



# Hexagonal Plasmonic Color Filter

## *Introduction*

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Color filters have many applications, for instance, for imaging and optical measurement systems. They can be designed for different types of filter characteristics, like bandpass, bandstop, longpass, shortpass, and so on.

This model demonstrates how to perform simulations of an absorbing bandstop color filter, based on a hexagonal array of holes in a thin aluminum layer. The structure is hexagonally periodic, but this example shows that the problem can be stated both as a hexagonally periodic problem and as a rectangularly periodic problem. Using the rectangular periodicity makes it simpler to use array datasets for visualization of the result from several unit cells. However, as the rectangular unit cell is larger than the hexagonal unit cell, the memory consumption is larger and the solution time is longer for the rectangular unit cell formulation.

## Model Definition

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Figure 1 shows seven hexagonal cells and visualizes the connection between the hexagonal cells, the corresponding Bravais lattice, and the rectangularly periodic cell that is also used in this model.

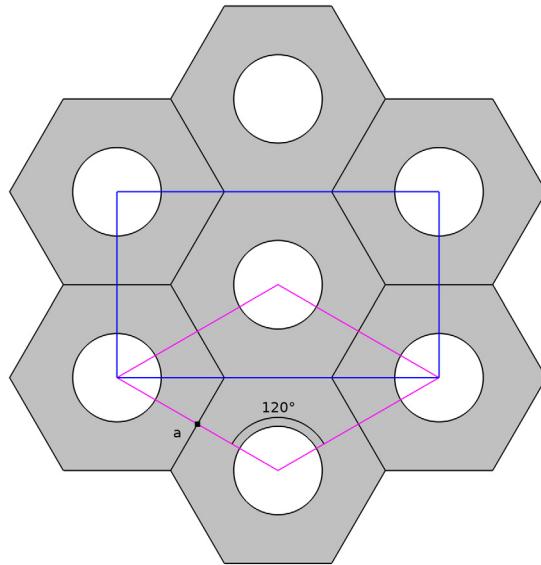


Figure 1: Seven hexagonal cells. The blue rectangle indicates the rectangularly periodic cell. The unit cell of the Bravais lattice for the hexagonal cell is indicated by the magenta rhombus shape. The distance between the hexagonal cell centers, the period length, is defined by the parameter  $a$ . The horizontal and vertical sides of the rectangular cell are  $\sqrt{3} \cdot a$  and  $a$ , respectively. The area of the rectangular cell is twice the area of the hexagonal cell (and the unit cell of the Bravais lattice).

For normal incidence, as in this model, the wave vector components in the port planes for the diffraction orders, are given by summing an integer number of the reciprocal lattice vectors for the unit cell. The integers used when constructing these wave vector components are the mode numbers for the diffraction orders.

To show that the larger rectangular cell can be used to represent the problem for the smaller hexagonal cell, first show that all points in the reciprocal lattice for the hexagonal case can be reached by appropriate addition of the reciprocal lattice vectors for the rectangular case.

To start, the primitive lattice vectors for the rectangular cell are

$$\mathbf{a}_{1r} = \sqrt{3}ax , \quad (1)$$

$$\mathbf{a}_{2r} = ay , \quad (2)$$

and

$$\mathbf{a}_{3r} = cz , \quad (3)$$

where  $a$  is the period in the hexagonal lattice,  $c \rightarrow \infty$ , and  $\mathbf{x}$ ,  $\mathbf{y}$ , and  $\mathbf{z}$  are the unit vectors in the  $x$ ,  $y$ , and  $z$  directions, respectively.

The reciprocal lattice vectors are then

$$\mathbf{b}_{1r} = 2\pi \frac{\mathbf{a}_{2r} \times \mathbf{a}_{3r}}{\mathbf{a}_{1r} \cdot (\mathbf{a}_{2r} \times \mathbf{a}_{3r})} = \frac{2\pi}{\sqrt{3}a} \mathbf{x} , \quad (4)$$

$$\mathbf{b}_{2r} = 2\pi \frac{\mathbf{a}_{3r} \times \mathbf{a}_{1r}}{\mathbf{a}_{1r} \cdot (\mathbf{a}_{2r} \times \mathbf{a}_{3r})} = \frac{2\pi}{a} \mathbf{y} , \quad (5)$$

$$\mathbf{b}_{3r} = 2\pi \frac{\mathbf{a}_{1r} \times \mathbf{a}_{2r}}{\mathbf{a}_{1r} \cdot (\mathbf{a}_{2r} \times \mathbf{a}_{3r})} = \frac{2\pi}{c} \mathbf{z} = \mathbf{0} . \quad (6)$$

For the hexagonal structure, with the rhombus Bravais lattice, the primitive lattice vectors are

$$\mathbf{a}_{1h} = \frac{\sqrt{3}}{2}ax + \frac{1}{2}ay , \quad (7)$$

$$\mathbf{a}_{2h} = -\frac{\sqrt{3}}{2}ax + \frac{1}{2}ay , \quad (8)$$

and

$$\mathbf{a}_{3rh} = cz . \quad (9)$$

Then, the reciprocal lattice vectors are

$$\mathbf{b}_{1h} = 2\pi \frac{\mathbf{a}_{2h} \times \mathbf{a}_{3h}}{\mathbf{a}_{1h} \cdot (\mathbf{a}_{2h} \times \mathbf{a}_{3h})} = \frac{2\pi}{a} \left( \frac{1}{\sqrt{3}} \mathbf{x} + \mathbf{y} \right) = \mathbf{b}_{1r} + \mathbf{b}_{2r} , \quad (10)$$

$$\mathbf{b}_{2h} = 2\pi \frac{\mathbf{a}_{3h} \times \mathbf{a}_{1h}}{\mathbf{a}_{1h} \cdot (\mathbf{a}_{2h} \times \mathbf{a}_{3h})} = \frac{2\pi}{a} \left( \mathbf{y} - \frac{\mathbf{x}}{\sqrt{3}} \right) = -\mathbf{b}_{1r} + \mathbf{b}_{2r} , \quad (11)$$

$$\mathbf{b}_{3h} = 2\pi \frac{\mathbf{a}_{1h} \times \mathbf{a}_{2h}}{\mathbf{a}_{1h} \cdot (\mathbf{a}_{2h} \times \mathbf{a}_{3h})} = \mathbf{0} . \quad (12)$$

Thus, from [Equation 10](#) and [Equation 11](#), it is clear that any point in reciprocal space from the hexagonal lattice can be written as

$$\mathbf{G}_{hmn} = m\mathbf{b}_{1h} + n\mathbf{b}_{2h} = (m-n)\mathbf{b}_{1r} + (m+n)\mathbf{b}_{2r} , \quad (13)$$

where  $m$  and  $n$  are the mode numbers for the particular diffraction order. All these points can be reached by combining the reciprocal lattice vectors for the rectangular unit cell, using integer coefficients. Thereby, all reciprocal lattice points for the hexagonal unit cell is part of the reciprocal lattice for the rectangular unit cell.

However, from [Equation 10](#) and [Equation 11](#) the reciprocal lattice vectors for the rectangular cell can be expressed from the reciprocal lattice vectors for the hexagonal cell as

$$\mathbf{b}_{1r} = \frac{1}{2}(\mathbf{b}_{1h} - \mathbf{b}_{2h}) \quad (14)$$

and

$$\mathbf{b}_{2r} = \frac{1}{2}(\mathbf{b}_{1h} + \mathbf{b}_{2h}) . \quad (15)$$

Thus, an arbitrary point in the reciprocal lattice of the rectangular cell can be written as

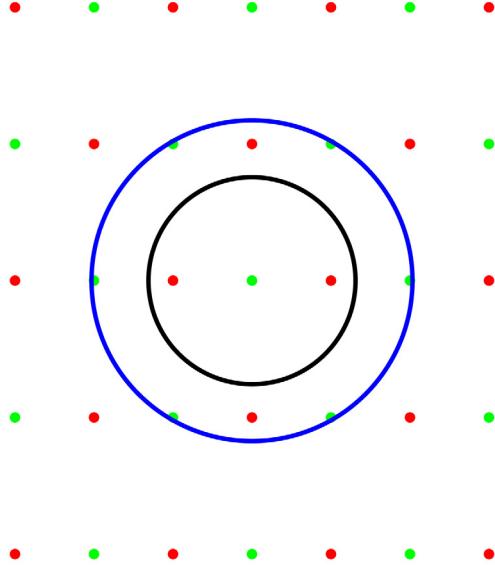
$$\mathbf{G}_{rmn} = m\mathbf{b}_{1r} + n\mathbf{b}_{2r} = \frac{m+n}{2}\mathbf{b}_{1h} + \frac{n-m}{2}\mathbf{b}_{2h} . \quad (16)$$

From [Equation 16](#), it is clear that there are points in the reciprocal space for the rectangular cell that are not part of the set of points in the reciprocal space for the hexagonal cell (as all reciprocal lattice points  $\mathbf{G}_{rmn}$  cannot be reached by combining the reciprocal lattice vectors  $\mathbf{b}_{1h}$  and  $\mathbf{b}_{2h}$  using integer coefficients). Thus, as expected, the smaller hexagonal cell has a reciprocal space that is a subset of the reciprocal space for the rectangular cell. [Figure 2](#) shows a picture of the points (modes) in the reciprocal lattice, for both the rectangular and the hexagonal unit cells. Notice, though, that the primitive vectors are defined as

$$\mathbf{a}_{1i} \times \mathbf{a}_{1i} = k\mathbf{n}, k > 0, i = r, h , \quad (17)$$

where  $\mathbf{n}$  is the port normal. Since the port normals point in opposite directions on Port 1 and Port 2, the primitive vectors are swapped on Port 2, compared to on Port 1. Thereby, also the reciprocal lattice vectors and the mode numbers are swapped on Port 2, compared

to Port 1. So, in [Figure 2](#) mode number  $m$  for Port 1 and mode number  $n$  for Port 2 are located on the horizontal axis, whereas mode number  $n$  for Port 1 and mode number  $m$  for Port 2 are located on the vertical axis.



*Figure 2: The reciprocal lattice. The dots represent points in the reciprocal lattice for the rectangular unit cell. The green points coincide with points in the reciprocal lattice for the hexagonal (rhombus) Bravais lattice, whereas the red dots are only available in the reciprocal lattice for the rectangular unit cell. The black line encircles the points (modes) available for Port 1, whereas the blue line encircles the points (modes) available for Port 2.*

In the model, all diffraction orders for the rectangular cell are computed. It is shown that for this model, with a normally incident field, the diffraction orders that do not correspond to modes for the hexagonal cell do not carry any power.

The incoming field is incident in the normal direction. Thus, continuity boundary conditions are used.

To excite the incoming wave and to absorb the outgoing waves, periodic ports and diffraction order ports are used. If the intention is not to compute the diffraction efficiencies for the different modes, perfectly matched layer (PML) backed slit ports can be used instead. This approach is demonstrated in the [Frequency Selective Surface, Periodic Complementary Split Ring Resonator](#) model.

Array datasets are used for visualizing the field from several unit cells. For the rectangular unit cell formulation, a single array dataset can be used. However, when using the hexagonal unit cell, three array datasets are combined to build the periodic hexagonal pattern.

## Results and Discussion

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Figure 3 shows the electric field in a single hexagonal unit cell, at the wavelength for maximum absorption. The field is concentrated to the top of the hole in the aluminum layer.

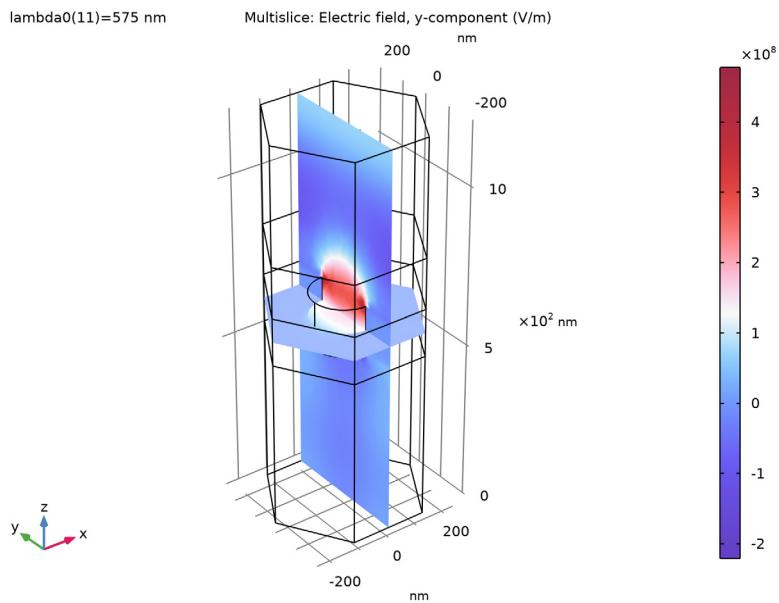
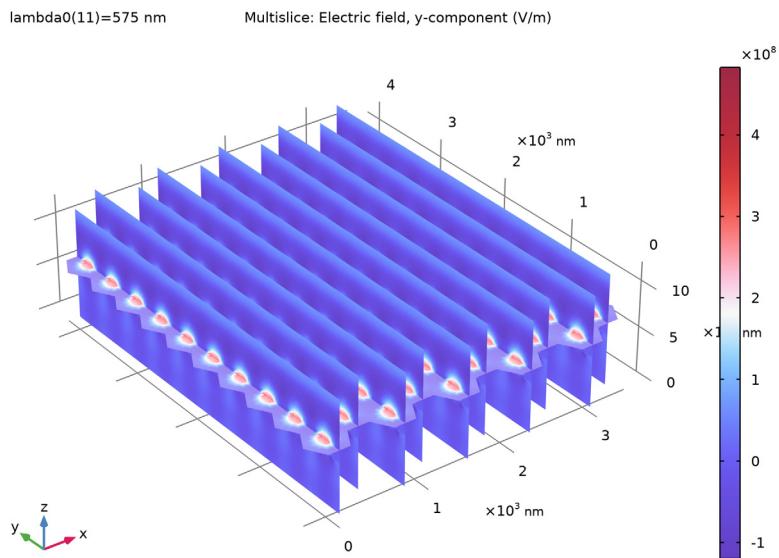


Figure 3: Plot of the y component of the electric field in a single hexagonal unit cell.

