2 shows the computed terminal capacitance and the equivalent parallel conductance as functions of the small signal frequency. The qualitative behavior of the equivalent parallel conductance compares well with Fig. 25 in Ref. 1 (The paper did not include capacitance in the figure.)

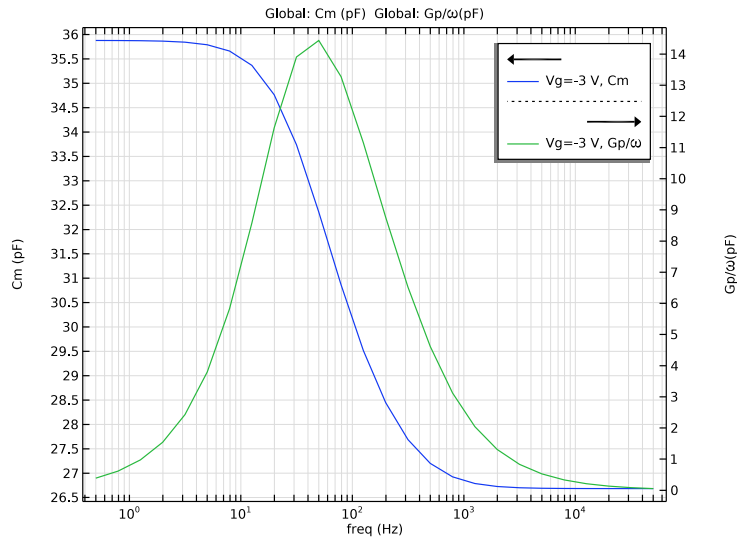


Figure 2: *Cm and Gp vs. frequency.*

Figure 3 shows the rectangular density of states for the traps.

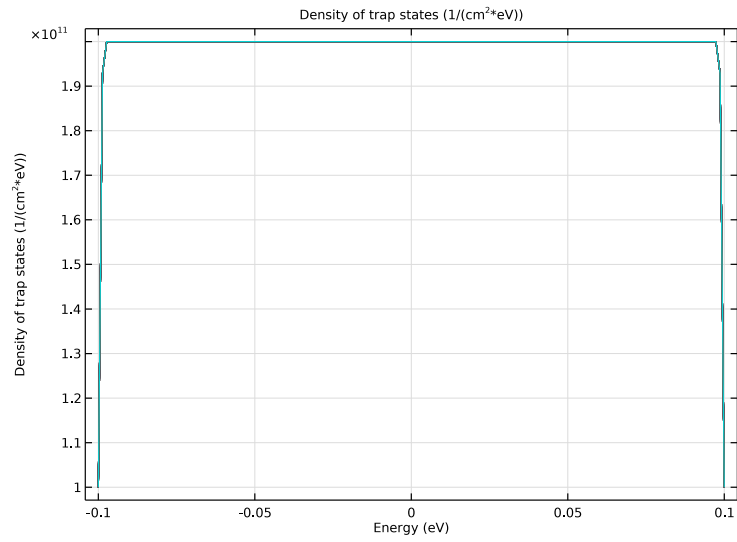


Figure 3: *Density of trap states along the energy axis.*

Figure 4 and Figure 5 shows the trap occupancy to gain some insight on the effect of the traps on the  $C_m$ - $V$  and  $G_p$ - $V$  curves. See the discussions in the section [Modeling Instructions](#) for more details.

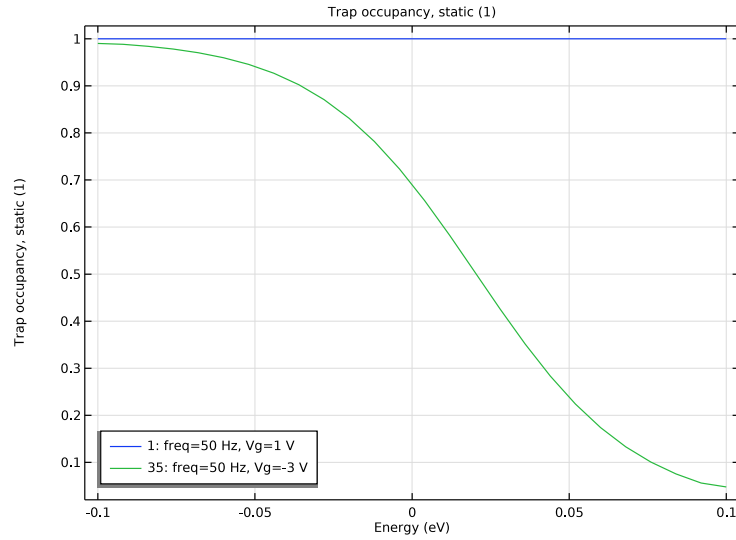


Figure 4: Trap occupancy in the static case.

