

Hexagonal Grating

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Introduction

A hexagonal grating is an infinite structure that is periodic with hexagonal (or rhomboid unit) cells. Figure 1 shows the hexagonal domain used for this model. The reflecting perfectly conducting surface consists of regularly spaced protruding semispheres.



Figure 1: The hexagonal domain, used for computing the diffraction from the hexagonal grating.

As shown in Figure 2, for a hexagonal cell of side length a, the corresponding unit cell is a rhomboid with side length $\sqrt{3}a$. In Figure 2, the side vectors for the hexagonal cell starts from the point P and are denoted \mathbf{a}_1 and \mathbf{a}_2 . The angle between \mathbf{a}_1 and \mathbf{a}_2 is 120 degrees. Similarly, for the rhomboid unit cell, the primitive vectors are denoted \mathbf{u}_1 and \mathbf{u}_2 and starts from the hexagon center point Q. The angle between the two primitive vectors is also 120 degrees.



Figure 2: Schematic showing the hexagonal cells with side length α and side vectors \mathbf{a}_1 and \mathbf{a}_2 . The primitive cells are defined by the primitive vectors \mathbf{u}_1 and \mathbf{u}_2 .

If the incident plane wave have a wave vector defined by

$$\mathbf{k} = \mathbf{k}_{\parallel} + \mathbf{k}_{\perp},\tag{1}$$

where $\mathbf{k}_{||}$ is the wave vector component parallel to the periodic boundary and \mathbf{k}_{\perp} is the component orthogonal to the periodic boundary, the in-plane wave vector component for diffraction order *mn* is given by

$$\mathbf{k}_{||mn} = \mathbf{k}_{||} + m\mathbf{G}_1 + n\mathbf{G}_2, \qquad (2)$$

where the reciprocal lattice vectors G_1 and G_2 are defined from the primitive vectors \boldsymbol{u}_1 and \boldsymbol{u}_2 as

$$\mathbf{G}_1 = 2\pi \frac{\mathbf{u}_2 \times \mathbf{n}}{\mathbf{u}_1 \cdot (\mathbf{u}_2 \times \mathbf{n})} \tag{3}$$

and

$$\mathbf{G}_2 = 2\pi \frac{\mathbf{n} \times \mathbf{u}_1}{\mathbf{u}_2 \cdot (\mathbf{n} \times \mathbf{u}_1)}, \tag{4}$$

where **n** is the normal vector (length 1) to the periodic boundary.

Since the out-of-plane wave vector component for mode *mn* is defined by

$$k_{\perp mn} = \sqrt{k^2 - k_{||mn}^2}, \qquad (5)$$

it is clear that for propagating modes, where the out-of-plane wave vector component above must be real, the length of the in-plane wave vector component must be smaller than the material wave number k. Figure 3 shows that it is only the modes inside the circle with radius k that will be propagating. In the example shown in Figure 3, there are five modes that will be propagating, in this case the modes m = n = 0 (the reflected wave), m = -1, n = 0, m = 0, n = -1, m = -1, n = -1, and m = -2, n = -1. All other modes will be evanescent and damped out.



Figure 3: The reciprocal lattice, showing the reciprocal lattice vectors \mathbf{G}_1 and \mathbf{G}_2 , the in-plane wave vector component $\mathbf{k}_{||}$, and the circle with radius k (the material wave number) enclosing the propagating mode points (larger dots. The dotted hexagon indicates that also the reciprocal lattice is a hexagonal point lattice. The dashed rhomboid indicates the unit cell spanned by the reciprocal lattice vectors.

Model Definition

In this model, the unit cell is small compared to the wavelength, so there will only be two modes that are propagating, the modes m = 0, n = -1 and m = -1, n = -1. For wavelengths longer than approximately 1.01 µm (the critical wavelength), the mode m = 0, n = -1 will be evanescent.

First a wavelength sweep will be made for an incident field having the polarization perpendicular to the plane of incidence (spanned by the wave vector for the incident wave and the normal to the periodic boundary) (so called s-polarization). Thereafter another wavelength sweep is made, but now with the polarization in the plane of incidence (p-polarization).

Results and Discussion

Figure 4 shows the electric field norm and the propagation directions for the incident, the reflected and the diffracted waves. Notice that the diffracted waves come in pairs (both have the same mode numbers), one wave having the polarization in the plane-of-diffraction and the other wave have orthogonal polarization to the plane-of-diffraction. The plane-of-diffraction is spanned by the wave vector for the diffracted wave and the normal to the periodic boundary. The wavelength is close the critical wavelength for the





Figure 4: The electric field norm and the propagation directions for the incident wave (red arrows), the reflected wave (blue arrows) and the two diffraction orders (green and yellow arrows). The wavelength is 1.01 μ m, which is close to the critical wavelength for the mode m = 0, n = -1, and the polarization of the incident wave is perpendicular to the plane of incidence.