[Figure 4](#) shows a plot similar to the plot in [Figure 3](#), but for many hexagonal unit cells. Three array datasets are combined to create the periodic hexagonal pattern.



*Figure 4: Plot of the electric field in an array of hexagonal unit cells.*

[Figure 5](#) shows the electric field in a single rectangular unit cell. As expected, the field pattern is similar to the field pattern displayed in [Figure 3](#). It is clear that the field is

periodic along the diagonals in the  $xy$  plane, from the left to the right boundary, and from the front to the back boundary.

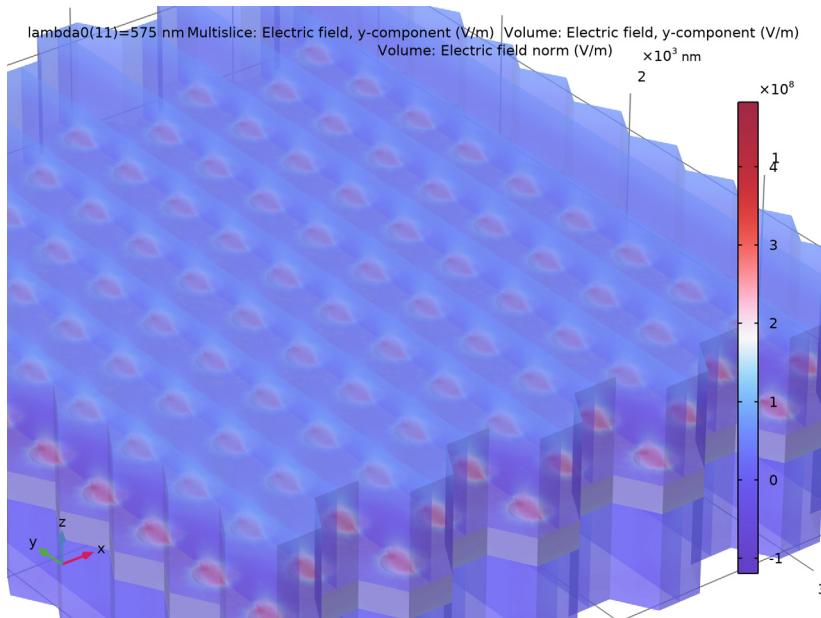
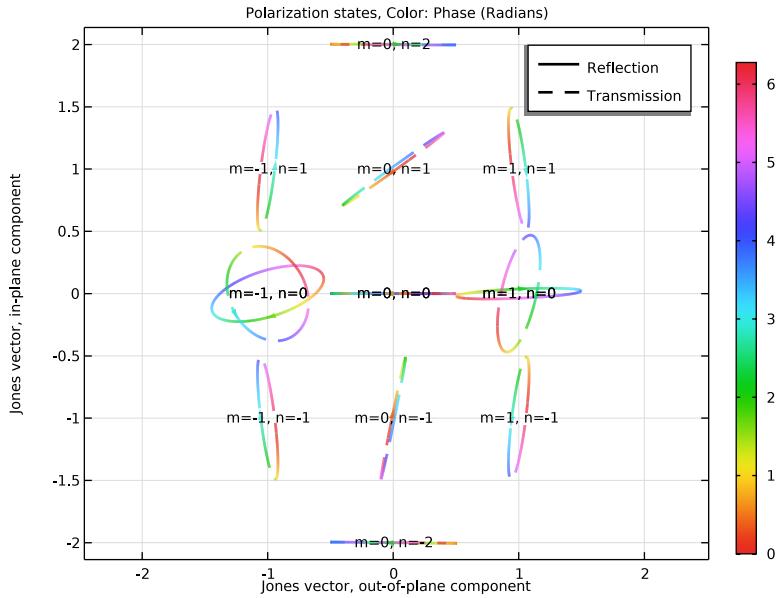


Figure 5: The  $y$  component of the electric field in one rectangular unit cell.

[Figure 6](#) shows that the reflectance, transmittance, and absorptance values are very similar for the two formulations.



[Figure 6](#): Comparison of the reflectance, transmittance, and absorptance spectra for the hexagonal and the rectangular unit cell formulations. The plots for the hexagonal unit cell use solid lines, whereas the plots for the rectangular unit cell use markers.

The diffraction efficiencies for the modes in the rectangular unit that do not correspond to any modes of the hexagonal unit cell are shown in [Figure 7](#). For all those modes, the

diffraction efficiency is less than  $10^{-4}$ , validating that, for this case, the rectangular unit cell indeed can be used for modeling the hexagonal unit cell.

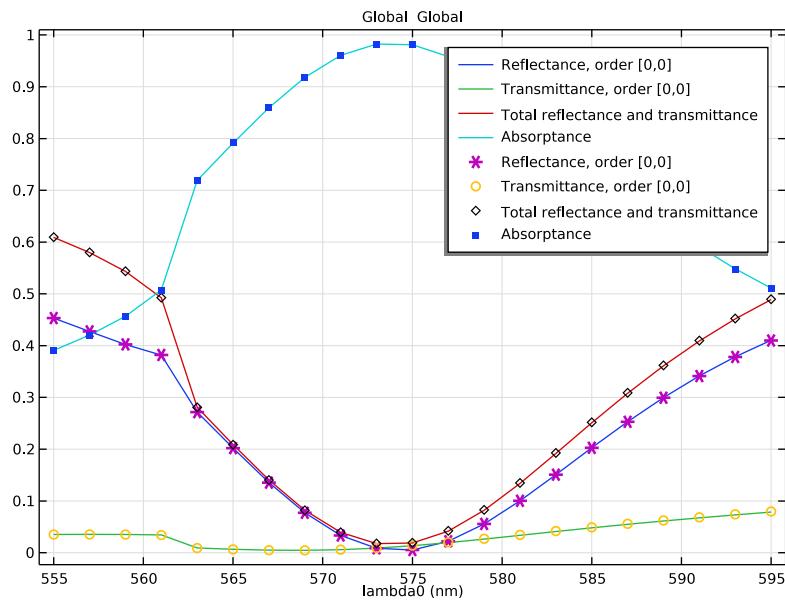
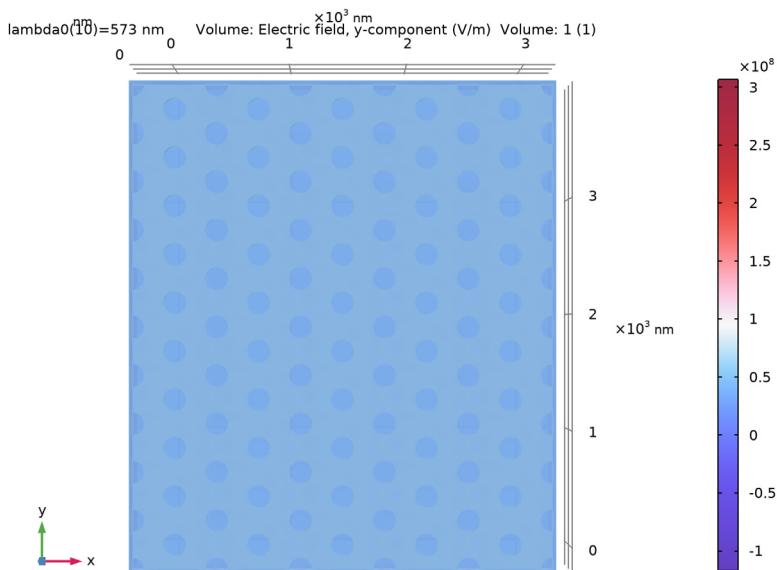


Figure 7: Plot of the diffraction efficiencies for modes from the rectangular unit cell that do not correspond to modes for the hexagonal unit cell.

Finally, [Figure 8](#) shows an electric field plot for an array of rectangular unit cells. The hexagonal periodicity is clearly seen in the hole pattern in the aluminum layer.



*Figure 8: The electric field (y component) for an array of rectangular unit cells.*

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**Application Library path:** Wave\_Optics\_Module/Gratings\_and\_Metamaterials/hexagonal\_plasmonic\_color\_filter

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### *Modeling Instructions*

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

#### **N E W**

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

#### **M O D E L   W I Z A R D**

- 1 In the **Model Wizard** window, click **3D**.
- 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 **Preset Studies for Selected Physics Interfaces> Wavelength Domain**.
- 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 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `hexagonal_plasmonic_color_filter_parameters.txt`.

## GEOMETRY 1

The geometry consists of a layered hexagonal pillar, with a cylinder in the second layer (from the bottom).

- 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**.

*Work Plane 1 (wp1)*

Create the hexagonal pillar, by first creating a 2D hexagon that is subsequently extruded to a pillar.

In the **Geometry** toolbar, click  **Work Plane**.

*Work Plane 1 (wp1)>Plane Geometry*

In the **Model Builder** window, click **Plane Geometry**.

*Work Plane 1 (wp1)>Polygon 1 (pol1)*

- 1 In the **Work Plane** toolbar, click  **Polygon**.
- 2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.

- 3** In the table, enter the following settings:

xw (nm)	yw (nm)
d_hex	0
d_hex/2	a/2
-d_hex/2	a/2
-d_hex	0
-d_hex/2	-a/2
d_hex/2	-a/2

*Extrude 1 (ext1)*

- 1** In the **Model Builder** window, under **Component 1 (comp1)>Geometry 1** right-click **Work Plane 1 (wp1)** and choose **Extrude**.

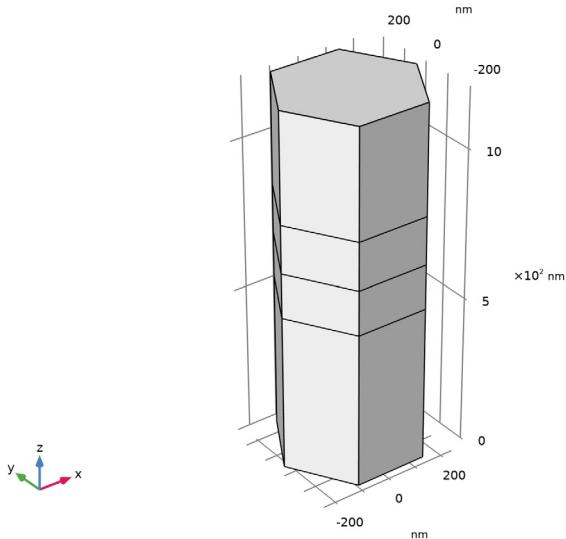
- 2** In the **Settings** window for **Extrude**, locate the **Distances** section.

- 3** In the table, enter the following settings:

Distances (nm)
height/2-t_A1/2
height/2+t_A1/2
height/2+t_A1/2+t_SOG
height

- 4** Click  **Build All Objects**.

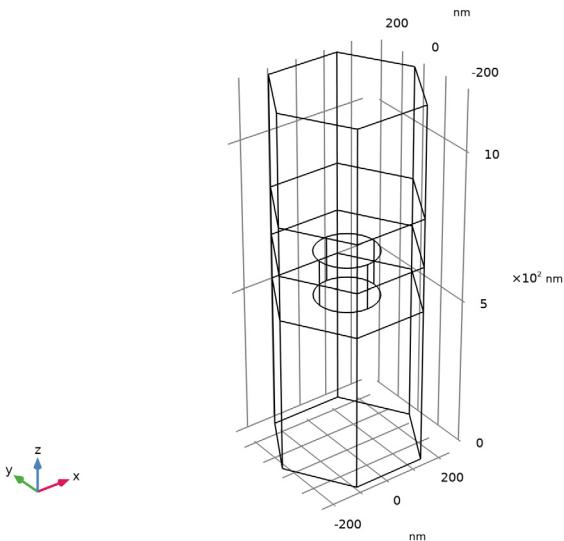
- 5 Click the  **Zoom Extents** button in the **Graphics** toolbar.



*Cylinder 1 (cyl1)*

- 1 In the **Geometry** toolbar, click  **Cylinder**.
- 2 In the **Settings** window for **Cylinder**, locate the **Size and Shape** section.
- 3 In the **Radius** text field, type `r0`.
- 4 In the **Height** text field, type `t_A1`.
- 5 Locate the **Position** section. In the **z** text field, type `height/2-t_A1/2`.
- 6 Click  **Build All Objects**.
- 7 Click the  **Zoom Extents** button in the **Graphics** toolbar.