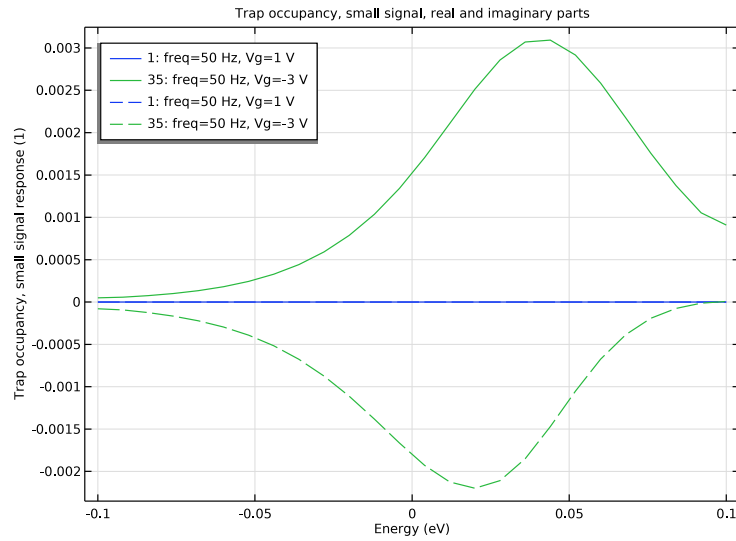


Figure 5: Small signal response of the trap occupancy.

## Reference

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1. E.H. Nicollian and A. Goetzberger, “The Si-SiO<sub>2</sub> interface – electrical properties as determined by the metal-insulator-silicon conductance technique,” *The Bell System Technical Journal*, vol. 46, no. 6, 1967.

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**Application Library path:** Semiconductor\_Module/Device\_Building\_Blocks/moscap\_1d\_interface\_traps


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## Modeling Instructions



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


### NEW

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

### MODEL WIZARD

- 1 In the **Model Wizard** window, click  **ID**.
- 2 In the **Select Physics** tree, select **Semiconductor > Semiconductor (semi)**.
- 3 Click **Add**.
- 4 Click  **Study**.

We will use the **Semiconductor Equilibrium** study to obtain the DC condition, and add a **Frequency Domain Perturbation** step later for the AC small signal analysis.

- 5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces > Semiconductor Equilibrium**.
- 6 Click  **Done**.

### GEOMETRY I


The Model Wizard exits and starts the COMSOL Desktop at the Geometry node. We can set the length scale to um 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 **µm**.

Load parameters and variables from files. The expressions for variables will be yellow-colored because the variable `semi.iomega` will not be available until the **Frequency Domain Perturbation** study step is solved.


## GLOBAL DEFINITIONS

### *Parameters 1*

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
- 2 In the **Settings** window for **Parameters**, locate the **Parameters** section.
- 3 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `moscap_1d_interface_traps_parameters.txt`.

## DEFINITIONS

### *Variables 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, locate the **Variables** section.
- 3 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `moscap_1d_interface_traps_variables.txt`.

Note the use of the `lindv` operator in the variable definitions to evaluate the complex-valued small-signal amplitude of the terminal charge `semi.Q0_2`. Note that when plotting a variable defined with the `lindv` operator, the **Compute differential** checkbox in the plot settings window should be cleared. We will show an example below.

Create line intervals in the geometry to represent the epilayer and the substrate, using the thickness parameters defined above in the **Parameters** node.

## 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 ( $\mu\text{m}$ )
0
t_epi
t_epi+t_sub

Add the default silicon material to the model.

#### ADD MATERIAL

- 1 In the **Materials** 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 Click the **Add to Component** button in the window toolbar.
- 5 In the **Materials** toolbar, click  **Add Material** to close the **Add Material** window.


Enter the cross-section area to the main physics node, and select the **Finite element quasi Fermi level** option for the discretization.

#### SEMICONDUCTOR (SEMI)

- 1 In the **Settings** window for **Semiconductor**, locate the **Cross-Section Area** section.
- 2 In the *A* text field, type area\_g.
- 3 Click to expand the **Discretization** section. From the **Formulation** list, choose **Finite element quasi Fermi level (quadratic shape function)**.

Create doping for the substrate and the epilayer, using the concentration parameters defined above.

