Created in COMSOL Multiphysics 6.1

Nanorods

Introduction

A Gaussian electromagnetic wave is incident on a dense array of very thin wires (or rods). The distance between the rods and, thus, also the rod diameter is much smaller than the wavelength. Under these circumstances, the rod array does not function as a diffraction grating (see the Plasmonic Wire Grating model). Instead, the rod array behaves as if it was a continuous metal sheet for light polarized along the rods, whereas for light polarized perpendicular to the rods, the array is almost transparent to the electromagnetic wave. However, for the latter case dipole coupling between the rods occurs, thereby coupling electromagnetic excitation between the rods also outside of the illuminated region.

Model Definition

Figure 1 shows the array of rods and the incident Gaussian beam. The beam propagates in negative y direction. The wavelength is 750 nm and the spot radius of the beam equals the wavelength. For a more detailed discussion about Gaussian beams, see the model Second Harmonic Generation of a Gaussian Beam.

For the tightly focused beam that is used in this example, a plane-wave expansion that approximates the well-known paraxial approximation of a Gaussian beam is used. The advantage of using the plane-wave expansion is that it is a true solution to the Helmholtz equation, as each plane wave is a solution to Helmholtz equation. Mathematically, what happens here is that the 2D Gaussian beam expression (the paraxial approximation)

$$\mathbf{E}_{\mathrm{Gauss}}(x, y) = E_0\sqrt{\frac{w_0}{w(y)}}e^{-(x/w(y))^2}\exp\left(-i\left(ky-\eta(y)+\frac{kx^2}{2R(y)}\right)\right)\mathbf{e} \tag{1}$$

is approximated by a plane wave expansion

$$\mathbf{E}_{PW} = \sum_{j=-M}^{M}\sum_{k=0}^{1} a_{jk}\hat{\mathbf{u}}_k(\mathbf{k}_j)\exp(-i(\mathbf{k}_j\cdot\mathbf{r})), \tag{2}$$

where each wave vector $\mathbf{k}_j$ points in different directions for each value of the index j and a_{jk} is the amplitude that has a different value for each wave vector and also for each of the two possible polarization directions per wave vector, $\hat{\mathbf{u}}_k(\mathbf{k}_j)$. So for a tightly focused beam, the paraxial approximation in Equation 1 does not approximate the Helmholtz equation well, whereas Equation 2 is a true solution to Helmholtz equation.

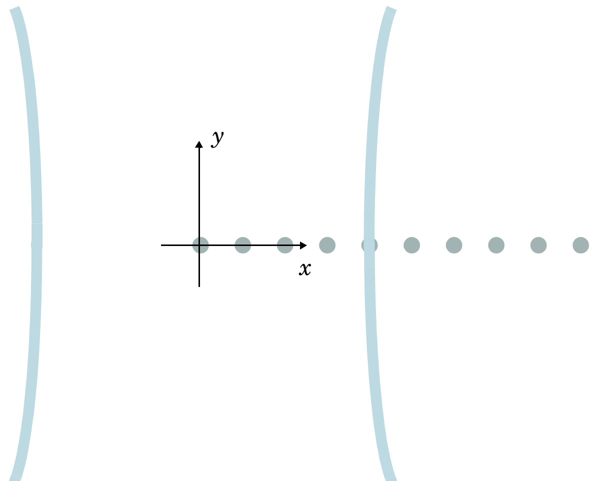

Figure 1: The modeled array of nanorods and the incident Gaussian beam. The model solves for the electric field in a 2D plane. Thus, the beam and rod properties are constant in the out-of-plane dimension.

The rods radius is 20 nm and the separation between the rods is 150 nm. Figure 1 shows that half of the beam illuminates the first part of the array of rods. Thus, most of the 40 rods in the model have a very low illumination.