- 8 Click the  **Wireframe Rendering** button in the **Graphics** toolbar, to better see the domains inside the unit cell.



#### GLOBAL DEFINITIONS

First add global materials. Later, add links to these materials from the two model components.

#### 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 Global Materials** in the window toolbar.
- 5 In the tree, select **Optical>Inorganic Materials>Al - Aluminium and aluminates>Models and simulations>Al (Aluminium) (Rakic et al. 1998: Brendel-Bormann model; n, k 0.0620-248 um).**
- 6 Click **Add to Global Materials** in the window toolbar.
- 7 In the tree, select **Optical>Inorganic Materials>O - Oxygen and oxides>Crystal>SiO2 (Silicon dioxide, Silica, Quartz) (Ghosh 1999: a-Quartz, n(o) 0.198-2.05 um).**
- 8 Click **Add to Global Materials** in the window toolbar.
- 9 In the **Home** toolbar, click  **Add Material** to close the **Add Material** window.

## **GLOBAL DEFINITIONS**

### *Spin-on Glass*

- 1 In the **Model Builder** window, under **Global Definitions** right-click **Materials** and choose **Blank Material**.
- 2 In the **Settings** window for **Material**, type **Spin-on Glass** in the **Label** text field.

At this point, you cannot easily add material parameters to this material. You will add the required material parameters, when a material link has been added that points to this material.

## **HEXAGONAL CELL**

- 1 In the **Model Builder** window, click **Component 1 (compl)**.
- 2 In the **Settings** window for **Component**, type **Hexagonal Cell** in the **Label** text field.

## **MATERIALS**

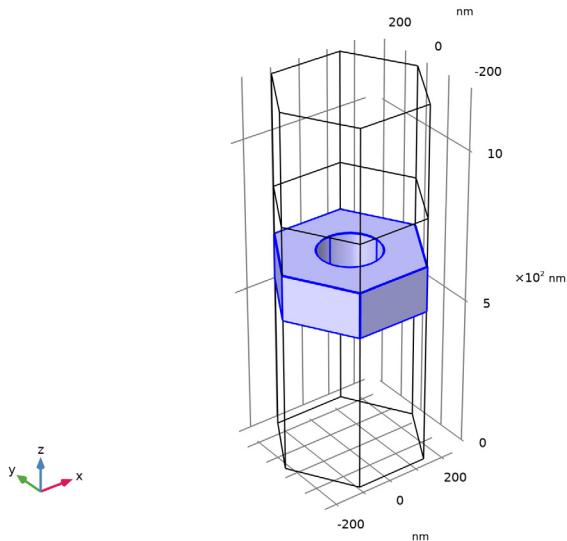
### *Air*

- 1 In the **Model Builder** window, under **Hexagonal Cell (compl)** right-click **Materials** and choose **More Materials>Material Link**.
- 2 In the **Settings** window for **Material Link**, type **Air** in the **Label** text field.

### *Al*

- 1 Right-click **Materials** and choose **More Materials>Material Link**.
- 2 In the **Settings** window for **Material Link**, type **Al** in the **Label** text field.

**3** Select Domain 2 only.

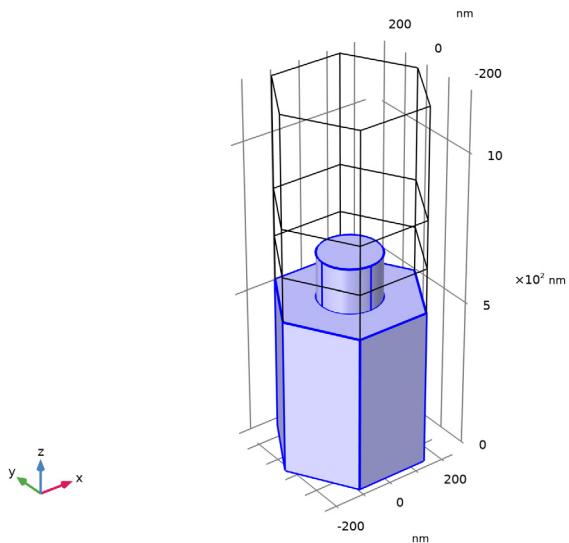


**4** Locate the **Link Settings** section. From the **Material** list, choose **Al (Aluminium) (Rakic et al. 1998: Brendel-Bormann model; n,k 0.0620-248 um) (mat2)**.

*SiO<sub>2</sub>*

- 1** Right-click **Materials** and choose **More Materials>Material Link**.
- 2** In the **Settings** window for **Material Link**, type **SiO<sub>2</sub>** in the **Label** text field.

**3** Select Domains 1 and 5 only.

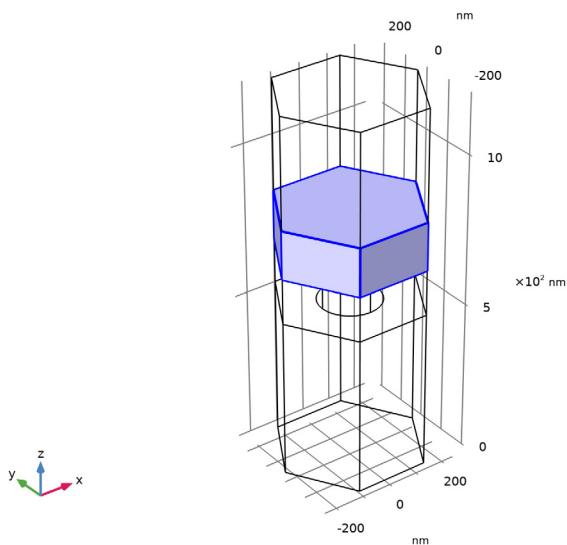


**4** Locate the **Link Settings** section. From the **Material** list, choose **SiO<sub>2</sub> (Silicon dioxide, Silica, Quartz) (Ghosh 1999: a-Quartz, n(o) 0.198-2.05 um) (mat3)**.

#### *Spin-on Glass*

- 1** Right-click **Materials** and choose **More Materials>Material Link**.
- 2** In the **Settings** window for **Material Link**, type **Spin-on Glass** in the **Label** text field.

**3** Select Domain 3 only.



**4** Locate the **Link Settings** section. From the **Material** list, choose **Spin-on Glass (mat4)**.

**5** Click **Go to Material**.

#### GLOBAL DEFINITIONS

##### *Spin-on Glass (mat4)*

Now, it is easy to add the missing material parameter, as a physics interface has specified what material parameters it needs.

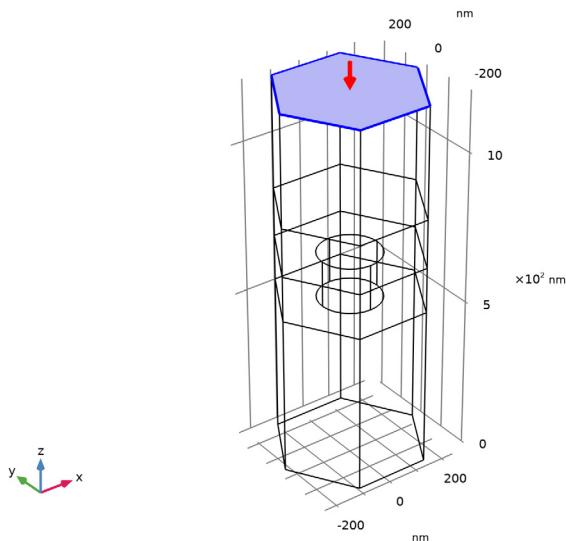
- 1** In the **Model Builder** window, under **Global Definitions>Materials** click **Spin-on Glass (mat4)**.
- 2** In the **Settings** window for **Material**, locate the **Material Contents** section.
- 3** In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Refractive index, real part	n_iso ; nii = n_iso, nij = 0	n_SOG		Refractive index

## ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EWFD)

### Port 1

- 1 In the **Model Builder** window, under **Hexagonal Cell (compl)** right-click **Electromagnetic Waves, Frequency Domain (ewfd)** and choose **Port**.
- 2 Select Boundary 13 only.



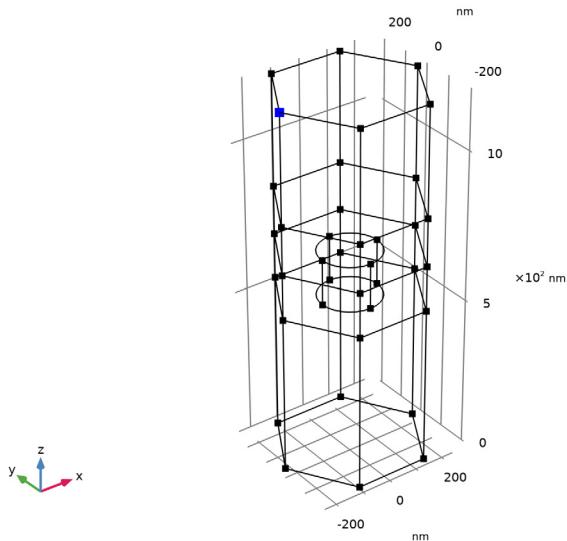
- 3 In the **Settings** window for **Port**, locate the **Port Properties** section.
- 4 From the **Type of port** list, choose **Periodic**.
- 5 Locate the **Port Mode Settings** section. Specify the  $\mathbf{E}_0$  vector as

0	x
1	y
0	z

### Periodic Port Reference Point 1

- 1 In the **Physics** toolbar, click **Attributes** and choose **Periodic Port Reference Point**.

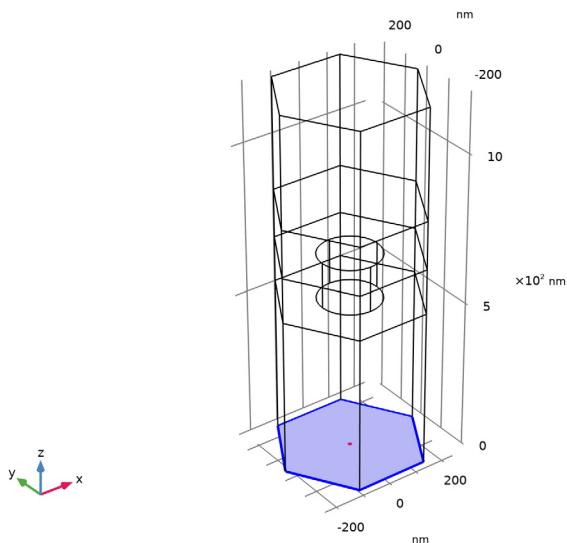
**2** Select Point 5 only.



*Port 2*

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

**2** Select Boundary 3 only.



**3** In the **Settings** window for **Port**, locate the **Port Properties** section.

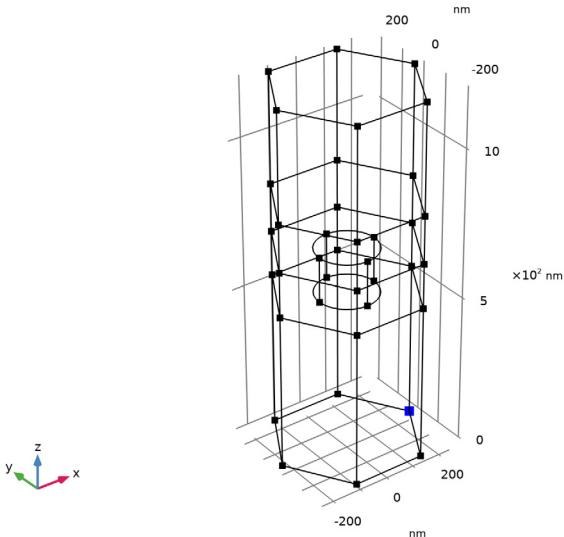
- From the **Type of port** list, choose **Periodic**.
- Locate the **Port Mode Settings** section. Specify the  $\mathbf{E}_0$  vector as

0	x
1	y
0	z

- Locate the **Automatic Diffraction Order Calculation** section. In the  $n$  text field, type `n_SiO2_max`.

*Periodic Port Reference Point /*

- In the **Physics** toolbar, click  **Attributes** and choose **Periodic Port Reference Point**.
- Select Point 34 only.

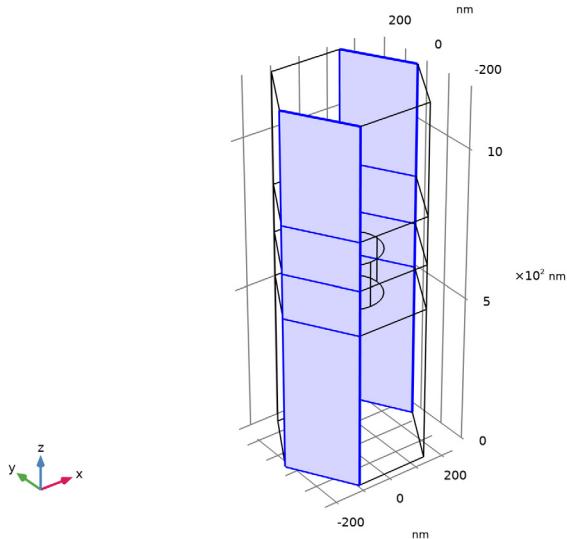


*Periodic Condition /*

Since normal incidence is considered, the field is assumed to be the same on opposing boundaries. Thus, continuity periodic conditions will be used.