Figure 5 shows the reflectance (for mode m = n = 0) and the diffraction efficiencies for the diffracted waves. Notice that both the reflectance and the diffraction efficiency for the in-

plane-polarized m = -1, n = -1 mode show resonances (peaks or dips) close to the critical wavelength for the m = 0, n = -1 modes.



Figure 5: Diffraction efficiencies for the reflected wave and the diffracted waves. The polarization of the incident wave is perpendicular to the plane of incidence.

Figure 6 and Figure 7 show polarization plots for the same case as Figure 4 and Figure 5. It is clear that even though the polarization for the incident wave is linear, the polarization for the reflected diffraction orders are elliptical.



Figure 6: Polarization plot showing the polarization ellipses for the three diffraction orders that are not evanescent at the first wavelength, $0.9 \ \mu m$.



Figure 7: Polarization plot for the same case as Figure 6, but at a wavelength of 1.01 μ m where only two diffraction orders are propagating.

Figure 8 shows a similar plot as Figure 4, but here the polarization of the incident wave is parallel with the plane of incidence.



Figure 8: Similar plot as in Figure 4, but here the polarization of the incident wave is parallel to the plane of incidence.

Figure 9 shows that for p-polarization both the reflected wave and the two m = -1, n = -1 modes show resonances close to the critical wavelength for the m = 0, n = -1 mode.



Figure 9: Similar plot as in Figure 5, but here the polarization of the incident wave is parallel to the plane of incidence.

Application Library path: Wave_Optics_Module/Gratings_and_Metamaterials/ hexagonal_grating

Modeling Instructions

From the File menu, choose New.

NEW

In the New window, click Model Wizard.

MODEL WIZARD

I In the Model Wizard window, click 间 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

First add some parameters that defines the geometry and the incident electric field.

Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 2 In the Settings window for Parameters, locate the Parameters section.
- **3** In the table, enter the following settings:

Name	Expression	Value	Description
lda0	1[um]	IE-6 m	Wavelength
а	lda0/2	5E-7 m	Hexagon side length
h0	3*lda0	3E-6 m	Air height
a1	a/2	2.5E-7 m	Sphere radius
theta	pi/3	1.0472	Elevation angle
phi	12[deg]	0.20944 rad	Azimuth angle
EO	1[V/m]	I V/m	Electric field amplitude
HO	1[A/m]	I A/m	Magnetic field amplitude

Notice that the azimuth angle phi above measures the angle for the wave vector of the incident wave from the *x*-axis.

STUDY I

Step 1: Wavelength Domain

- I In the Model Builder window, under Study I click Step I: Wavelength Domain.
- 2 In the Settings window for Wavelength Domain, locate the Study Settings section.
- 3 Click Range.
- 4 In the Range dialog box, type 0.9[um] in the Start text field.
- 5 In the **Step** text field, type 0.01[um].

- 6 In the **Stop** text field, type 1.1[um].
- 7 Click Replace.

GEOMETRY I

- I In the Model Builder window, under Component I (compl) click Geometry I.
- 2 In the Settings window for Geometry, locate the Units section.
- **3** From the **Length unit** list, choose **µm**.

The geometry consists of an extruded hexagon, with a semisphere removed from it at the bottom.

Work Plane I (wp1)

I In the Geometry toolbar, click 🖶 Work Plane.

2 In the Settings window for Work Plane, click 🛁 Show Work Plane.

Work Plane I (wpI)>Plane Geometry

In the Model Builder window, click Plane Geometry.

Work Plane I (wp1)>Polygon I (poll)

- I 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 (µm)	yw (µm)	
а	0	
a/2	sqrt(3)/2*a	
-a/2	sqrt(3)/2*a	
-a	0	
-a/2	-sqrt(3)/2*a	
a/2	-sqrt(3)/2*a	

Extrude I (extI)

I In the Model Builder window, right-click Geometry I and choose Extrude.

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

3 In the table, enter the following settings:

Distances (µm)

h0

Sphere I (sphI)

- I In the **Geometry** toolbar, click \bigoplus **Sphere**.
- 2 In the Settings window for Sphere, locate the Size section.
- 3 In the Radius text field, type a1.