The rods are metallic, with a dispersion formula for the relative permittivity given by

$$\varepsilon(\omega) = 1 - \frac{\omega_P^2}{\omega^2}$$

where the angular frequency is defined by

$$\omega = \frac{2\pi c}{\lambda}$$

and ω_p is the plasma frequency. The plasma frequency is set to $\sqrt{21}\omega$, resulting in a negative relative permittivity similar to that of gold.

Results and Discussion

Figure 2 shows the norm of the electric field for the Gaussian beam. In this configuration, the light beam is polarized in the x direction, that is, in the direction of the grating vector.

As seen from the surface plot, the nanorod array illuminates half of the Gaussian light beam. However, for this polarization there is no noticeable reflection nor diffraction from the nanorod array.

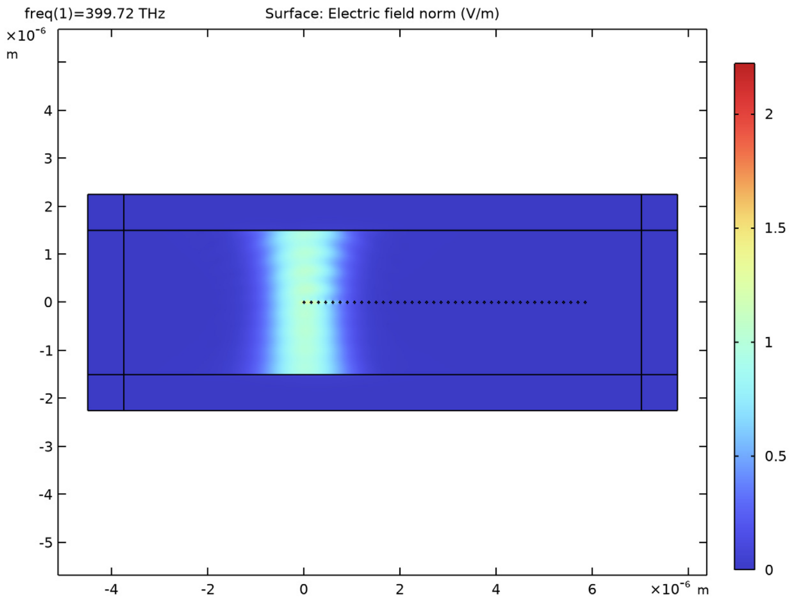

Figure 2: Surface plot of the electric field norm. The electric field of the Gaussian light beam is polarized in the x direction (along the grating vector).

Figure 3 shows a zoom-in of the leftmost part of the nanorod array and the center of the light beam. The plot shows that there is a dipolar coupling between the rods. Figure 4 shows that the coupling between the nanorods extends much longer than the intensity distribution of the exciting Gaussian light beam.

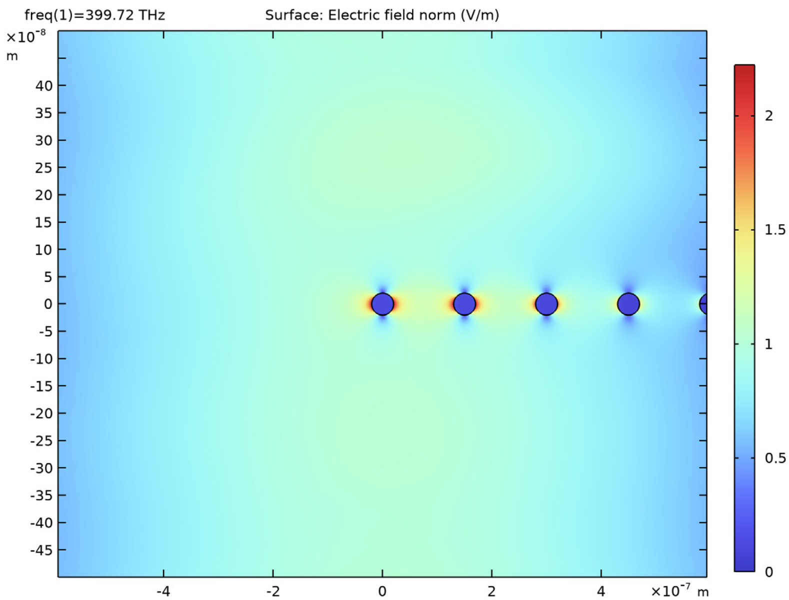

Figure 3: Zoom-in on the center of the Gaussian beam and the leftmost nanorods. As for Figure 2*, the polarization of the beam is in the x direction.*