- In the **Physics** toolbar, click  **Boundaries** and choose **Periodic Condition**.

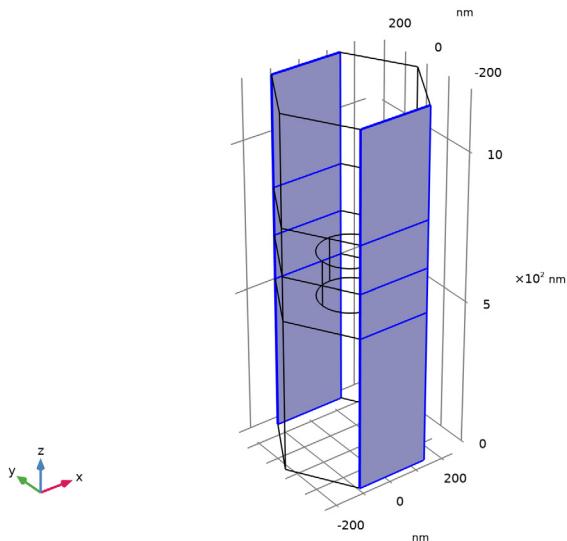
**2** Select Boundaries 1, 4, 7, 10, and 32–35 only.



#### *Periodic Condition 2*

**1** In the **Physics** toolbar, click **Boundaries** and choose **Periodic Condition**.

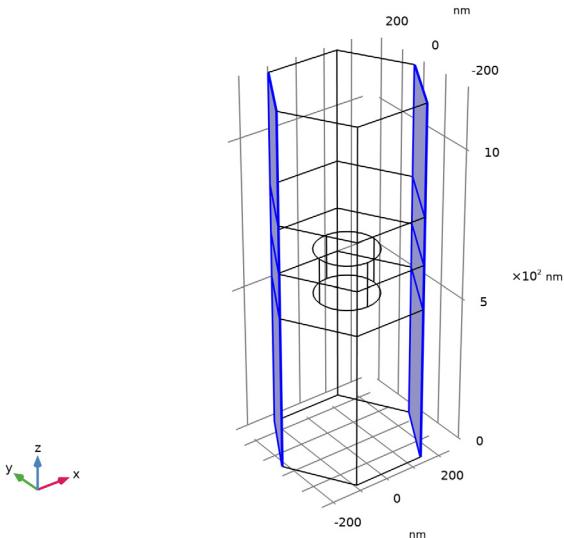
**2** Select Boundaries 14–21 only.



### Periodic Condition 3

1 In the **Physics** toolbar, click  **Boundaries** and choose **Periodic Condition**.

2 Select Boundaries 2, 5, 8, 11, and 28–31 only.



### STUDY 1

#### Step 1: Wavelength Domain

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

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

3 From the **Wavelength unit** list, choose **nm**.

4 In the **Wavelengths** text field, type `range(lda_min,lda_step,lda_max)`.

Now, the wavelength range has been given. Thus, the maximum frequency is known and it is possible to automatically add the necessary diffraction orders.

### ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EWFD)

#### Port 1

1 In the **Model Builder** window, under **Hexagonal Cell (comp1)>Electromagnetic Waves, Frequency Domain (ewfd)** click **Port 1**.

2 In the **Settings** window for **Port**, locate the **Automatic Diffraction Order Calculation** section.

3 Click **Add Diffraction Orders**.

## STUDY 1

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

## RESULTS

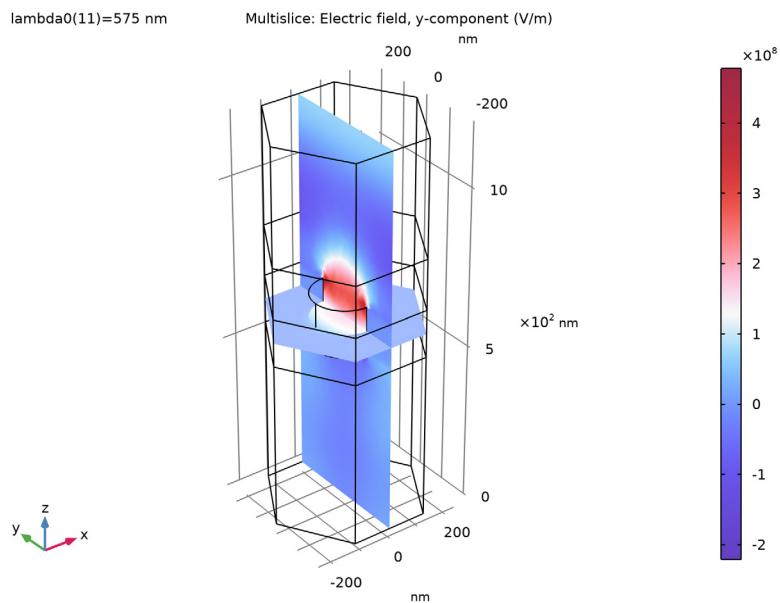
### *Electric Field (ewfd)*

- 1 In the **Settings** window for **3D Plot Group**, locate the **Data** section.
- 2 From the **Parameter value (lambda0 (nm))** list, choose **575**. This correspond to the peak absorption wavelength.

### *Multislice 1*

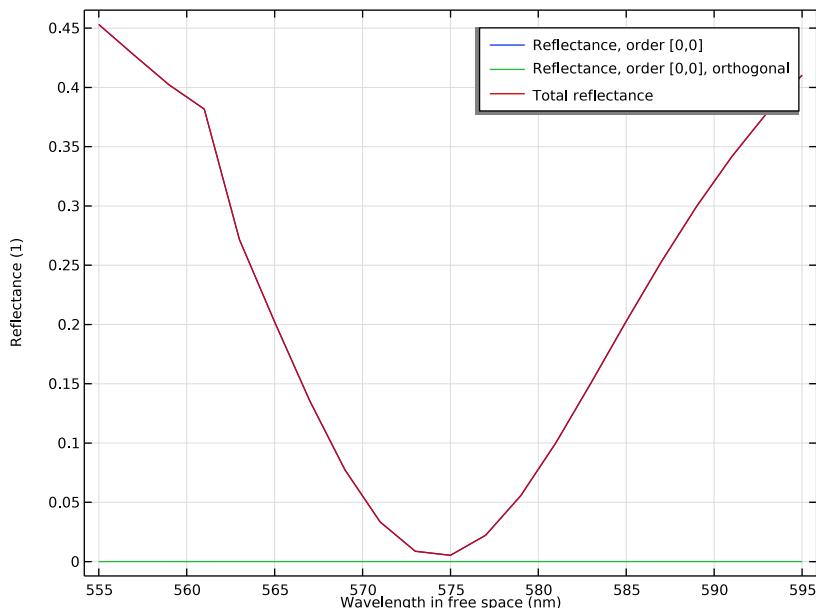
- 1 In the **Model Builder** window, expand the **Electric Field (ewfd)** node, then click **Multislice 1**.
- 2 In the **Settings** window for **Multislice**, locate the **Expression** section.
- 3 In the **Expression** text field, type **ewfd.Ey**.
- 4 Locate the **Multiplane Data** section. Find the **Y-planes** subsection. In the **Planes** text field, type **0**.
- 5 Locate the **Coloring and Style** section. Click  **Change Color Table**.
- 6 In the **Color Table** dialog box, select **Wave>WaveLight** in the tree.
- 7 Click **OK**.

8 In the **Electric Field (ewfd)** toolbar, click  **Plot**.



### Reflectance (ewfd)

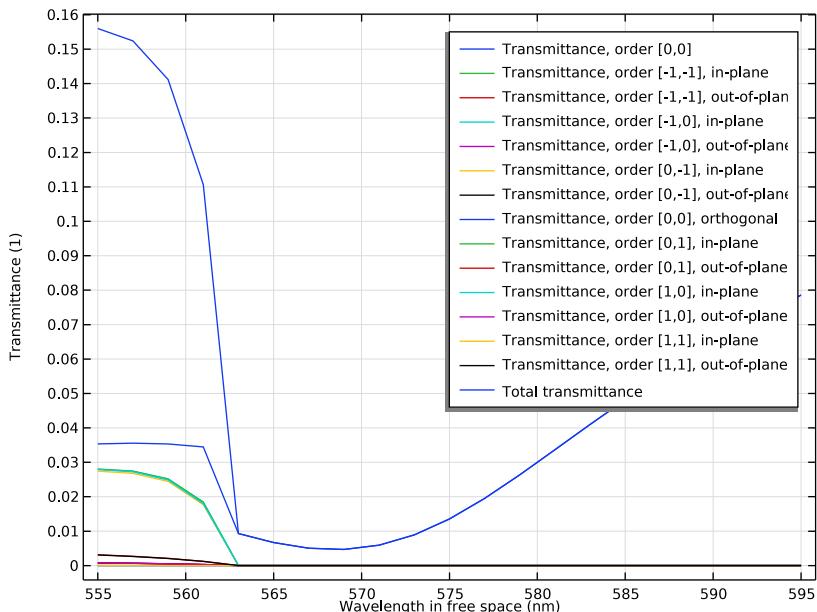
In the **Model Builder** window, under **Results** click **Reflectance (ewfd)**.



This plot shows that the reflectance at 575 nm is close to zero.

### *Transmittance (ewfd)*

- In the **Model Builder** window, click **Transmittance (ewfd)**.



This plot shows that also the transmittance is very small at 575 nm.

### *Reflectance, Transmittance, and Absorptance (ewfd)*

Now, make a plot including also the absorptance.

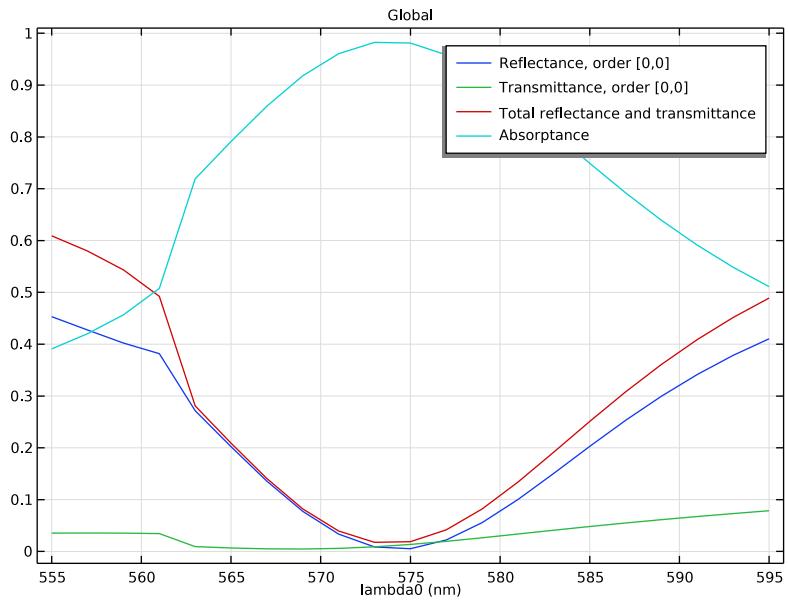
- In the **Home** toolbar, click **Add Plot Group** and choose **ID Plot Group**.
- In the **Settings** window for **ID Plot Group**, type Reflectance, Transmittance, and Absorptance (ewfd) in the **Label** text field.

#### *Global |*

- Right-click **Reflectance, Transmittance, and Absorptance (ewfd)** and choose **Global**.
- In the **Settings** window for **Global**, locate the **y-Axis Data** section.
- In the table, enter the following settings:

Expression	Unit	Description
ewfd.Rorder_0_0	1	Reflectance, order [0,0]
ewfd.Torder_0_0	1	Transmittance, order [0,0]
ewfd.RTtotal	1	Total reflectance and transmittance
ewfd.Atotal	1	Absorptance

**4** In the **Reflectance, Transmittance, and Absorptance (ewfd)** toolbar, click  **Plot**.

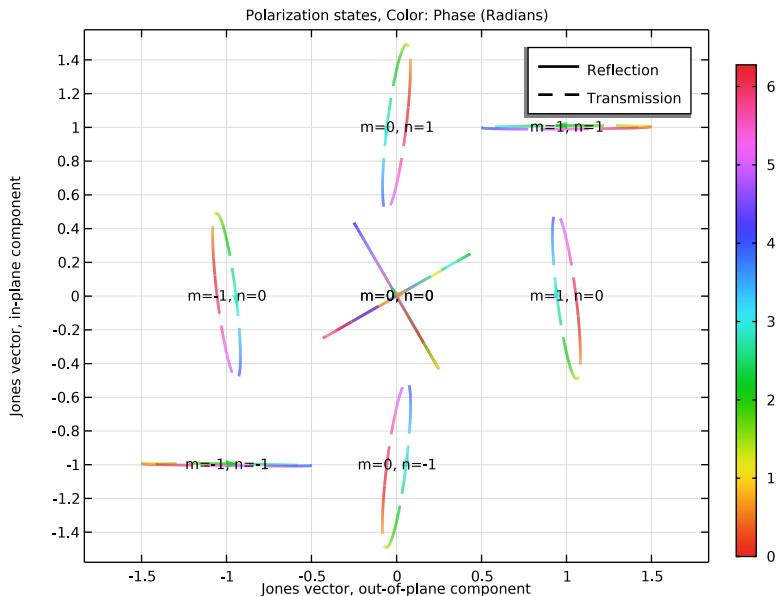


At 575 nm, almost all the power is absorbed.