Difference I (dif I)

- I In the Geometry toolbar, click 📃 Booleans and Partitions and choose Difference.
- 2 Select the object extl only.
- 3 In the Settings window for Difference, locate the Difference section.
- **4** Find the **Objects to subtract** subsection. Select the **Delivate Selection** toggle button.
- 5 Select the object **sph1** only.
- 6 Click 🟢 Build All Objects.
- 7 Click the 🗤 Go to Default View button in the Graphics toolbar.
- 8 Click the 🔁 Wireframe Rendering button in the Graphics toolbar.



ADD MATERIAL

- I 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)

Port I

- I In the Model Builder window, under Component I (compl) right-click Electromagnetic Waves, Frequency Domain (ewfd) and choose Port.
- **2** Select Boundary 4 only.



- 3 In the Settings window for Port, locate the Port Properties section.
- 4 From the Type of port list, choose Periodic.

For the first port, wave excitation is **on** by default.

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

-EO*sin(phi)	x
E0*cos(phi)	у
0	z

6 In the α_1 text field, type theta.

7 In the α₂ text field, type phi+pi/3, as this angle is measured from the first side vector of the port (not the *x*-axis).

Periodic Port Reference Point I

Before creating the diffraction orders ports, a reference point must be defined on the periodic port.

- I In the Physics toolbar, click 📃 Attributes and choose Periodic Port Reference Point.
- **2** In the Settings window for Periodic Port Reference Point, locate the Point Selection section.
- 3 Click Clear Selection.
- 4 Select Point 2 only. This point selection makes the angle previously provided for alpha_2 consistent with the intended angle of incidence for the incident wave.



Port I

- I In the Model Builder window, click Port I.
- **2** In the Settings window for Port, locate the Automatic Diffraction Order Calculation section.
- **3** Click Add Diffraction Orders.

Periodic Condition 1

- I In the Physics toolbar, click 📄 Boundaries and choose Periodic Condition.
- 2 In the Settings window for Periodic Condition, locate the Periodicity Settings section.
- **3** From the **Type of periodicity** list, choose **Floquet periodicity**.
- 4 From the k-vector for Floquet periodicity list, choose From periodic port.

5 Select Boundaries 1 and 12 only.



Periodic Condition 2

- I In the Physics toolbar, click 📄 Boundaries and choose Periodic Condition.
- 2 In the Settings window for Periodic Condition, locate the Periodicity Settings section.
- **3** From the **Type of periodicity** list, choose **Floquet periodicity**.
- **4** From the **k-vector for Floquet periodicity** list, choose **From periodic port**.

5 Select Boundaries 5 and 8 only.



Periodic Condition 3

- I In the Physics toolbar, click 📄 Boundaries and choose Periodic Condition.
- 2 In the Settings window for Periodic Condition, locate the Periodicity Settings section.
- **3** From the **Type of periodicity** list, choose **Floquet periodicity**.
- **4** From the **k-vector for Floquet periodicity** list, choose **From periodic port**.

5 Select Boundaries 2 and 11 only.



MESH I

y 🚺

In the Model Builder window, under Component I (compl) right-click Mesh I and choose Build All.





STUDY I

Step 1: Wavelength Domain In the Home toolbar, click **= Compute**.

RESULTS

Electric Field (ewfd)

Add Arrow Surface plots showing the wave vector directions for the incident field, the reflected field and the diffracted fields. Notice that the diffracted fields come in pairs, where each pair have the same wave vector. Thus, only two wave vectors for the diffraction orders need to be added in this case.

Arrow Surface 1

- I Right-click Electric Field (ewfd) and choose Arrow Surface.
- 2 In the Settings window for Arrow Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Electromagnetic Waves, Frequency Domain>Ports>ewfd.klncx_l,...,ewfd.klncz_l Incident wave vector.
- 3 Locate the Expression section. Select the Description check box.
- 4 In the associated text field, type Incident wave (red).

Arrow Surface 2

- I Right-click Arrow Surface I and choose Duplicate.
- 2 In the Settings window for Arrow Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Electromagnetic Waves, Frequency Domain>Ports>ewfd.kModex_I,...,ewfd.kModez_I Port mode wave vector.
- 3 Locate the Coloring and Style section. From the Color list, choose Blue.
- 4 Locate the Expression section. In the Description text field, type Reflected wave (blue).

Arrow Surface 3

- I Right-click Arrow Surface 2 and choose Duplicate.
- 2 In the Settings window for Arrow Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Electromagnetic Waves, Frequency Domain>Ports>ewfd.kModex_2,...,ewfd.kModez_2 Port mode wave vector.
- 3 Locate the Coloring and Style section. From the Color list, choose Green.