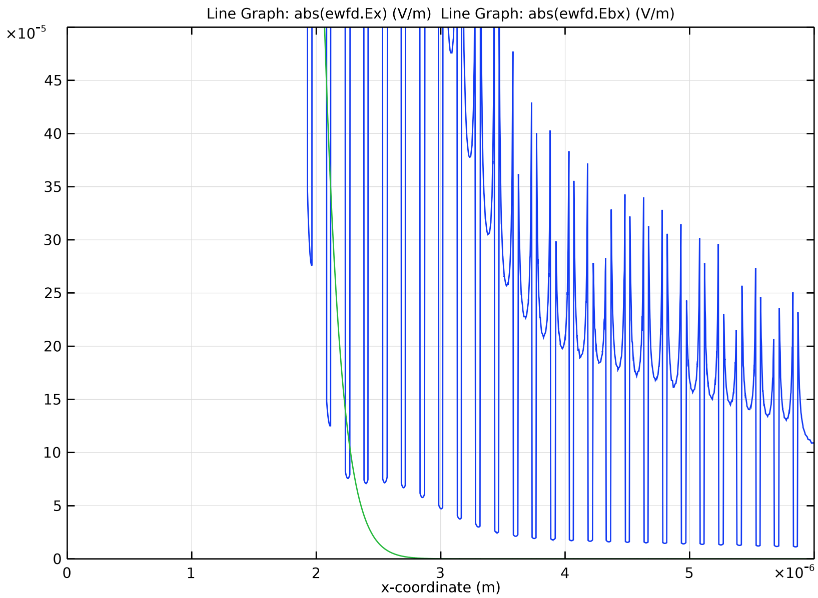

Figure 4: Line plot of the x component of the electric field (blue line) and the Gaussian beam background field (green line). The beam is polarized in the x direction.

When the light beam is polarized along the rods, that is, in the *z* direction (the out-of-plane direction), the interaction between the beam and the nanorod array is much stronger. As a comparison to Figure 3, Figure 5 shows a zoom-in of the center of the Gaussian beam and the leftmost nanorods. When the beam is polarized in the out-of-plane direction, the nanorod array appears for the beam almost as an opaque metal sheet. Thus, the beam is reflected and there is strong edge diffraction.