#### *Polarization Plot (ewfd)*

**I** In the **Model Builder** window, under **Results** click **Polarization Plot (ewfd)**.

- 2 In the **Polarization Plot (ewfd)** toolbar, click  **Plot**.



The modes shown in this plot, correspond to the modes (the green points encircled by the blue circle) in [Figure 2](#). However, when converting mode numbers for the hexagonal structure, the theory discussed in the [Model Definition](#) must be used. Thus, for instance, mode ( $m = -1, n = -1$ ) in this plot corresponds to mode ( $m = 0, n = -2$ ) in [Figure 2](#).

### *Array 3D /*

Now, build an array plot of the electric field in many unit cells. This is done using three array datasets.

- 1 In the **Results** toolbar, click  **More Datasets** and choose **Array 3D**.
- 2 In the **Settings** window for **Array 3D**, locate the **Array Size** section.
- 3 From the **Array type** list, choose **Linear**.
- 4 In the **Size** text field, type 10.
- 5 Locate the **Displacement** section. From the **Method** list, choose **Manual**.
- 6 In the **Y** text field, type  $a$ .

This dataset produces a row of hexagonal cells in  $y$  direction.

### *Array 3D 2*

- 1 In the **Results** toolbar, click  **More Datasets** and choose **Array 3D**.
- 2 In the **Settings** window for **Array 3D**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Array 3D 1**.
- 4 Locate the **Array Size** section. From the **Array type** list, choose **Linear**.
- 5 In the **Size** text field, type **2**.
- 6 Locate the **Displacement** section. From the **Method** list, choose **Manual**.
- 7 In the **x** text field, type  **$\sqrt{3} * a / 2$** .
- 8 In the **y** text field, type  **$a / 2$** .
- 9 Click to expand the **Advanced** section. Clear the **Check for overlap between cells** check box, to avoid error messages from the algorithm that checks if cells overlap.

This dataset produces a row in the *y* direction with two staggered hexagonal cells in the *x* direction.

### *Array 3D 3*

- 1 In the **Results** toolbar, click  **More Datasets** and choose **Array 3D**.
- 2 In the **Settings** window for **Array 3D**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Array 3D 2**.
- 4 Locate the **Array Size** section. From the **Array type** list, choose **Linear**.
- 5 In the **Size** text field, type **5**.
- 6 Locate the **Displacement** section. From the **Method** list, choose **Manual**.
- 7 In the **x** text field, type  **$\sqrt{3} * a$** .
- 8 Locate the **Advanced** section. Clear the **Check for overlap between cells** check box.

This is the dataset that will be used in the plot group.

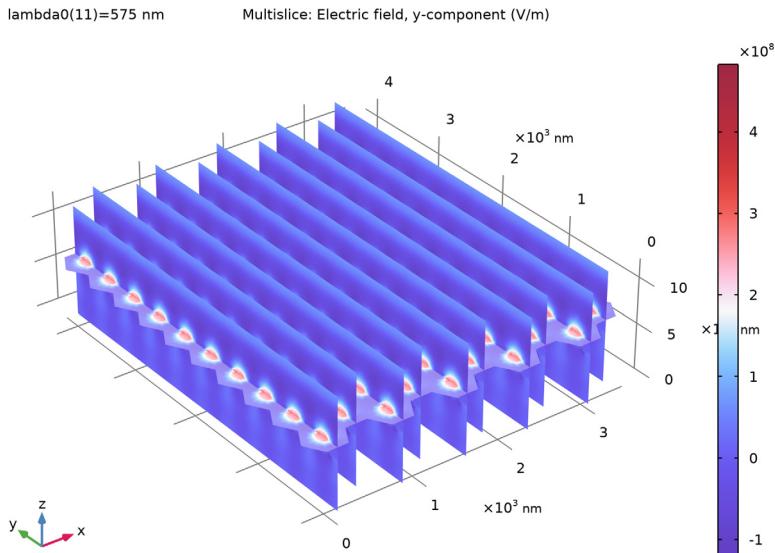
### *Hexagonally Arrayed Field Plot*

- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type **Hexagonally Arrayed Field Plot** in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Array 3D 3**.
- 4 From the **Parameter value (lambda0 (nm))** list, choose **575**.
- 5 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

### *Multislice 1*

- 1 In the **Hexagonally Arrayed Field Plot** toolbar, click  **More Plots** and choose **Multislice**.

- 2 In the **Settings** window for **Multislice**, locate the **Expression** section.
- 3 In the **Expression** text field, type `ewfd.Ey`.
- 4 Locate the **Multiplane Data** section. Find the **x-planes** subsection. From the **Entry method** list, choose **Coordinates**.
- 5 In the **Coordinates** text field, type `range(0[nm],sqrt(3)*a/2,9*sqrt(3)*a/2)`.
- 6 Find the **y-planes** subsection. In the **Planes** text field, type `0`.
- 7 Find the **z-planes** subsection. From the **Entry method** list, choose **Coordinates**.
- 8 In the **Coordinates** text field, type `height/2+t_A1/2`.
- 9 Locate the **Coloring and Style** section. Click  **Change Color Table**.
- 10 In the **Color Table** dialog box, select **Wave>WaveLight** in the tree.
- 11 Click **OK**.
- 12 In the **Hexagonally Arrayed Field Plot** toolbar, click  **Plot**.



Add a transparency node to get a better view of the field in all cells.

#### *Transparency I*

Right-click **Multislice I** and choose **Transparency**.

#### *Hexagonally Arrayed Field Plot*

Add a volume plot to see more of the contours of the hexagonal cells.

### *Volume 1*

- 1 In the **Model Builder** window, right-click **Hexagonally Arrayed Field Plot** and choose **Volume**.
- 2 In the **Settings** window for **Volume**, locate the **Expression** section.
- 3 In the **Expression** text field, type `ewfd.Ey`.
- 4 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Multislice 1**.

### *Transparency 1*

Right-click **Volume 1** and choose **Transparency**.

### *Hexagonally Arrayed Field Plot*

Finally, add a volume plot indicating the aluminum layer.

### *Volume 2*

- 1 In the **Model Builder** window, right-click **Hexagonally Arrayed Field Plot** and choose **Volume**.
- 2 In the **Settings** window for **Volume**, locate the **Coloring and Style** section.
- 3 From the **Coloring** list, choose **Uniform**.
- 4 From the **Color** list, choose **Gray**.

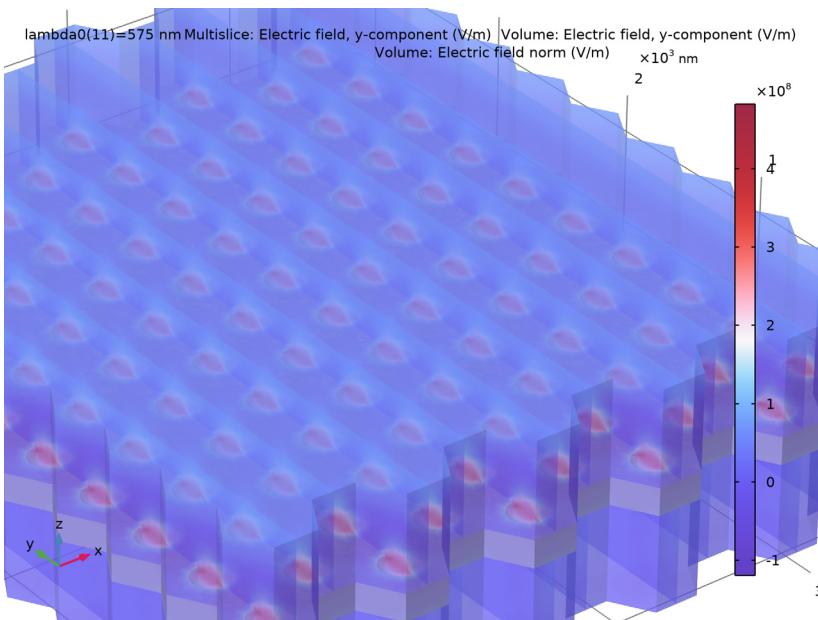
### *Selection 1*

- 1 Right-click **Volume 2** and choose **Selection**.
- 2 Select Domain 2 only, to only show the aluminum layer.

### *Volume 2*

- 1 In the **Model Builder** window, click **Volume 2**.
- 2 In the **Settings** window for **Volume**, click to expand the **Quality** section.
- 3 From the **Resolution** list, choose **No refinement**.  
It enables elements not to split into smaller patches during rendering.
- 4 In the **Hexagonally Arrayed Field Plot** toolbar, click  **Plot**.

- 5 Click the  **Zoom In** button in the **Graphics** toolbar.



This concludes the first part of this model.

## ROOT

Now, model the hexagonal structure using a rectangular unit cell.

### ADD COMPONENT

In the **Model Builder** window, right-click the root node and choose **Add Component>3D**.

### RECTANGULAR CELL

In the **Settings** window for **Component**, type **Rectangular Cell** in the **Label** text field.

### GEOMETRY 2

1 In the **Model Builder** window, under **Rectangular Cell (comp2)** click **Geometry 2**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

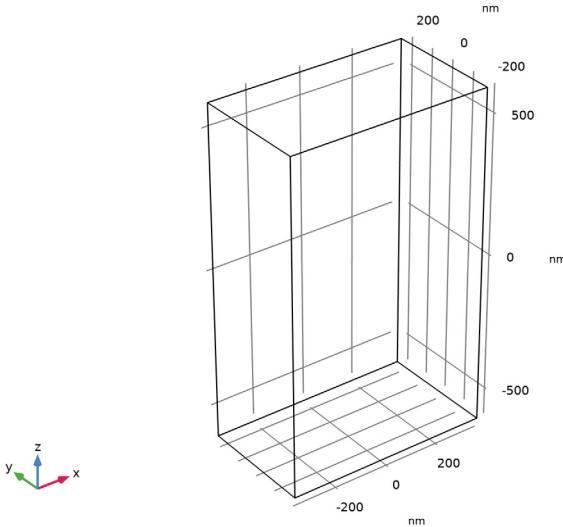
3 From the **Length unit** list, choose **nm**.

#### Block 1 (blk1)

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

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

- 3 In the **Width** text field, type `d_rect_x`.
- 4 In the **Depth** text field, type `d_rect_y`.
- 5 In the **Height** text field, type `height`.
- 6 Locate the **Position** section. From the **Base** list, choose **Center**.
- 7 Click  **Build Selected**.
- 8 Click the  **Wireframe Rendering** button in the **Graphics** toolbar.

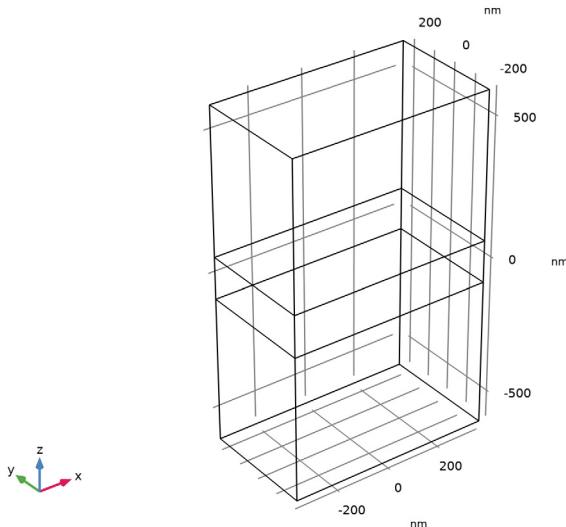


- 9 Right-click **Block 1 (blk1)** and choose **Duplicate**.

#### *Block 2 (blk2)*

- 1 In the **Model Builder** window, click **Block 2 (blk2)**.
- 2 In the **Settings** window for **Block**, locate the **Size and Shape** section.
- 3 In the **Height** text field, type `t_A1`.

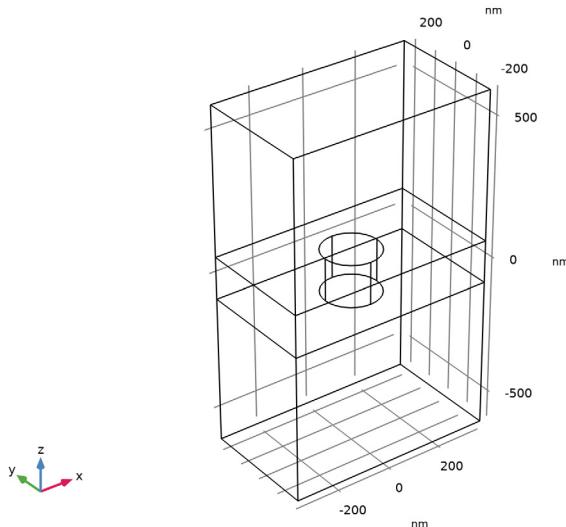
4 Click  **Build Selected**.



#### Cylinder 1 (cyl1)

- 1 In the **Geometry** toolbar, click  **Cylinder**.
- 2 In the **Settings** window for **Cylinder**, locate the **Size and Shape** section.
- 3 In the **Radius** text field, type `r0`.
- 4 In the **Height** text field, type `t_A1`.
- 5 Locate the **Position** section. In the **z** text field, type `-t_A1/2`.