#### *Analytic Doping Model 1*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Analytic Doping Model**.
- 2 Select Domain 2 only.
- 3 In the **Settings** window for **Analytic Doping Model**, locate the **Impurity** section.
- 4 From the **Impurity type** list, choose **Donor doping (n-type)**.
- 5 In the  $N_{D0}$  text field, type Nd\_sub.

#### *Analytic Doping Model 2*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Analytic Doping Model**.
- 2 Select Domain 1 only.


- 3 In the **Settings** window for **Analytic Doping Model**, locate the **Impurity** section.
- 4 From the **Impurity type** list, choose **Donor doping (n-type)**.
- 5 In the  $N_{D0}$  text field, type Nd\_epi.

Ground the bottom surface of the substrate and add a **Thin Insulator Gate** boundary condition on the top surface of the epilayer, using parameters defined above for the gate properties.

#### *Metal Contact 1*


- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Metal Contact**.
- 2 Select Boundary 3 only.

#### *Thin Insulator Gate 1*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Thin Insulator Gate**.
- 2 Select Boundary 1 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  $\epsilon_{ins}$  text field, type epsr\_ox.
- 6 In the  $d_{ins}$  text field, type t\_ox.
- 7 In the  $\Phi$  text field, type phiM.


Add a **Harmonic Perturbation** subnode to the gate for the small signal analysis.

#### *Harmonic Perturbation 1*

- 1 In the **Physics** toolbar, click  **Attributes** and choose **Harmonic Perturbation**.
- 2 In the **Settings** window for **Harmonic Perturbation**, locate the **Terminal** section.
- 3 In the  $V_0$  text field, type Vac.


Use a **Surface Charge Density** boundary condition to take into account the fixed charges in the gate oxide.

#### *Surface Charge Density 1*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Surface Charge Density**.
- 2 Select Boundary 1 only.
- 3 In the **Settings** window for **Surface Charge Density**, locate the **Surface Charge Density** section.
- 4 In the  $\rho_s$  text field, type rhos\_ox.


Finally use a **Trap-Assisted Surface Recombination** boundary condition to take into account the effect of the interface traps, which form a continuum of levels around the middle of the band gap.

#### *Trap-Assisted Surface Recombination 1*

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

The **Explicit trap distribution** option requires one or more subnodes to specify the distribution of the trap energy level(s), in order for the boundary condition to take effect.

#### *Continuous Energy Levels 1*

- 1 In the **Physics** toolbar, click  **Attributes** and choose **Continuous Energy Levels**.
- 2 In the **Settings** window for **Continuous Energy Levels**, locate the **Traps** section.
- 3 In the  $N_t$  text field, type  $N_{ss} * E_{w0} * e_{const}$ .
- 4 From the **Trap density distribution** list, choose **Rectangle**.
- 5 In the  $E_w$  text field, type  $E_{w0}$ .
- 6 In the  $\Delta E_{tran}$  text field, type  $E_{w0} / 100$ .


We can shrink the range of discretization to be the same as the one for the rectangle distribution that we have just specified above, to make more efficient use of the extra dimension, which by default approximates the continuous energy distribution by 25 discrete levels distributed within the range. The number of discrete levels can be adjusted using the input field **Continuous energy discretization, number of mesh points**.

- 7 In the  $E_{t,min}$  text field, type  $semi.tasr1.ctb1.Et0 - E_{w0} / 2$ .
- 8 In the  $E_{t,max}$  text field, type  $semi.tasr1.ctb1.Et0 + E_{w0} / 2$ .
- 9 Locate the **Carrier Capture** section. In the  $\sigma <_n >$  text field, type  $sigma_n$ .
- 10 In the  $V_n^{th}$  text field, type  $v\_th$ .
- 11 In the  $V_p^{th}$  text field, type  $v\_th$ .
- 12 In the  $\sigma <_p >$  text field, type  $sigma_p$ .

Set up a user-defined mesh for a better compromise between discretization error and roundoff error.

## **MESH 1**


### *Edge 1*

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

### *Distribution 1*

- 1 Right-click **Edge 1** and choose **Distribution**.
- 2 Select Domain 1 only.
- 3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 4 In the **Number of elements** text field, type 100.

### *Distribution 2*


- 1 In the **Model Builder** window, right-click **Edge 1** and choose **Distribution**.
- 2 Select Domain 2 only.
- 3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 4 In the **Number of elements** text field, type 20.
- 5 Click  **Build All**.

In the first study, we fix the small signal analysis frequency at 50 Hz and sweep the gate voltage from accumulation to inversion.