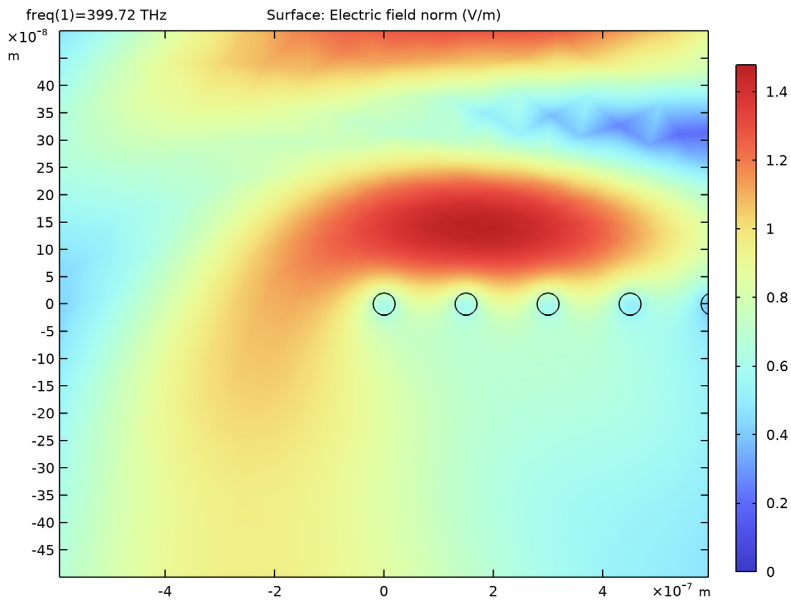

Figure 5: Zoom-in of the electric field norm for the center of the Gaussian beam and the leftmost nanorods. The Gaussian light beam is polarized along the rods (out-of-plane in the z direction).

The effects of reflection and edge diffraction is very obvious from Figure 6. Above the array there is a standing wave, formed by the incident beam and the beam reflected from the array, and below the array edge diffraction is evident.

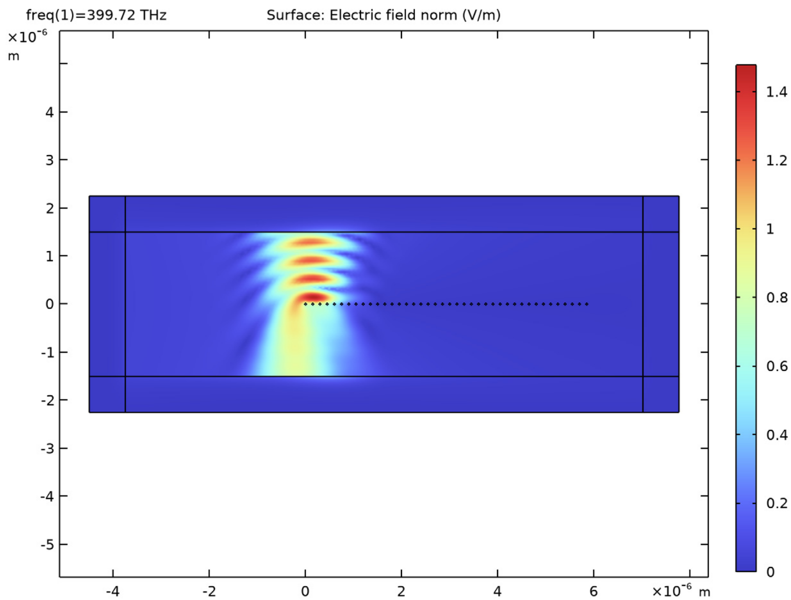

Figure 6: Surface plot of the full Gaussian beam and all the nanorods. The beam is polarized in the out-of-plane (z) direction.

Notes About the COMSOL Implementation

This application implementation demonstrates the use of perfectly matched layers for absorbing a propagating wave. Furthermore, when defining the relative permittivity, the Drude–Lorentz dispersion model is used. This setting is found in the wave equation feature.

Application Library path: `Wave_Optics_Module/Optical_Scattering/nanorods`

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**.
2 In the **Select Physics** tree, select **Optics>Wave Optics>Electromagnetic Waves, Frequency Domain (ewfd)**.
3 Click **Add**.
4 Click **Study**.
5 In the **Select Study** tree, select **General Studies>Frequency Domain**.
6 Click **Done**.

GLOBAL DEFINITIONS

Add parameters for the Gaussian light beam, the geometry, and the materials.