**6** Click  **Build Selected**.

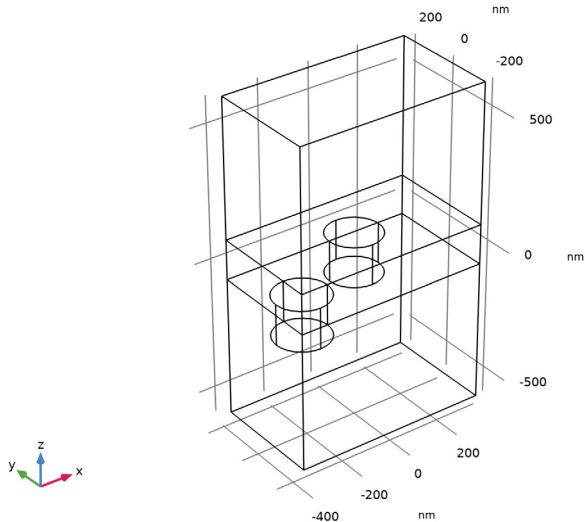


**7** Right-click **Cylinder 1 (cyl1)** and choose **Duplicate**.

*Cylinder 2 (cyl2)*

- 1** In the **Model Builder** window, click **Cylinder 2 (cyl2)**.
- 2** In the **Settings** window for **Cylinder**, locate the **Position** section.
- 3** In the **x** text field, type  $-d_{rect\_x}/2$ .
- 4** In the **y** text field, type  $-d_{rect\_y}/2$ .

**5** Click  **Build Selected.**



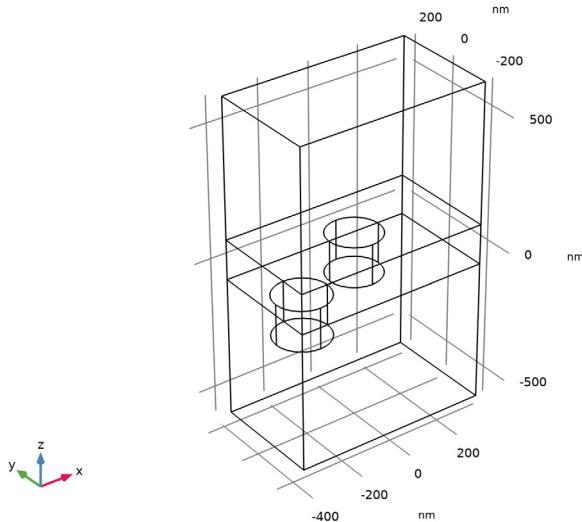
#### *Block 2 (blk2)*

In the **Model Builder** window, right-click **Block 2 (blk2)** and choose **Duplicate**.

#### *Block 3 (blk3)*

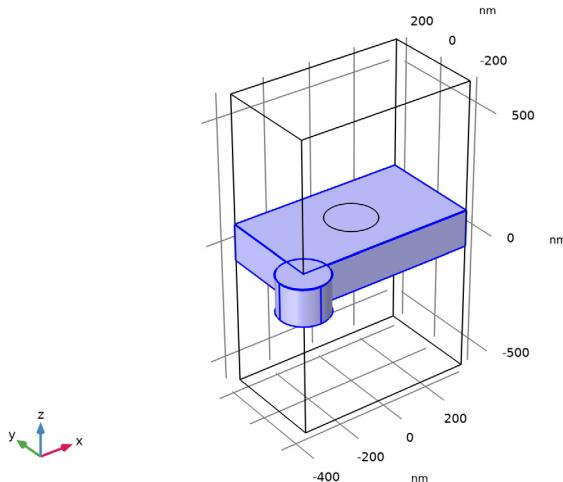
I In the **Model Builder** window, click **Block 3 (blk3)**.

- 2 In the **Settings** window for **Block**, click  **Build Selected**.

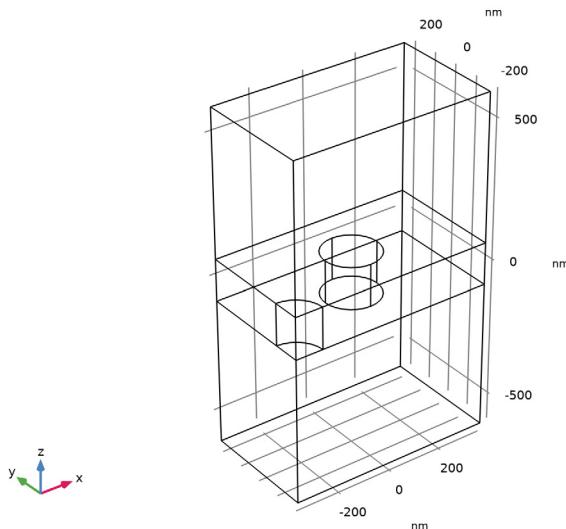


*Intersection 1 (int1)*

- 1 In the **Geometry** toolbar, click  **Booleans and Partitions** and choose **Intersection**.  
2 Select the objects **blk3** and **cyl2** only.



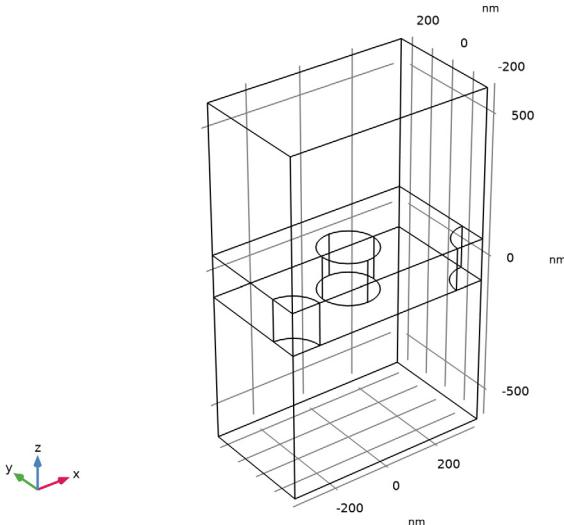
- 3 In the **Settings** window for **Intersection**, click  **Build Selected**.



#### *Mirror 1 (mir1)*

- 1 In the **Geometry** toolbar, click  **Transforms** and choose **Mirror**.
- 2 Select the object **int1** only.
- 3 In the **Settings** window for **Mirror**, locate the **Input** section.
- 4 Select the **Keep input objects** check box.
- 5 Locate the **Normal Vector to Plane of Reflection** section. In the **x** text field, type **1**.
- 6 In the **z** text field, type **0**.

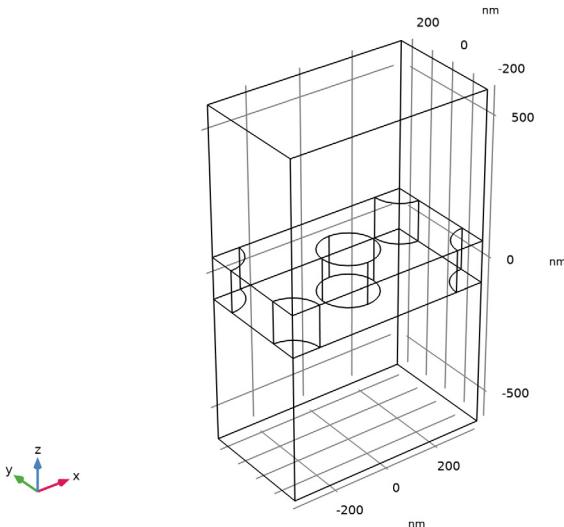
7 Click  **Build Selected**.



#### *Mirror 2 (mir2)*

- 1 In the **Geometry** toolbar, click  **Transforms** and choose **Mirror**.
- 2 Select the objects **int1** and **mir1** only.
- 3 In the **Settings** window for **Mirror**, locate the **Input** section.
- 4 Select the **Keep input objects** check box.
- 5 Locate the **Normal Vector to Plane of Reflection** section. In the **y** text field, type **1**.
- 6 In the **z** text field, type **0**.

7 Click  **Build Selected**.



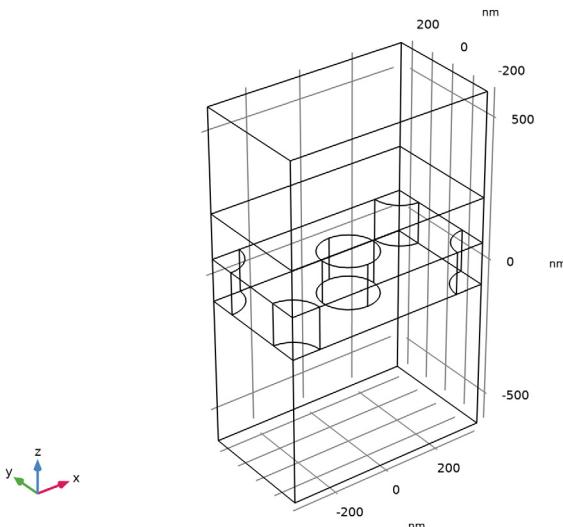
#### *Block 3 (blk3)*

Right-click **Block 3 (blk3)** and choose **Duplicate**.

#### *Block 4 (blk4)*

- 1 In the **Model Builder** window, click **Block 4 (blk4)**.
- 2 In the **Settings** window for **Block**, locate the **Size and Shape** section.
- 3 In the **Height** text field, type `t_SOG`.
- 4 Locate the **Position** section. In the **z** text field, type `(t_A1+t_SOG)/2`.

- 5 Click  **Build All Objects**.



#### ADD PHYSICS

- 1 In the **Home** toolbar, click  **Add Physics** to open the **Add Physics** window.
- 2 Go to the **Add Physics** window.
- 3 In the tree, select **Optics>Wave Optics>Electromagnetic Waves, Frequency Domain (ewfd)**.
- 4 Click **Add to Rectangular Cell** in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Physics** to close the **Add Physics** window.

#### STUDY 1

##### Step 1: Wavelength Domain

Just make sure that the newly added physics interface is not used with the first study.

- 1 In the **Model Builder** window, under **Study 1** click **Step 1: Wavelength Domain**.
- 2 In the **Settings** window for **Wavelength Domain**, locate the **Physics and Variables Selection** section.

- 3** In the table, enter the following settings:

Physics interface	Solve for	Equation form
Electromagnetic Waves, Frequency Domain (ewfd)	✓	Automatic (Frequency domain)
Electromagnetic Waves, Frequency Domain 2 (ewfd2)		Automatic (Frequency domain)

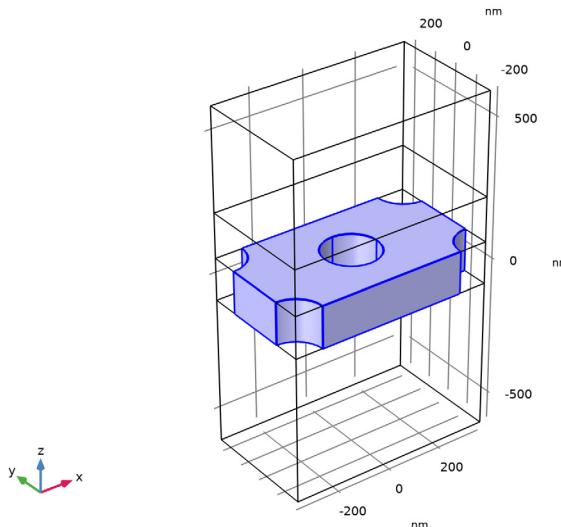
## MATERIALS

Air

- In the **Model Builder** window, under **Rectangular Cell (comp2)** right-click **Materials** and choose **More Materials>Material Link**.
- In the **Settings** window for **Material Link**, type Air in the **Label** text field.

Al

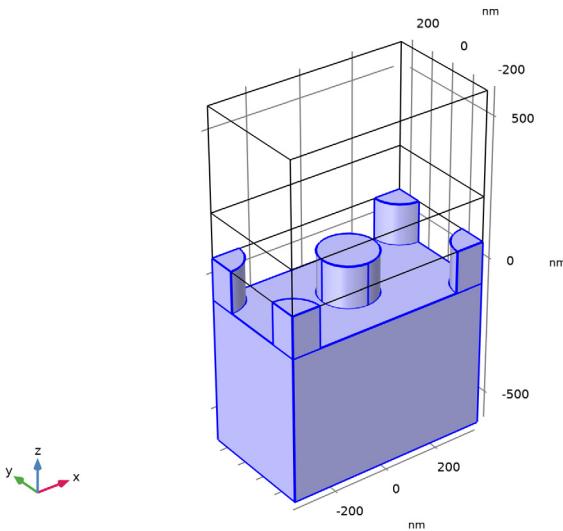
- Right-click **Materials** and choose **More Materials>Material Link**.
- In the **Settings** window for **Material Link**, type Al in the **Label** text field.
- Select Domain 5 only.



- Locate the **Link Settings** section. From the **Material** list, choose **Al (Aluminium) (Rakic et al. 1998: Brendel-Bormann model; n,k 0.0620-248 um) (mat2)**.

## *SiO<sub>2</sub>*

- 1 Right-click **Materials** and choose **More Materials>Material Link**.
- 2 In the **Settings** window for **Material Link**, type **SiO<sub>2</sub>** in the **Label** text field.
- 3 Select Domains 1, 2, and 6–9 only.