## **STUDY 1 - VG SWEEP AT 50 HZ**

- 1 In the **Model Builder** window, click **Study 1**.
- 2 In the **Settings** window for **Study**, type Study 1 - Vg sweep at 50 Hz in the **Label** text field.

### *Step 1: Semiconductor Equilibrium*


- 1 In the **Model Builder** window, under **Study 1 - Vg sweep at 50 Hz** 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(1, -0.2, -2) range(-2.1, -0.05, -4) range(-4.2, -0.2, -5)	V

Add a **Frequency Domain Perturbation** study step for the small signal analysis. Make sure to specify the same gate voltage swept values.

*Step 2: Frequency-Domain Perturbation*

- 1 In the **Study** toolbar, click  **More Study Steps** and choose **Frequency Domain > Frequency-Domain Perturbation**.
- 2 In the **Settings** window for **Frequency-Domain Perturbation**, locate the **Study Settings** section.
- 3 In the **Frequencies** text field, type f0.
- 4 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.
- 5 Click **+ Add**.
- 6 In the table, enter the following settings:


Parameter name	Parameter value list	Parameter unit
Vg (Gate voltage)	range(1, -0.2, -2) range(-2.1, -0.05, -4) range(-4.2, -0.2, -5)	V

- 7 In the table, click to select the cell at row number 1 and column number 3.
- 8 In the **Study** toolbar, click  **Compute**.


**RESULTS**

*Energy Levels (semi)*

By default for the **Frequency Domain Perturbation** study step, the plots show the small signal variation of the quantities being plotted. To look at the static solution, either change the list in each of the plots, or just change the dataset for the plot group. We will do the latter for simplicity.


- 1 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 2 From the **Dataset** list, choose **Study 1 - Vg sweep at 50 Hz/Solution Store 1 (sol2)**.
- 3 Locate the **Legend** section. Clear the **Show legends** checkbox.
- 4 In the **Energy Levels (semi)** toolbar, click  **Plot**.

*Carrier Concentrations (semi)*

- 1 In the **Model Builder** window, click **Carrier Concentrations (semi)**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 1 - Vg sweep at 50 Hz/Solution Store 1 (sol2)**.
- 4 Locate the **Legend** section. Clear the **Show legends** checkbox.
- 5 In the **Carrier Concentrations (semi)** toolbar, click  **Plot**.

The plots of the energy levels and carrier concentrations show that the voltage sweep indeed covers the range from accumulation to inversion.

*Electric Potential (semi)*

- 1 In the **Model Builder** window, click **Electric Potential (semi)**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 1 - Vg sweep at 50 Hz/Solution Store 1 (sol2)**.
- 4 In the **Electric Potential (semi)** toolbar, click  **Plot**.


*Net Dopant Concentration (semi)*

The model has a uniform n-doping therefore, we remove the generated default plot, Net Dopant Concentration.

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

Now create a plot for the measured capacitance and the equivalent parallel conductance to compare with Fig. 23 in the reference paper. The two quantities can have different magnitudes. So we will use two separate Global plots and two y-axes; one for each quantity.

*Cm and Gp vs. Vg*

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Cm and Gp vs. Vg in the **Label** text field.

*Global 1*

- 1 Right-click **Cm and Gp vs. Vg** 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
Cm	pF	Cm

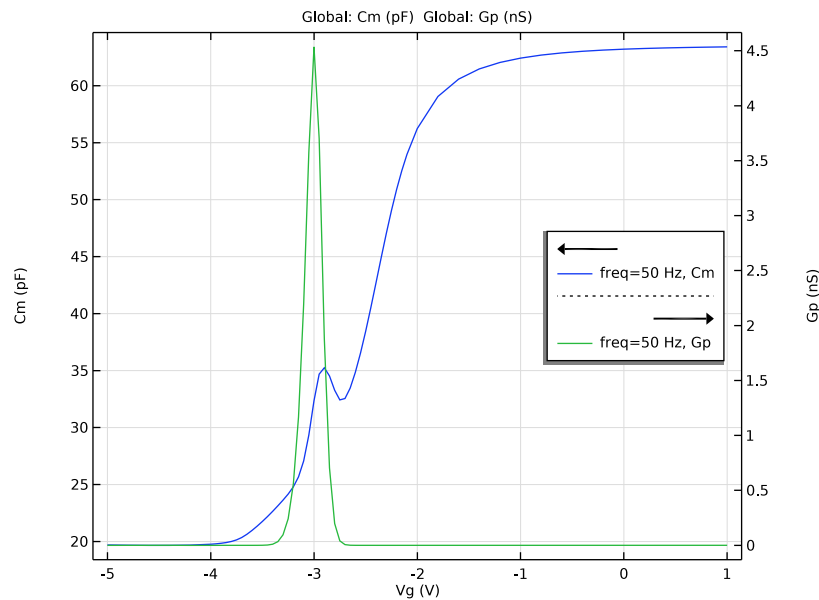
*Global 2*

- 1 In the **Model Builder** window, right-click **Cm and Gp vs. Vg** 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
Gp	nS	Gp