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
lda0	750[nm]	7.5E-7 m	Wavelength
f	c_const/lda0	3.9972E14 1/s	Frequency
w0	lda0	7.5E-7 m	Spot radius
z0	pi*w0^2/lda0	2.3562E-6 m	Rayleigh range
k	2*pi/lda0	8.3776E6 1/m	Propagation constant
E0	1[V/m]	1 V/m	Electric field amplitude
r_NP	20[nm]	2E-8 m	Radius of nanorods
N_NP	40	40	Number of nanorods
dx_NP	150[nm]	1.5E-7 m	Separation between nanorods
omega_p	sqrt(21)*2*pi*f	1.1509E16 1/s	Plasma frequency for nanorod material
w_air_left	5*w0	3.75E-6 m	Width of air domain for x < 0
w_air_right	max(5*w0,1.2*(N_NP-1)*dx_NP)	7.02E-6 m	Width of air domain for x > 0
w_air	w_air_left+w_air_right	1.077E-5 m	Width of air domain

Name	Expression	Value	Description
h_air	4*lda0	3E-6 m	Height of air domain
d_PML	lda0	7.5E-7 m	Thickness of PML domains

GEOMETRY 1

Rectangle 1 (r1)

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

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

3 In the **Width** text field, type `w_air+2*d_PML`.

4 In the **Height** text field, type `h_air+2*d_PML`.

5 Locate the **Position** section. In the **x** text field, type `-w_air_left-d_PML`.

6 In the **y** text field, type `-h_air/2-d_PML`.

Now create layers surrounding the rectangle for the perfectly matched layers (PMLs).

7 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	d_PML

8 Select the **Layers to the left** check box.

9 Select the **Layers to the right** check box.

10 Select the **Layers on top** check box.

The check box for the bottom layer is selected by default.

Circle 1 (c1)

Create the nanorods by first defining a circle, and then create a linear array of those circles.

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

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

3 In the **Radius** text field, type `r_NP`.

Nanorods

1 In the **Geometry** toolbar, click **Transforms** and choose **Array**.

2 In the **Settings** window for **Array**, type `Nanorods` in the **Label** text field.

The circle, representing a nanorod, is very small. Thus, you probably need to zoom in to select it.

3 Select the object **c1** only.

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

5 Locate the **Size** section. From the **Array type** list, choose **Linear**.

6 In the **Size** text field, type `N_NP`.

7 Locate the **Displacement** section. In the **x** text field, type `dx_NP`.

8 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box, to simplify later selection of the nanorods.

9 Click **Build Selected**.

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

DEFINITIONS

Create a view to be used later for zooming-in on the rods.

View 2

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

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

3 Select the **Lock axis** check box.

Axis

1 In the **Model Builder** window, expand the **View 2** node, then click **Axis**.

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

3 In the **x minimum** text field, type `-0.5e-6`.

4 In the **x maximum** text field, type `0.5e-6`.

5 In the **y minimum** text field, type `-0.5e-6`.

6 In the **y maximum** text field, type `0.5e-6`.

Switch back to the regular view now.

7 In the **Graphics** window toolbar, click ▼ next to **Go to Default View**, then choose **Go to View 1**.

Perfectly Matched Layer 1 (pml1)

Define the layers surrounding the central rectangular domain as PML regions.

1 In the **Definitions** toolbar, click **Perfectly Matched Layer**.

Let the default material be air. The material properties of the nanorods will later be defined in a wave equation feature.

2 Select Domains 1–4 and 6–9 only.

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 **Built-in>Air**.

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

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

ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EWFD)

Calculate the first solution for light polarized along the out-of-plane z direction. Solve for the scattered field and set the background field to a 2D Gaussian beam propagating in the negative y direction.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Electromagnetic Waves, Frequency Domain (ewfd)**.

2 In the **Settings** window for **Electromagnetic Waves, Frequency Domain**, locate the **Formulation** section.

3 From the list, choose **Scattered field**.

4 From the **Background wave type** list, choose **Gaussian beam**.

5 From the **Gaussian beam type** list, choose **Plane wave expansion**. This makes the Gaussian beam background field be a true solution to the Helmholtz equation.

6 From the **Wave vector distribution type** list, choose **User defined**. In the $N_{\mathbf{k}}$ text field, type `51`.

7 In the $k_{t,max}$ text field, type `1.5*ewfd.k0`.

The two settings above makes sure that the period for the Gaussian beam background field is larger than the computing domain in the x direction and that the field falls of smoothly also for very low field strengths.