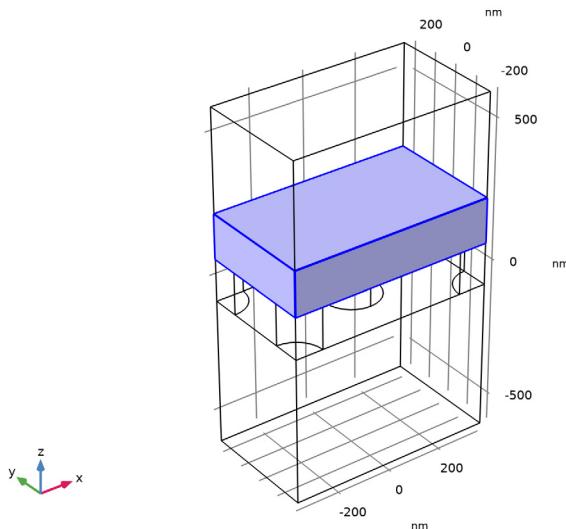


- 4 Locate the **Link Settings** section. From the **Material** list, choose **SiO<sub>2</sub> (Silicon dioxide, Silica, Quartz) (Ghosh 1999: a-Quartz, n(o) 0.198-2.05 um) (mat3)**.

## *Spin-on Glass*

- 1 Right-click **Materials** and choose **More Materials>Material Link**.
- 2 In the **Settings** window for **Material Link**, type **Spin-on Glass** in the **Label** text field.

**3** Select Domain 3 only.



**4** Locate the **Link Settings** section. From the **Material** list, choose **Spin-on Glass (mat4)**.

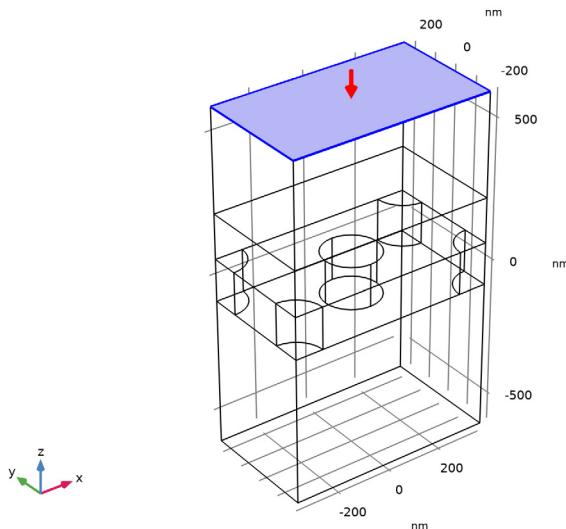
#### ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN 2 (EWFD2)

In the **Model Builder** window, under **Rectangular Cell (comp2)** click **Electromagnetic Waves, Frequency Domain 2 (ewfd2)**.

*Port 1*

I In the **Physics** toolbar, click **Boundaries** and choose **Port**.

**2** Select Boundary 13 only.



**3** In the **Settings** window for **Port**, locate the **Port Properties** section.

**4** From the **Type of port** list, choose **Periodic**.

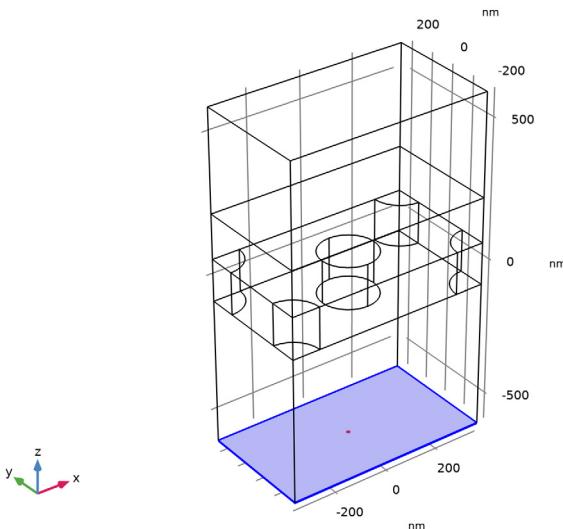
**5** Locate the **Port Mode Settings** section. Specify the  $\mathbf{E}_0$  vector as

0	x
1	y
0	z

*Port 2*

I In the **Physics** toolbar, click **Boundaries** and choose **Port**.

**2** Select Boundary 3 only.



**3** In the **Settings** window for **Port**, locate the **Port Properties** section.

**4** From the **Type of port** list, choose **Periodic**.

**5** Locate the **Port Mode Settings** section. Specify the  $\mathbf{E}_0$  vector as

0	x
1	y
0	z

**6** Locate the **Automatic Diffraction Order Calculation** section. In the *n* text field, type `n_SiO2_max`.

#### *Periodic Condition 1*

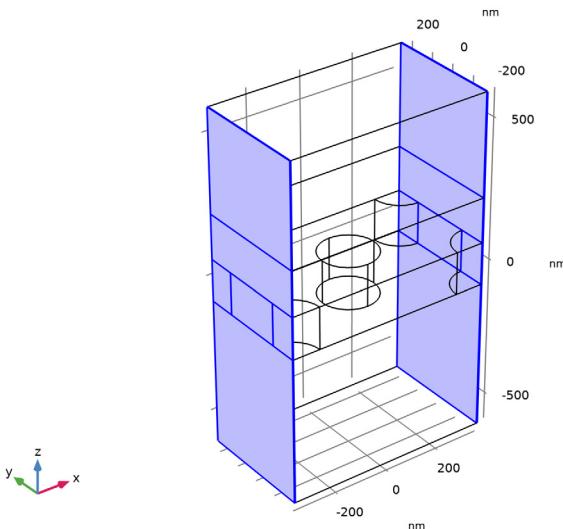
**1** In the **Physics** toolbar, click **Boundaries** and choose **Periodic Condition**.

**2** In the **Settings** window for **Periodic Condition**, locate the **Boundary Selection** section.

**3** Click **Paste Selection**.

**4** In the **Paste Selection** dialog box, type `1, 4, 7, 10, 14, 18, 42-47` in the **Selection** text field.

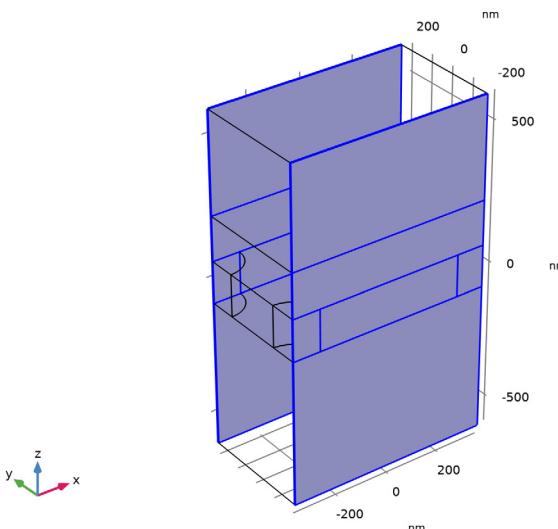
**5** Click **OK**.



#### *Periodic Condition 2*

- 1** In the **Physics** toolbar, click **Boundaries** and choose **Periodic Condition**.
- 2** In the **Settings** window for **Periodic Condition**, locate the **Boundary Selection** section.
- 3** Click **Paste Selection**.
- 4** In the **Paste Selection** dialog box, type **2, 5, 8, 11, 22-27, 34, 39** in the **Selection** text field.

**5** Click **OK**.



#### 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>Wavelength Domain**.
- 4** Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Electromagnetic Waves, Frequency Domain (ewfd)**.
- 5** Click **Add Study** in the window toolbar.
- 6** In the **Model Builder** window, click the root node.
- 7** In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.

#### STUDY 2

##### Step 1: Wavelength Domain

- 1** In the **Settings** window for **Wavelength Domain**, locate the **Study Settings** section.
- 2** From the **Wavelength unit** list, choose **nm**.
- 3** In the **Wavelengths** text field, type `range(lda_min,lda_step,lda_max)`.

## ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN 2 (EWFD2)

### Port 1

- 1 In the **Model Builder** window, under **Rectangular Cell (comp2)>Electromagnetic Waves, Frequency Domain 2 (ewfd2)** click **Port 1**.
- 2 In the **Settings** window for **Port**, locate the **Automatic Diffraction Order Calculation** section.
- 3 Click **Add Diffraction Orders**. Now, that the wavelength range has been specified in the study, the diffraction orders can be automatically generated.

### STUDY 2

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

### RESULTS

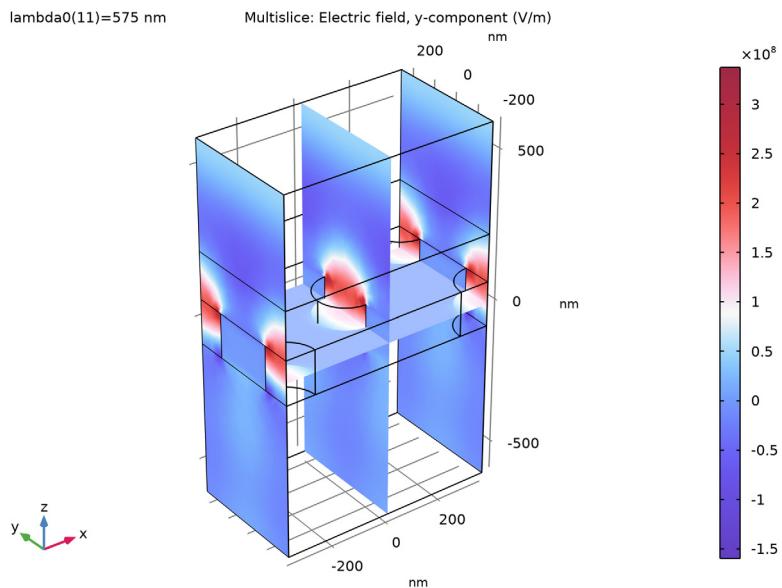
#### Electric Field (ewfd2)

- 1 In the **Settings** window for **3D Plot Group**, locate the **Data** section.
- 2 From the **Parameter value (lambda0 (nm))** list, choose **575**.

#### Multislice 1

- 1 In the **Model Builder** window, expand the **Electric Field (ewfd2)** node, then click **Multislice 1**.
- 2 In the **Settings** window for **Multislice**, locate the **Expression** section.
- 3 In the **Expression** text field, type **ewfd2.Ey**.
- 4 Locate the **Multiplane Data** section. Find the **X-planes** subsection. From the **Entry method** list, choose **Coordinates**.
- 5 In the **Coordinates** text field, type **-d\_rect\_x/2 0 d\_rect\_x/2**.
- 6 Find the **Y-planes** subsection. In the **Planes** text field, type **0**.
- 7 Locate the **Coloring and Style** section. Click  **Change Color Table**.
- 8 In the **Color Table** dialog box, select **Wave>WaveLight** in the tree.
- 9 Click **OK**.

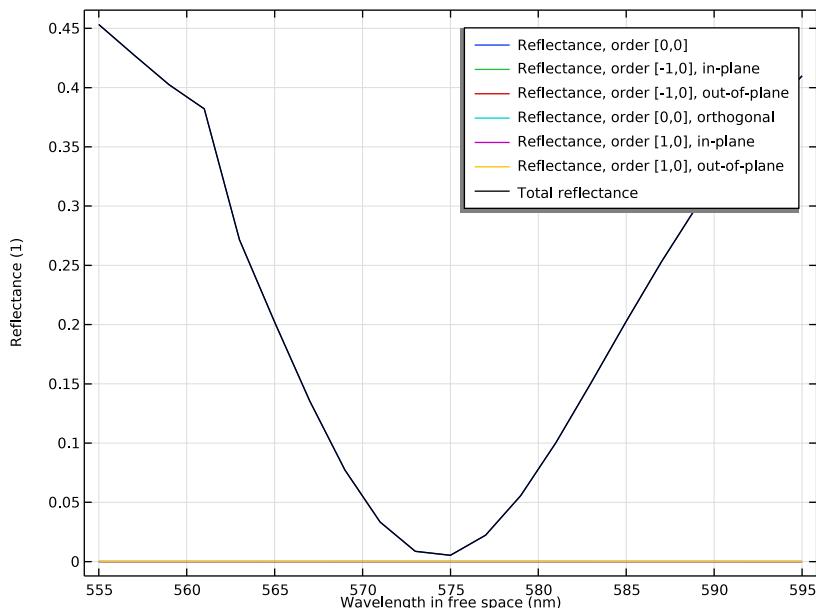
10 In the **Electric Field (ewfd2)** toolbar, click  **Plot**.



This plot shows that the field is indeed periodic along the diagonals in the  $xy$  plane, and from the leftmost boundary to the rightmost boundary, and from the front to the back boundary.