*Cm and Gp vs. Vg*

- 1 In the **Model Builder** window, click **Cm and Gp vs. Vg**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Plot Settings** section.
- 3 Select the **Two y-axes** checkbox.
- 4 In the table, select the **Plot on secondary y-axis** checkbox for **Global 2**.
- 5 Locate the **Legend** section. From the **Position** list, choose **Middle right**.
- 6 In the **Cm and Gp vs. Vg** toolbar, click  **Plot**.





The peaking of the equivalent parallel conductance and the distinct wiggle of the measured capacitance curve are clearly seen to be qualitatively similar to the figure in the reference paper with comparable magnitudes. As mentioned earlier, since the variables being plotted have been defined using the `lindev` operator to evaluate the

complex-valued small-signal amplitude, the **Compute differential** checkbox in the plot settings window should be cleared, as is the case here by default.

Now create a study to sweep the frequency while keeping the gate voltage constant.

#### 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 > Small-Signal Analysis, Frequency Domain**.
- 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

##### *Step 1: Stationary*

By default a **Stationary** step is included when adding the **Compute differential** study. Here we can remove the step and set up the solver sequence to use the static solution already computed in the previous study for the small signal analysis. In this case select the solution for the gate voltage of -3 V.

- 1 In the **Model Builder** window, under **Study 2** right-click **Step 1: Stationary** and choose **Delete**.
- 2 In the **Model Builder** window, click **Study 2**.
- 3 In the **Settings** window for **Study**, type Study 2 - Freq sweep at -3 V in the **Label** text field.

##### *Step 1: Frequency-Domain Perturbation*

- 1 In the **Model Builder** window, under **Study 2 - Freq sweep at -3 V** click **Step 1: Frequency-Domain Perturbation**.
- 2 In the **Settings** window for **Frequency-Domain Perturbation**, locate the **Study Settings** section.
- 3 In the **Frequencies** text field, type  $f_0 * 10^{\text{range}(-2, 0.2, 3)}$ .
- 4 Locate the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.
- 5 Click **+ Add**.

6 In the table, enter the following settings:


Parameter name	Parameter value list	Parameter unit
Vg (Gate voltage)	-3	V

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

*Solution 3 (sol3)*

In the **Study** toolbar, click  **Show Default Solver**.

*Step 1: Frequency-Domain Perturbation*

- 1 In the **Model Builder** window, expand the **Solution 3 (sol3)** node, then click **Study 2 - Freq sweep at -3 V > Step 1: Frequency-Domain Perturbation**.
- 2 In the **Settings** window for **Frequency-Domain Perturbation**, locate the **Values of Linearization Point** section.
- 3 From the **Settings** list, choose **User controlled**.
- 4 From the **Method** list, choose **Solution**.
- 5 From the **Study** list, choose **Study 1 - Vg sweep at 50 Hz, Frequency-Domain Perturbation**.
- 6 From the **Solution** list, choose **Solution 1 (sol1)**.
- 7 From the **Use** list, choose **Solution Store 1 (sol2)**.
- 8 From the **Parameter value (Vg (V))** list, choose **-3 V**.
- 9 In the **Study** toolbar, click  **Compute**.

## RESULTS

*Net Dopant Concentration (semi)*

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

Create a plot for the equivalent parallel conductance to compare with Fig. 25 in the reference paper. The measured capacitance will also be plotted for the fun of it.

*Cm and Gp vs. Freq*

- 1 In the **Model Builder** window, right-click **Cm and Gp vs. Vg** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type Cm and Gp vs. Freq in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 2 - Freq sweep at -3 V/ Solution 3 (sol3)**.
- 4 Locate the **Legend** section. From the **Position** list, choose **Upper right**.