8 From the **Beam orientation** list, choose **Along the y-axis**.

9 In the w_0 text field, type `w0`.

10 In the k text field, type `-ewfd.k0`.

Because there are no in-plane field components in this case, it suffices to compute the solution for the out-of-plane component.

11 Locate the **Components** section. From the **Electric field components solved for** list, choose **Out-of-plane vector**.

Wave Equation, Electric 2

Create a separate wave equation feature for the nanorod domains.

1 In the **Physics** toolbar, click **Domains** and choose **Wave Equation, Electric**.

2 In the **Settings** window for **Wave Equation, Electric**, locate the **Domain Selection** section.

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

Select the Drude-Lorentz dispersion model. The material parameters will result in a negative real part of the relative permittivity. This is normal for many metals, for frequencies below the plasma frequency.

4 Locate the **Electric Displacement Field** section. From the **Electric displacement field model** list, choose **Drude-Lorentz dispersion model**.

5 In the ω_P text field, type `omega_p`.

6 In the table, enter the following settings:

Oscillator strength (1)	Resonance frequency (rad/s)	Damping in time (rad/s)
1	0	0

STUDY 1

Step 1: Frequency Domain

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

2 In the **Settings** window for **Frequency Domain**, locate the **Study Settings** section.

3 In the **Frequencies** text field, type `f`.

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

RESULTS

Electric Field (ewfd)

Compare the results with that in Figure 6. The rod array appears for the field almost as a metal sheet. Thus, there are effects of edge diffraction and the reflection leads to standing wave effects in the region above the nanorod array.

Select the previously defined view, to zoom in on the center of the beam and the leftmost rods.

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

2 From the **View** list, choose **View 2**.

3 In the **Electric Field (ewfd)** toolbar, click **Plot** and compare the result with that in Figure 5. The zoom-in shows that light is blocked by the nanorod array and that light is diffracted by the edge of the array.

ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EWFD)

Repeat the simulation with the electric field set to in-plane polarization.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Electromagnetic Waves, Frequency Domain (ewfd)**.

2 In the **Settings** window for **Electromagnetic Waves, Frequency Domain**, locate the **Components** section.

3 From the **Electric field components solved for** list, choose **In-plane vector**.

STUDY 1

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

RESULTS

Electric Field (ewfd)

Compare the result with the graph in Figure 3. The zoomed-in view shows that the nanorods act as dipoles that enhance the field strength between the rods.

1 Click the **Zoom Extents** button in the **Graphics** toolbar and compare the graph with Figure 2. In the zoomed-out view the Gaussian beam seems to be almost unperturbed by the nanorod array that cuts into half of the beam.

Make a cut line through the centers of the rods, to make a detailed line graph of the field distribution along the line.

Cut Line 2D 1

1 In the **Results** toolbar, click **Cut Line 2D**.

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

3 In row **Point 1**, set **X** to `-w_air_left`.

4 In row **Point 2**, set **X** to `w_air_right`.

1D Plot Group 2

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

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

3 From the **Dataset** list, choose **Cut Line 2D 1**.

Line Graph 1

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

   Plot the magnitude of the electric field, polarized in the *x* direction, and compare with the background electric field.

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

3 In the **Expression** text field, type `abs(ewfd.Ex)`.

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

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

Line Graph 2

1 Right-click **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 `abs(ewfd.Ebx)`.

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

1D Plot Group 2

Set the axis limits to get a detailed view of the field distribution. Notice the field enhancement along the array of the rods.

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

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

3 Select the **Manual axis limits** check box.

4 In the **x minimum** text field, type `0`.

5 In the **x maximum** text field, type `6E-6`.

6 In the **y minimum** text field, type `0`.

7 In the **y maximum** text field, type `5e-4`.

8 In the **1D Plot Group 2** toolbar, click **Plot** and compare the graph with Figure 4.