### Reflectance (ewfd2)

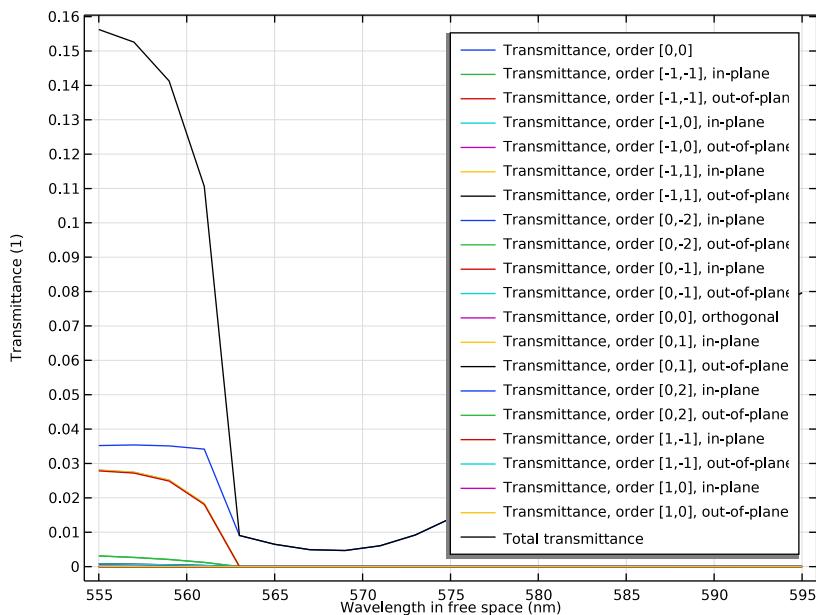
In the **Model Builder** window, under **Results** click **Reflectance (ewfd2)**.



Almost zero reflectance is observed at 575 nm.

## Transmittance (ewfd2)

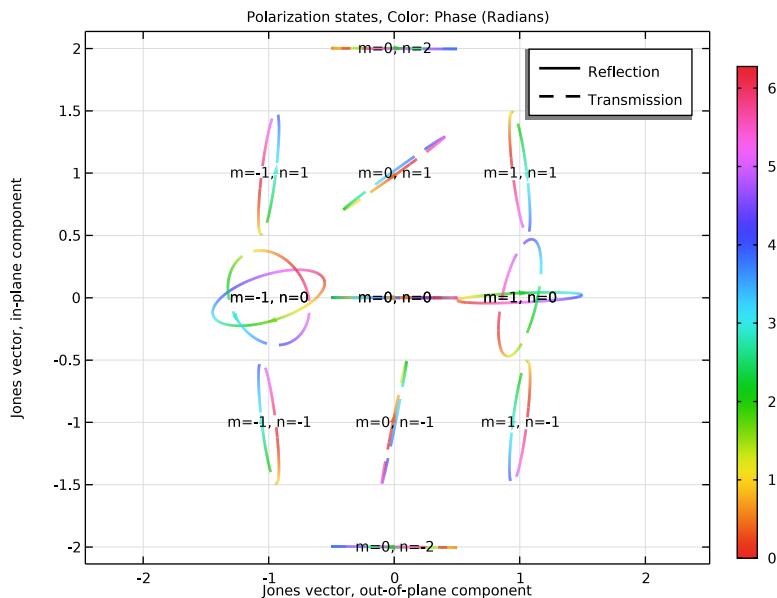
In the **Model Builder** window, click **Transmittance (ewfd2)**.



The transmittance is also small at 575 nm.

### Polarization Plot (ewfd2)

- In the **Model Builder** window, click **Polarization Plot (ewfd2)**.



For normal incidence, the in-plane and out-of-plane polarization directions are degenerate. However, for this model, we specified the exciting field to be polarized in the  $y$  direction. Thus, we can deduce that the out-of-plane direction points in the  $y$  direction, and the in-plane direction points in the  $x$  direction.

The polarization states are the same for the modes that coincides with those for the hexagonal cell. The modes ( $m = 0, n = +/-1$ ) and ( $m = +/-1, n = 0$ ) are not proper hexagonal modes and do not carry any power, as will be shown later.

### Global 2

- In the **Model Builder** window, right-click **Reflectance, Transmittance, and Absorptance (ewfd)** and choose **Global**.
- In the **Settings** window for **Global**, locate the **Data** section.
- From the **Dataset** list, choose **Study 2/Solution 2 (3) (sol2)**.

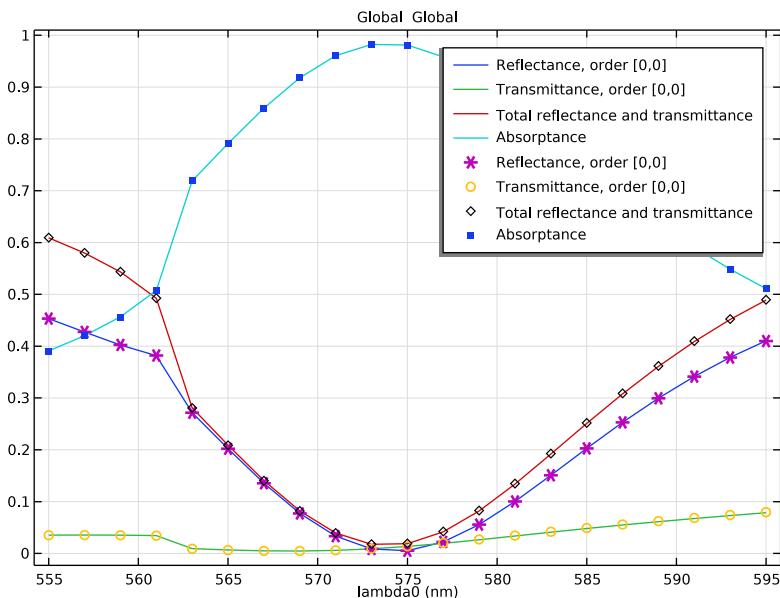
**4** Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
ewfd2.Rorder_0_0	1	Reflectance, order [0,0]
ewfd2.Torder_0_0	1	Transmittance, order [0,0]
ewfd2.RTtotal	1	Total reflectance and transmittance
ewfd2.Atotal	1	Absorptance

**5** Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

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

**7** In the **Reflectance, Transmittance, and Absorptance (ewfd)** toolbar, click  **Plot**.



The reflectance, transmittance, and absorptance plots are very similar although they do not completely overlap.

#### Invalid Diffraction Orders

Now, show that the diffraction efficiencies are very small for modes that are available for the rectangular unit cell, but not for the hexagonal unit cell.

**I** In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.

**2** In the **Settings** window for **ID Plot Group**, type Invalid Diffraction Orders in the **Label** text field.

**3** Locate the **Data** section. From the **Dataset** list, choose **Study 2/Solution 2 (3) (sol2)**.

*Global |*

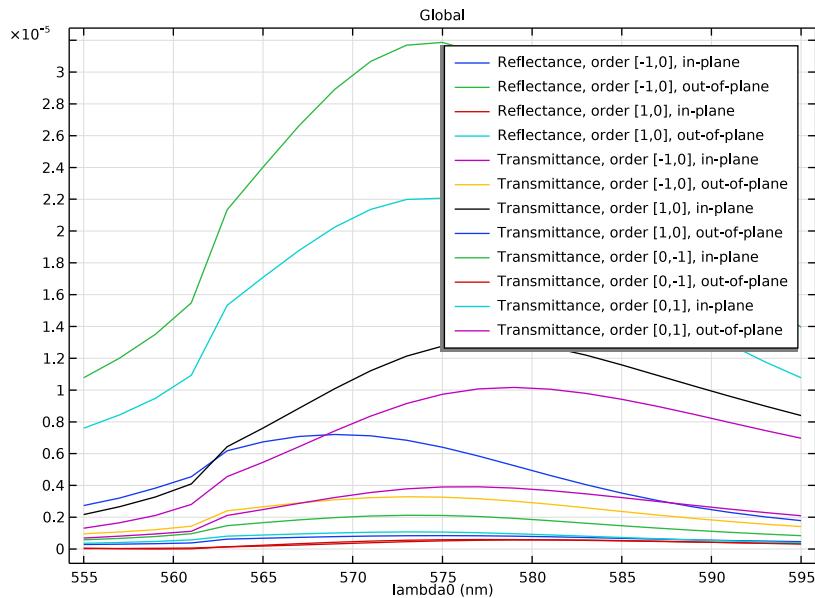
**1** Right-click **Invalid Diffraction Orders** and choose **Global**.

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

**3** In the table, enter the following settings:

<b>Expression</b>	<b>Unit</b>	<b>Description</b>
ewfd2.Rorder_n1_0_ip	1	Reflectance, order [-1,0], in-plane
ewfd2.Rorder_n1_0_op	1	Reflectance, order [-1,0], out-of-plane
ewfd2.Rorder_p1_0_ip	1	Reflectance, order [1,0], in-plane
ewfd2.Rorder_p1_0_op	1	Reflectance, order [1,0], out-of-plane
ewfd2.Torder_n1_0_ip	1	Transmittance, order [-1,0], in-plane
ewfd2.Torder_n1_0_op	1	Transmittance, order [-1,0], out-of-plane
ewfd2.Torder_p1_0_ip	1	Transmittance, order [1,0], in-plane
ewfd2.Torder_p1_0_op	1	Transmittance, order [1,0], out-of-plane
ewfd2.Torder_0_n1_ip	1	Transmittance, order [0,-1], in-plane
ewfd2.Torder_0_n1_op	1	Transmittance, order [0,-1], out-of-plane
ewfd2.Torder_0_p1_ip	1	Transmittance, order [0,1], in-plane
ewfd2.Torder_0_p1_op	1	Transmittance, order [0,1], out-of-plane

- 4 In the **Invalid Diffraction Orders** toolbar, click  **Plot**.



Indeed, the diffraction efficiencies for these modes are all less than  $10^{-4}$ .

#### *Array 3D 4*

Finally, build a field plot over many periodic cells, using an array dataset.

- 1 In the **Results** toolbar, click  **More Datasets** and choose **Array 3D**.
- 2 In the **Settings** window for **Array 3D**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 2/Solution 2 (3) (sol2)**.
- 4 Locate the **Array Size** section. In the **X size** text field, type 5.
- 5 In the **Y size** text field, type 10.

#### *Rectangularly Arrayed Field Plot*

- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type *Rectangularly Arrayed Field Plot* in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Array 3D 4**.
- 4 From the **Parameter value ( $\lambda_0$  (nm))** list, choose **573**.
- 5 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

### *Volume 1*

- 1 Right-click **Rectangularly Arrayed Field Plot** and choose **Volume**.
- 2 In the **Rectangularly Arrayed Field Plot** toolbar, click  **Plot**.
- 3 In the **Model Builder** window, click **Volume 1**.
- 4 In the **Settings** window for **Volume**, locate the **Expression** section.
- 5 In the **Expression** text field, type `ewfd2.Ey`.
- 6 Locate the **Coloring and Style** section. Click  **Change Color Table**.
- 7 In the **Color Table** dialog box, select **Wave>WaveLight** in the tree.
- 8 Click **OK**.

### *Transparency 1*

- 1 Right-click **Volume 1** and choose **Transparency**.
- 2 In the **Settings** window for **Transparency**, locate the **Transparency** section.
- 3 Set the **Transparency** value to **0.2**.

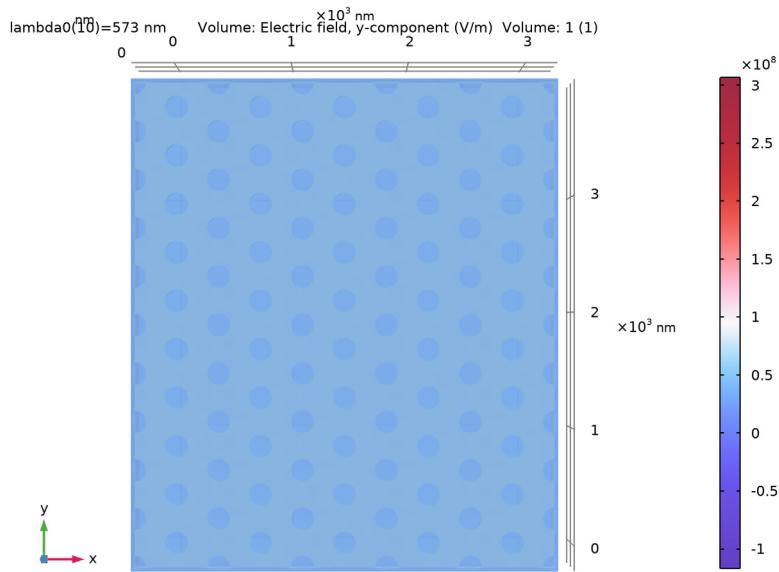
### *Volume 2*

- 1 In the **Model Builder** window, right-click **Rectangularly Arrayed Field Plot** and choose **Volume**.
- 2 In the **Settings** window for **Volume**, locate the **Expression** section.
- 3 In the **Expression** text field, type `1`.
- 4 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
- 5 From the **Color** list, choose **Gray**.
- 6 Locate the **Quality** section. From the **Resolution** list, choose **No refinement**.

### *Selection 1*

- 1 Right-click **Volume 2** and choose **Selection**.
- 2 Select Domain 5 only, to include only the aluminum layer.
- 3 In the **Rectangularly Arrayed Field Plot** toolbar, click  **Plot**.

- 4 Click the  **Go to XY View** button in the **Graphics** toolbar.



This view clearly shows the hexagonal cell pattern.

- 5 Click the  **Go to Default View** button in the **Graphics** toolbar.  
6 Click the  **Zoom In** button in the **Graphics** toolbar.

7 In the **Rectangularly Arrayed Field Plot** toolbar, click  **Plot**.