*Global 2*

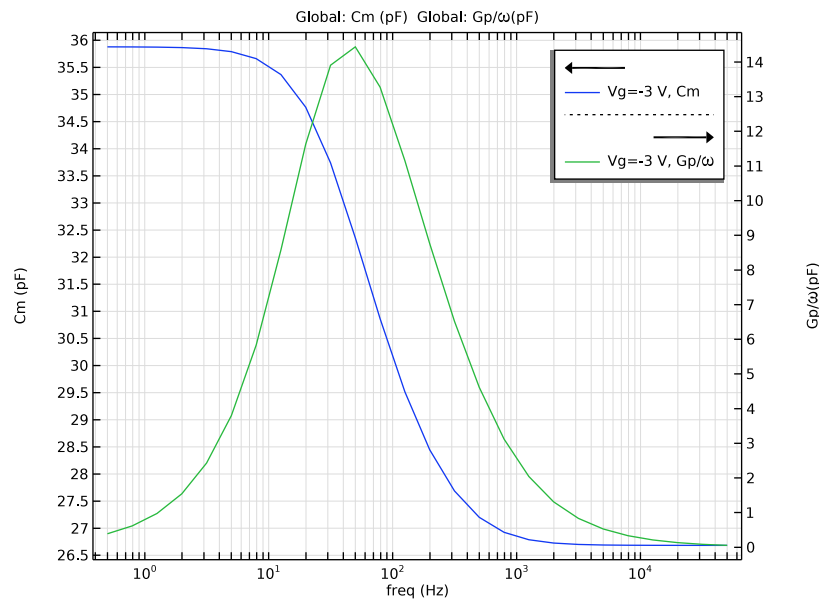
- 1 In the **Model Builder** window, expand the **Cm and Gp vs. Freq** node, then click **Global 2**.
- 2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
$Gp / (2 * \pi * \text{freq})$	pF	$Gp / \omega$

- 4 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **freq**.

*Global 1*

- 1 In the **Model Builder** window, click **Global 1**.
- 2 In the **Settings** window for **Global**, locate the **x-Axis Data** section.
- 3 From the **Axis source data** list, choose **freq**.
- 4 Click the  **x-Axis Log Scale** button in the **Graphics** toolbar.
- 5 In the **Cm and Gp vs. Freq** toolbar, click  **Plot**.




To gain some insight on the behavior of the capacitance and conductance shown in the plots above, it helps to plot the trap occupancy along the energy axis. The energy axis is added to the model by the physics interface using an extra dimension component. To plot any quantity along the energy axis, we need to create a dataset pointing to the extra

dimension component where the quantity is defined. We will first plot the density of states of the traps as an example.

#### *Study 1 - Vg sweep at 50 Hz/Solution 1 XD*


- 1 In the **Model Builder** window, expand the **Results > Datasets** node.
- 2 Right-click **Results > Datasets > Study 1 - Vg sweep at 50 Hz/Solution 1 (sol1)** and choose **Duplicate**.
- 3 In the **Settings** window for **Solution**, type Study 1 - Vg sweep at 50 Hz/Solution 1 XD in the **Label** text field.
- 4 Locate the **Solution** section. From the **Component** list, choose **Extra Dimension from Continuous Energy Levels 1 (semi\_tasr1\_ctb1\_xdim)**.

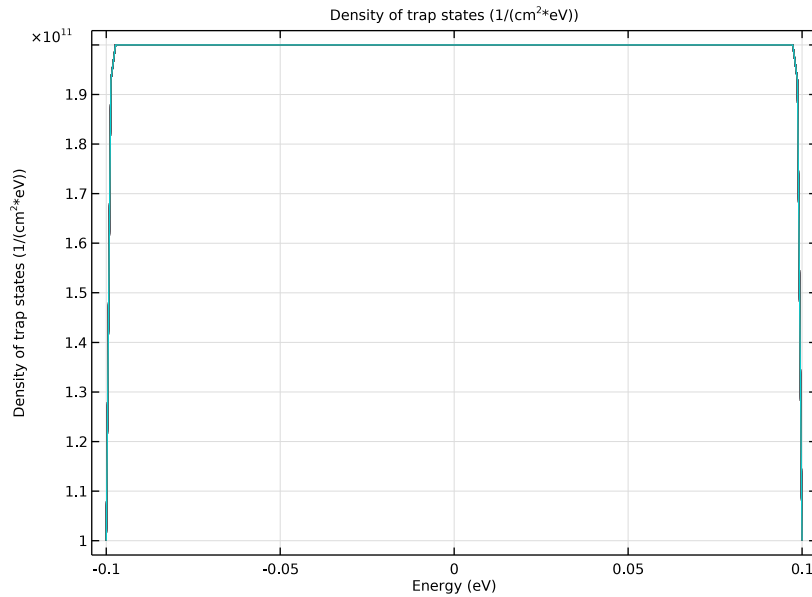
#### *Density of trap states vs. Energy*

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Density of trap states vs. Energy in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 1 - Vg sweep at 50 Hz/Solution 1 XD (sol1)**.

