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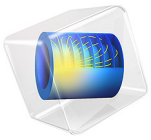

Schottky Contact

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This benchmark simulates the behavior of an ideal Schottky barrier diode made of a tungsten contact deposited on a silicon wafer. The resulting J–V (current density versus applied voltage) curve obtained from the model under forward bias is compared with experimental measurements found in the literature.

Introduction

When a metal is brought in contact to a semiconductor, a potential barrier forms at the contact. This is mainly a consequence of the work function difference between the metal and the semiconductor.

In this model, the ideal Schottky contact is used to model the behavior of a simple Schottky barrier diode. The use of the word "ideal" implies here that surface states, image force lowering, tunneling, and diffusion effects are neglected in the computation of the current transferred between the semiconductor and the metal at the interface.

Note that ideal Schottky contacts are characterized by a thermionic current that depends mostly on the applied bias and barrier height of the metal–semiconductor contact. These contacts usually occur in nondegenerate semiconductors with doping concentrations less than 1×10^{16} cm^{-3} at room temperature.

Model Definition

This model simulates the behavior of a tungsten–semiconductor Schottky barrier diode. Figure 1 shows the geometry of the modeled devices. It consists of an n-doped silicon wafer (N_d=1×10^{16} cm^{-3}) on top of which a tungsten contact has been deposited.

The model computes the current density obtained under forward bias (from 0 to 0.25 V) and compares the resulting J–V curve with experimental measurements presented in Ref. 1.

This model uses the default silicon material properties as well as an ideal barrier height defined by:

$$\Phi_B = \Phi_m - \chi_0$$

Where Φ_B is the barrier height, Φ_m is the metal work function, and χ_0 is the electron affinity of the semiconductor.

The work function of the tungsten contact has been chosen to be $\Phi_m = 4.72$ V, which gives a barrier height of $\Phi_B = 0.67$ V.

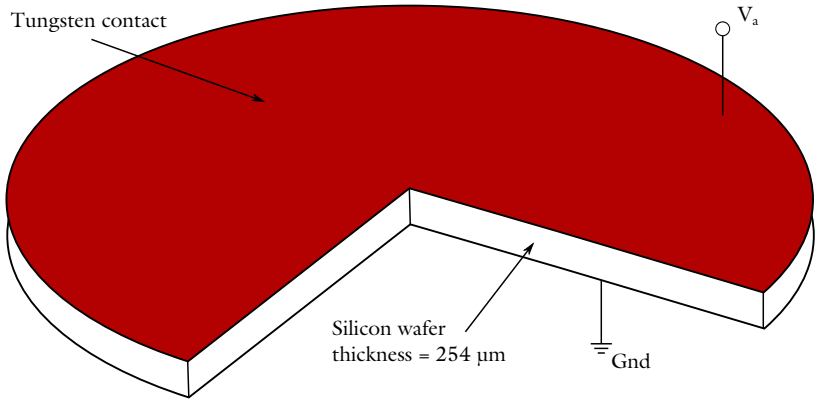

Figure 1: Schematic of the geometry. The Schottky contact is displayed in red and the silicon wafer in white. The thickness of the n-doped silicon wafer is 254 µm (0.01 inches) and the diameter of the diode is twenty times larger than its thickness.

Results and Discussion

Figure 2 shows the current density obtained under forward bias with our model (solid line) and compares it with the experimental measurements presented in Ref. 1 (circles).

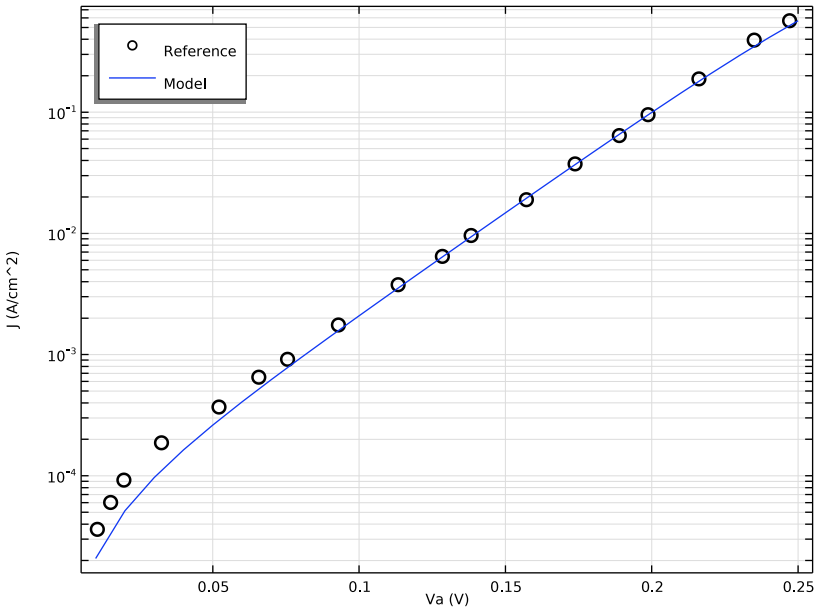

Figure 2: The current density obtained with the model (solid line) and the measurements (circles) presented in Ref. 1 *under forward bias.*

Reference

1. C.R. Crowell, J.C. Sarace, and S.M. Sze, "Tungsten-Semiconductor Schottky-Barrier Diodes," *Transaction of the Metallurgical Society of AIME*, vol. 233, pp. 478–481, 1965.