4 Locate the Expression section. In the Description text field, type Mode m = -1, n = -1 (green).

Arrow Surface 4

- I Right-click Arrow Surface 3 and choose Duplicate.
- 2 In the Settings window for Arrow Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Electromagnetic Waves, Frequency Domain>Ports>ewfd.kModex_4,...,ewfd.kModez_4 Port mode wave vector.
- 3 Locate the Coloring and Style section. From the Color list, choose Yellow.
- 4 Locate the Expression section. In the Description text field, type Mode m = 0, n = -1 (yellow).

Electric Field (ewfd)

Select the wavelength closest to the critical wavelength for the mode m = 0, n = -1.

- I In the Model Builder window, click Electric Field (ewfd).
- 2 In the Settings window for 3D Plot Group, locate the Data section.
- **3** From the **Parameter value (lambda0 (μm))** list, choose **1.01**.
- 4 In the Electric Field (ewfd) toolbar, click **O** Plot.



Your plot should look the same as Figure 4.

Reflectance (ewfd)

The reflectance and the diffraction efficiencies for the diffracted waves are plotted by default.

- I In the Model Builder window, click Reflectance (ewfd).
- 2 In the Settings window for ID Plot Group, click to expand the Title section.
- **3** From the **Title type** list, choose **None**.
- **4** Locate the **Plot Settings** section. In the **y-axis label** text field, type Diffraction efficiency.
- **5** Locate the Legend section. From the Position list, choose Upper left.

6 In the **Reflectance (ewfd)** toolbar, click **I** Plot.



Your plot should look like Figure 5.

Polarization Plot (ewfd)

- I In the Model Builder window, click Polarization Plot (ewfd).
- 2 In the Settings window for ID Plot Group, locate the Legend section.
- 3 From the Position list, choose Upper left.

4 In the Polarization Plot (ewfd) toolbar, click **O** Plot.



The polarization plot shows that all three modes are elliptically polarized, but with different orientations for the polarization ellipse.

5 Locate the Data section. In the Parameter values (lambda0 (µm)) list, select 1.01.

6 In the Polarization Plot (ewfd) toolbar, click 🗿 Plot.



At this wavelength, mode m = 0, n = -1 is evanescent, so there is no polarization ellipse for that mode.

To really understand the polarization direction, you can also plot the Jones base vectors. First create a view zoomed in on the port boundary and then use the view in the created plot.

- 7 Click the 🐱 Show More Options button in the Model Builder toolbar.
- 8 In the Show More Options dialog box, select Results>Views in the tree.
- 9 In the tree, select the check box for the node Results>Views.
- IO Click OK.

View 3D 3

- I In the Model Builder window, right-click Views and choose View 3D.
- 2 Click the **Zoom Box** button in the **Graphics** toolbar and then use the mouse to zoom in on the port boundary.

Polarization Base Vectors

I In the Home toolbar, click 📠 Add Plot Group and choose 3D Plot Group.

- 2 In the Settings window for 3D Plot Group, type Polarization Base Vectors 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. From the View list, choose View 3D 3.

Out-of-Plane Base Vector

- I Right-click Polarization Base Vectors and choose Arrow Surface.
- 2 In the Settings window for Arrow Surface, type Out-of-Plane Base Vector in the Label text field.
- 3 Click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (comp1)>Electromagnetic Waves, Frequency Domain>Ports> Polarization state>Jones base vectors>ewfd.eJROOPx_0_0,...,ewfd.eJROOPz_0_0 Jones base vector on reflection side, out-of-plane direction, order [0,0].
- 4 Locate the Arrow Positioning section. In the Number of arrows text field, type 1.

In-Plane Base Vector

- I Right-click Out-of-Plane Base Vector and choose Duplicate.
- 2 In the Settings window for Arrow Surface, type In-Plane Base Vector in the Label text field.
- 3 Click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (comp1)>Electromagnetic Waves, Frequency Domain>Ports> Polarization state>Jones base vectors>ewfd.eJRIPx_0_0,...,ewfd.eJRIPz_0_0 Jones base vector on reflection side, in-plane direction, order [0,0].
- 4 Locate the Coloring and Style section. From the Color list, choose Green.
- 5 Click to expand the Inherit Style section. From the Plot list, choose Out-of-Plane Base Vector.
- 6 Clear the **Color** check box.