#### *Line Graph 1*

- 1 Right-click **Density of trap states vs. Energy** and choose **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **Selection** section.
- 3 From the **Selection** list, choose **All domains**.
- 4 Locate the **y-Axis Data** section. In the **Expression** text field, type  $\text{atxd0}(0[\text{um}], (\text{semi.tasr1.ctb1.gt}/(\text{e\_const}*\text{Ew0})))$ .
- 5 In the **Unit** field, type  $1/(\text{cm}^2*\text{eV})$ .
- 6 Select the **Description** checkbox. In the associated text field, type Density of trap states.
- 7 From the **Expression evaluated for** list, choose **Static solution**.
- 8 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
- 9 In the **Expression** text field, type  $\text{atxd0}(0[\text{um}], \text{semi.tasr1.ctb1.Vxd} - \text{semi.tasr1.ctb1.Et0})*\text{e\_const}$ .
- 10 From the **Unit** list, choose **eV**.
- 11 Select the **Description** checkbox. In the associated text field, type Energy.
- 12 From the **Expression evaluated for** list, choose **Static solution**.

**B** In the **Density of trap states vs. Energy** toolbar, click  **Plot**.



Note that the operator `atxd0` is used with a "0" because the energy axis (extra dimension) is defined in a boundary condition, which has a dimension of 0 in the 1D model. The first argument for the operator is `0[um]` since the boundary condition is applied on the boundary located at 0 um. The *x*-axis for the energy is centered around the center of the trap energy level distribution. The density of trap states shows a rectangular distribution of  $2e11 [cm^{-2} \cdot eV^{-1}]$  as specified. The option of **Static solution** is selected for both the *x*- and *y*-axes.


Now we plot the trap occupancy along the energy axis and compare two cases: gate voltage = 1 V (accumulation) and gate voltage = -3 V (peak of equilibrium parallel conductance). First the static solution.

*Trap occupancy, static*

- 1** In the **Model Builder** window, right-click **Density of trap states vs. Energy** and choose **Duplicate**.
- 2** In the **Settings** window for **ID Plot Group**, type `Trap occupancy, static` in the **Label** text field.
- 3** Locate the **Data** section. From the **Parameter selection (Vg)** list, choose **From list**.
- 4** In the **Parameter values (Vg (V))** list, choose **1** and **-3**.

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

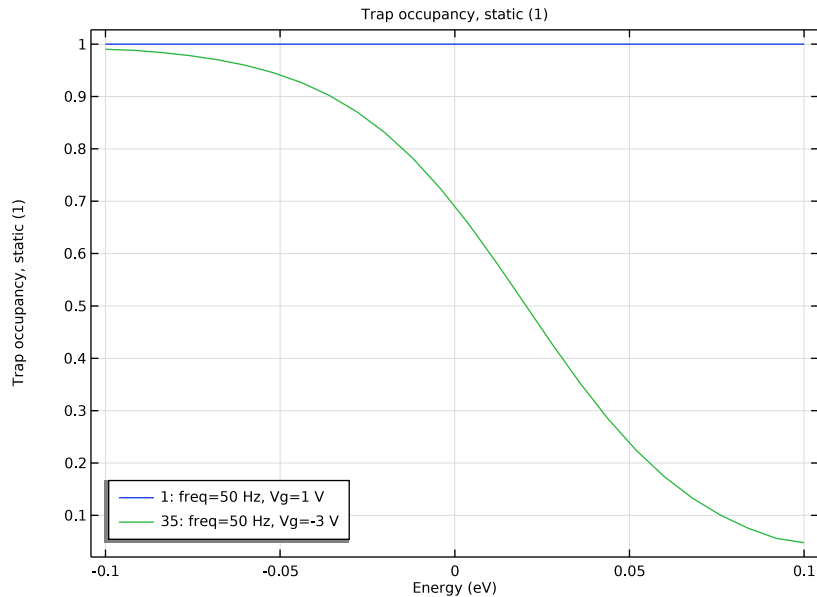
#### *Line Graph 1*

- 1 In the **Model Builder** window, expand the **Trap occupancy, static** node, then click **Line Graph 1**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `atxd0(0[um], (semi.tasr1.ctb1.ft))`.
- 4 In the **Description** text field, type `Trap occupancy, static`.
- 5 Click to expand the **Legends** section. Select the **Show legends** checkbox.
- 6 In the **Trap occupancy, static** toolbar, click  **Plot**.