Application Library path: `Semiconductor_Module/Device_Building_Blocks/schottky_contact`

Modeling Instructions

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

NEW

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

MODEL WIZARD

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

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

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
Va	0[V]	0 V	Voltage
phim	4.72[V]	4.72 V	Work function
th	0.01[in]	2.54E-4 m	Thickness
w	th	2.54E-4 m	Radius
T0	298[K]	298 K	Temperature

Choose um as default length units.

GEOMETRY 1

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**.

Rectangle 1 (r1)

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

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

3 In the **Width** text field, type w.

4 In the **Height** text field, type th.

5 Right-click **Rectangle 1 (r1)** and choose **Duplicate**.

Rectangle 2 (r2)

Create another rectangle in order to resolve the depletion region near the Schottky contact.

1 In the **Model Builder** window, click **Rectangle 2 (r2)**.

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

3 In the **Height** text field, type `1[um]`.

4 Locate the **Position** section. In the **z** text field, type `th-1[um]`.

5 In the **Geometry** toolbar, click **Build All**.

Create an integration coupling variable. This will be used to display the normal current density at the boundary.

DEFINITIONS

Integration 1 (intop1)

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

2 In the **Settings** window for **Integration**, locate the **Source Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 5 only.

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

Load the material properties of silicon.

ADD MATERIAL

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

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

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

4 Click **Add to Component** in the window toolbar.

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

MATERIALS

Si - Silicon (mat1)

Set the lattice temperature to T0.

SEMICONDUCTOR (SEMI)

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`.

Add a doping model. Keep the default values, that is, n-type with impurity concentration of 1E16 cm^-3.

Analytic Doping Model 1

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

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

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

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

Since the doping feature adds a highly nonlinear contribution to the equation system, it is better to ramp the impurity concentration up from a small value. First set the continuation option to use the interface continuation parameter.

5 Click to expand the **Continuation Settings** section. Next set the interface continuation parameter as a parameter "ramp" at the main physics node.

6 In the **Model Builder** window, click **Semiconductor (semi)**.

7 In the **Settings** window for **Semiconductor**, click to expand the **Continuation Settings** section.

8 In the C_p text field, type `ramp`.

9 From the **Doping and trap density continuation parameter** list, choose **Use interface continuation parameter**.

Finally enter the parameter "ramp" in the parameter table. Later on this can be used in an auxiliary sweep in a study step to ramp the impurity concentration up from a small value.

GLOBAL DEFINITIONS

Parameters 1

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
ramp	1	1	

SEMICONDUCTOR (SEMI)

Metal Contact 1

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

Add an ideal Schottky contact. Set the metal work function to phim and the applied voltage to Va.

2 Select Boundary 5 only.

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

4 From the **Type** list, choose **Ideal Schottky**.

5 Locate the **Terminal** section. In the V_0 text field, type `Va`.

6 Locate the **Contact Properties** section. In the Φ text field, type `phim`.

Metal Contact 2

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

Set the potential on the ohmic side of the silicon wafer to $V = 0$ V.

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

3 Select Boundary 2 only.

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

MESH 1

Mapped 1

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

2 In the **Settings** window for **Mapped**, locate the **Domain Selection** section.

3 From the **Geometric entity level** list, choose **Entire geometry**.

Distribution 1

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

Add a fine mesh along the thickness of the top rectangle where the depletion region will occur.

2 Select Boundaries 3 and 7 only.

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

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

5 In the **Number of elements** text field, type 40.

6 In the **Element ratio** text field, type 50.

7 From the **Growth rate** list, choose **Exponential**.

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

Distribution 2

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

2 Select Boundaries 1 and 6 only.

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

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

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

6 In the **Element ratio** text field, type 100.

7 From the **Growth rate** list, choose **Exponential**.

8 Select the **Symmetric distribution** check box.

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

Distribution 3

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

2 Select Boundary 5 only.

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

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

5 In the **Model Builder** window, right-click **Mesh 1** and choose **Build All**.

STUDY 1

Step 1: Stationary

Set up an auxiliary continuation sweep for the 'ramp' parameter.

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

2 In the **Settings** window for **Stationary**, 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
ramp	`10^range(-6,2,0)`	

Add a second study step to perform an auxiliary continuation sweep for the 'Va' parameter.

Step 2: Stationary 2

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

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

3 Select the **Auxiliary sweep** check box.

4 Click **Add**.

5 Click **Range**.

6 In the **Range** dialog box, type `0.01` in the **Start** text field.

7 In the **Step** text field, type `0.01`.

8 In the **Stop** text field, type `0.25`.

9 Click **Add**.

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

11 From the **Run continuation for** list, choose **No parameter**.

12 From the **Reuse solution from previous step** list, choose **Yes**.

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

RESULTS

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, under **Results** right-click **Net Dopant Concentration (semi)** and choose **Delete**.

Table 1

1 In the **Results** toolbar, click **Table**.

Load the measurements from the reference in a table.

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

3 Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `schottky_contact_1d_ref.txt`.

J vs. V

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

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

3 Click to expand the **Title** section. From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section.

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

6 Select the **y-axis label** check box. In the associated text field, type `J (A/cm^2)`.

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

Table Graph 1

1 Right-click **J vs. V** and choose **Table Graph**.

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

3 Find the **Line style** subsection. From the **Line** list, choose **None**.

4 From the **Color** list, choose **Black**.

5 From the **Width** list, choose **3**.

6 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

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

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

9 In the table, enter the following settings:

Legends
Reference

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

Global 1

1 In the **Model Builder** window, right-click **J vs. V** 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
`-intop1(semi.nJ)/intop1(1)`	A/cm^2	

4 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

5 In the table, enter the following settings:

Legends
Model

6 In the **J vs. V** toolbar, click **Plot**.