Normalized Mode Wave Vector

- I Right-click In-Plane Base Vector and choose Duplicate.
- 2 In the Settings window for Arrow Surface, type Normalized Mode Wave Vector in the Label text field.
- 3 Locate the Expression section. In the X component text field, type ewfd.kModex_1/ ewfd.k.
- 4 In the Y component text field, type ewfd.kModey_1/ewfd.k.
- 5 In the Z component text field, type ewfd.kModez_1/ewfd.k.

6 Locate the Coloring and Style section. From the Color list, choose Blue.

Boundary Normal

- I Right-click Normalized Mode Wave Vector and choose Duplicate.
- 2 In the Settings window for Arrow Surface, type Boundary Normal in the Label text field.

Selection I

- I Right-click **Boundary Normal** and choose **Selection**, to only show the normal on the port boundary.
- **2** Select Boundary 4 only.



Boundary Normal

- I In the Model Builder window, click Boundary Normal.
- 2 In the Settings window for Arrow Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Electromagnetic Waves, Frequency Domain>Geometry and mesh>ewfd.nx,ewfd.ny, ewfd.nz Normal vector.
- 3 Locate the Coloring and Style section. From the Color list, choose Black.
- **4** In the **Polarization Base Vectors** toolbar, click **OM Plot**.



5 Zoom-in and move the plot, to make the vectors appear as in the picture below.

As shown, the out-of-plane base vector (red) is orthogonal to the plane spanned by the port normal (black) and the mode's wave vector (blue). The in-plane base vector (green) is parallel to the plane spanned by the port normal and the mode's wave vector.

Out-of-Plane Base Vector

Change the arrow expressions to visualize the behavior for mode m = -1, n = -1 to demonstrate that the base vectors are different for the different modes.

- I In the Model Builder window, click Out-of-Plane Base Vector.
- 2 In the Settings window for Arrow Surface, locate the Expression section.
- **3** In the **X** component text field, type ewfd.eJR00Px_n1_n1.
- 4 In the Y component text field, type ewfd.eJR00Py_n1_n1.
- **5** In the **Z** component text field, type ewfd.eJR00Pz_n1_n1.

Here, the variable suffix n1_n1 represents the mode number m = -1, n = -1.

In-Plane Base Vector

- I In the Model Builder window, click In-Plane Base Vector.
- 2 In the Settings window for Arrow Surface, locate the Expression section.
- **3** In the **X** component text field, type ewfd.eJRIPx_n1_n1.

- **4** In the **Y** component text field, type ewfd.eJRIPy_n1_n1.
- 5 In the Z component text field, type ewfd.eJRIPz_n1_n1.

Normalized Mode Wave Vector

- I In the Model Builder window, click Normalized Mode Wave Vector.
- 2 In the Settings window for Arrow Surface, locate the Expression section.
- 3 In the X component text field, type ewfd.kModex_2/ewfd.k.
- 4 In the Y component text field, type ewfd.kModey_2/ewfd.k.
- 5 In the Z component text field, type ewfd.kModez_2/ewfd.k.

Here, the variable suffix is the port name, not the mode number.



6 In the Polarization Base Vectors toolbar, click **O** Plot.

As shown, the wave vector and the polarization vectors are different for this mode, compared to the vectors for the zero order mode.

ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EWFD)

Port I

Now, repeat the simulation for an incoming wave with p-polarization (the electric field polarized in the plane of incidence).

- In the Model Builder window, under Component I (comp1)>Electromagnetic Waves, Frequency Domain (ewfd) click Port I.
- 2 In the Settings window for Port, locate the Port Mode Settings section.
- 3 From the Input quantity list, choose Magnetic field.
- **4** Specify the \mathbf{H}_0 vector as

-HO*sin(phi)	x
HO*cos(phi)	у
0	z

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

RESULTS

Electric Field (ewfd)

I Click the 4 Zoom Extents button in the Graphics toolbar, and verify that your plot look the same as Figure 8.



Reflectance (ewfd)

I In the Model Builder window, click Reflectance (ewfd).

2 In the **Reflectance (ewfd)** toolbar, click **Plot**, and verify that your plot look the same as Figure 9.



Polarization Plot (ewfd)

Finally, take a look at the polarization states when the input wave is p-polarized.

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



2 In the Settings window for ID Plot Group, click 🛏 Plot First.

Also in this case, the polarization is elliptical for the different modes.

3 Locate the Data section. In the Parameter values (lambda0 (µm)) list, select 1.01.





At this wavelength, close the resonance, the polarization for the m = 0, n = 0 mode switches to almost out-of-plane polarization, whereas the m = -1, n = -1 mode has almost circular polarization. The relative magnitude of the Jones vector elements is also reflected in the diffraction efficiency plot above.