The staircase like shape of the green curve is an indication of the 25 discrete levels used to approximate the continuous energy distribution as mentioned earlier. It is useful for developing purposes to be able to see these levels explicitly. Sometimes it is useful to smooth out the discretization for presentation purposes. This can be easily done by changing the **Resolution** option for the plot to **No refinement**.

- 7 Click to expand the **Quality** section. From the **Evaluation settings** list, choose **Manual**.
- 8 From the **Resolution** list, choose **No refinement**.

9 In the **Trap occupancy, static** toolbar, click  **Plot**.



We see that at the gate voltage of 1 V, since the Fermi level is far above the trap energy levels, the traps are fully occupied (blue curve). In this case one would not expect any significant contribution to the small signal response from the traps. On the other hand, at the gate voltage of -3 V, the Fermi level goes through the middle of the trap energy levels so that many trap levels are partially occupied (green curve). In this case one would expect the traps to contribute significantly to the small signal response, consistent with the peaking of the equivalent parallel conductance and the distinct wiggle of the measured capacitance curve seen in the earlier figure.

Finally, plot the small signal response of the trap occupancy along the energy axis and compare the same two cases: gate voltage = 1 V (accumulation) and gate voltage = -3 V (peak of equilibrium parallel conductance). Since the small signal response is complex valued, we plot both the real part (in solid curves) and the imaginary part (in dashed curves). Remember to select the **Compute differential** checkbox for the correct evaluation of the small signal response.

*Trap occupancy, small signal response*

- 1 In the **Model Builder** window, right-click **Trap occupancy, static** and choose **Duplicate**.
- 2 In the **Model Builder** window, click **Trap occupancy, static 1**.

- 3 In the **Settings** window for **ID Plot Group**, type Trap occupancy, small signal response in the **Label** text field.
- 4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.
- 5 In the **Title** text area, type Trap occupancy, small signal, real and imaginary parts.
- 6 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

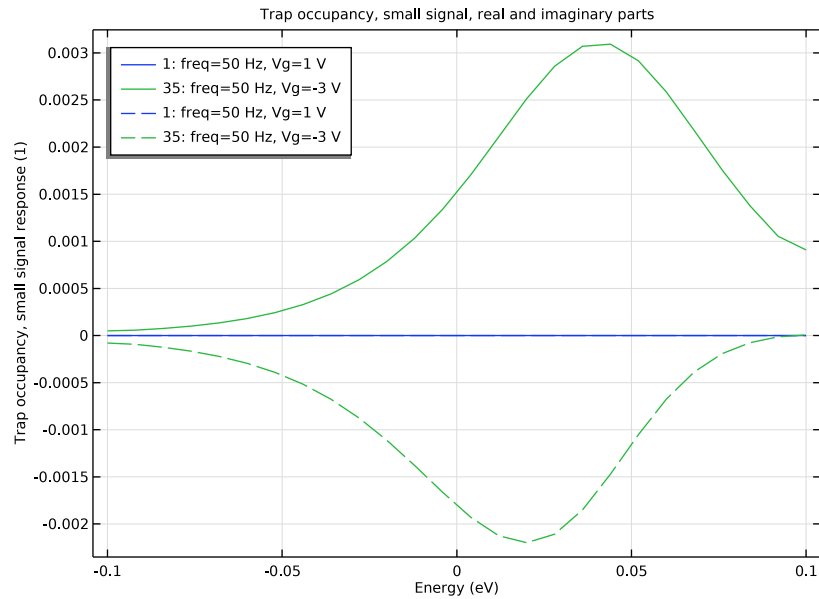
#### *Line Graph 1*

- 1 In the **Model Builder** window, click **Line Graph 1**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Description** text field, type Trap occupancy, small signal response.
- 4 From the **Expression evaluated for** list, choose **Harmonic perturbation**.
- 5 Select the **Compute differential** checkbox.

#### *Line Graph 2*

- 1 Right-click **Results > Trap occupancy, small signal response > Line Graph 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type  $\text{atxd0}(0[\text{um}], \text{imag}(\text{semi.tasr1.ctb1.ft}))$ .
- 4 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- 5 From the **Color** list, choose **Cycle (reset)**.

6 In the **Trap occupancy, small signal response** toolbar, click  **Plot**.



We see that at the gate voltage of 1 V, both the real and imaginary parts of the small signal response of the trap occupancy are very small (blue curves). On the other hand, at the gate voltage of -3 V, both the real and imaginary parts of the small signal response of the trap occupancy are significant (green curves). All of these are consistent with the discussion above.