Bandgap Analysis of a Photonic Crystal

This application performs a bandgap analysis of a photonic crystal similar to the one used in the Photonic Crystal model.

Introduction

The model investigates the wave propagation in a photonic crystal that consists of GaAs pillars placed equidistant from each other. The distance between the pillars determines a relationship between the wave number and the frequency of the light that prevents light of certain wavelengths to propagate inside the crystal structure. This frequency range is called the photonic bandgap (Ref. 2). There are several bandgaps for a certain structure, and this application extracts the bandgaps for the lowest bands of the crystal.

Model Definition

This application is similar to the Photonic Crystal waveguide model. The difference is that in this application the crystal itself is analyzed instead of a waveguide. Because it has a repeated pattern it is possible to use periodic boundary conditions. As a result, only one pillar is needed for this simulation.

There are two main complications with this bandgap analysis. Firstly, the refractive index of GaAs is frequency dependent. Secondly, the wave vector must be ramped for the band diagram. Although you can solve each of these complications with the eigenvalue solver separately, the two complications combined make it difficult without reformulating the problem. Thus, formulate a nonlinear eigenvalue problem, using a stationary solver with the eigenvalue as an unknown. The equation for the eigenvalue is a normalization of the electric field, so the average field is unity over the domain. The nonlinear solver finds the correct eigenvalue with an updated refractive index to the found eigenvalue. Furthermore, the parametric solver can sweep the wave vector, $\boldsymbol{k}$.

The wave vector for the propagating wave, $\boldsymbol{k}$, enters the simulation as Floquet periodicity boundary conditions (Ref. 1),

$$E_z(2) = E_z(1)e^{-i\beta}$$

where β is a phase factor determined by the wave vector and the distance, d, between the periodic boundaries:

$$\beta = kd$$

The range for the swept k is determined by the reciprocal lattice vectors of the photonic crystal, and these are determined from the primitive lattice vectors. For a 2D crystal there are two lattice vectors, $\mathbf{a}_1$ and $\mathbf{a}_2$, defined in Figure 1.

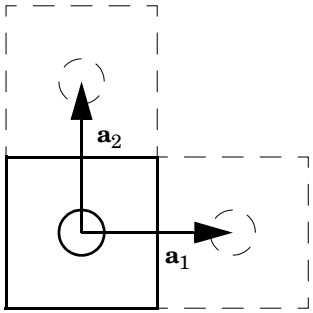


Figure 1: Definition of the square primitive cells ant the lattice vectors $\mathbf{a}_1$ *and* $\mathbf{a}_2$.

The reciprocal lattice vectors are calculated from $\mathbf{a}_1$ and $\mathbf{a}_2$ using the relations

$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

where $\mathbf{a}_3$ is assumed to be the unit vector $\mathbf{e}_z$. When $\mathbf{a}_1$ and $\mathbf{a}_2$ are perpendicular to each other and to $\mathbf{a}_3$, $\mathbf{b}_1$ and $\mathbf{b}_2$ become

$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_1}{|\mathbf{a}_1||\mathbf{a}_1|}$$

$$\mathbf{b}_2 = 2\pi\frac{\mathbf{a}_2}{|\mathbf{a}_2||\mathbf{a}_2|}$$

Results and Discussion

Figure 2 shows the z-component of the electric field, as determined by the eigenfrequency solver for k=0.

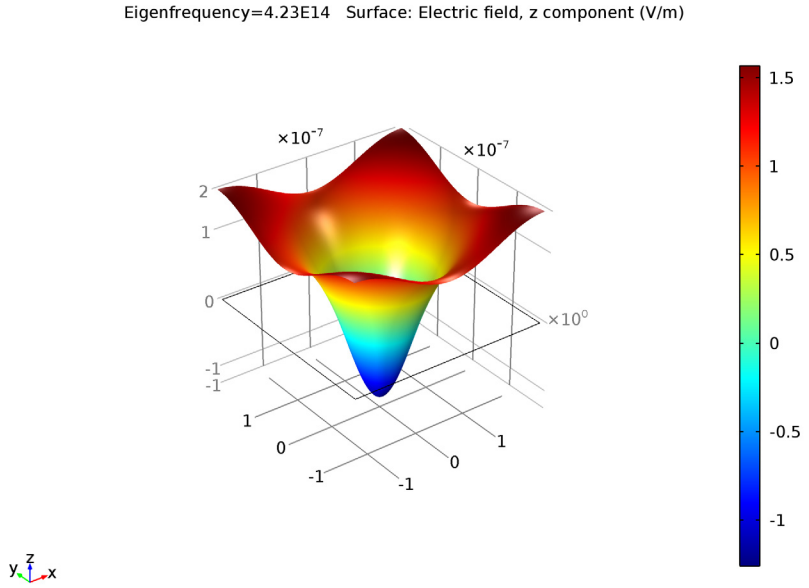


Figure 2: Z-component of the electric field for k = 0.

Figure 3 shows the z-component of the electric field for k=0.5 for the fifth band, as determined by the nonlinear solver.

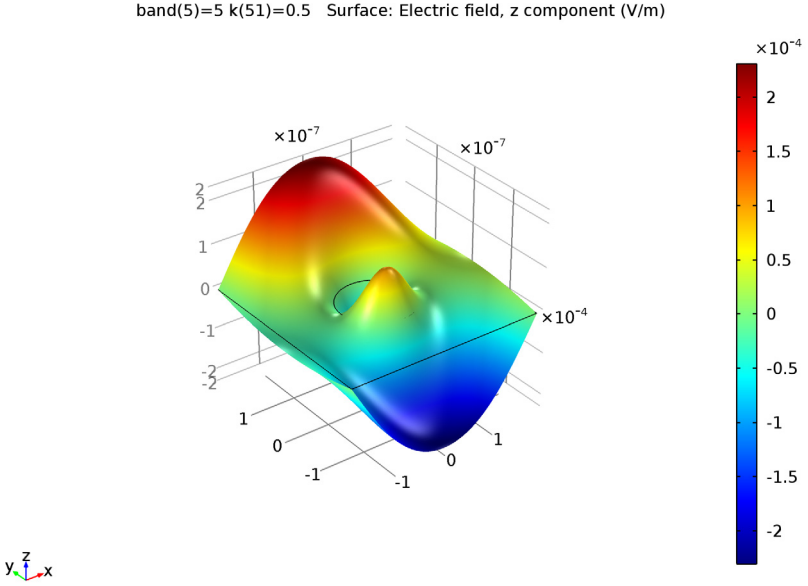


Figure 3: Z-component of the electric field for the fifth band and k = 0.5.

Finally, Figure 4 shows the band diagram for k swept from 0 to 0.5 in the (1,1) direction. Notice that band two and three are degenerate for k=0, and that band one and two and four and five are degenerate at k=0.5.

Between band three and four there is a frequency range for which there are no states. This frequency range corresponds to a band gap in the structure, as there can be no propagating waves in the (1,1) propagation direction for that frequency range.

Notice that there is actually a band with a lower frequency than for the lowest band in Figure 4. However, this band has so small frequencies that the approximation for the

frequency-dependent refractive index of GaAs is no longer valid. Thus, this band has not been included in the calculations.

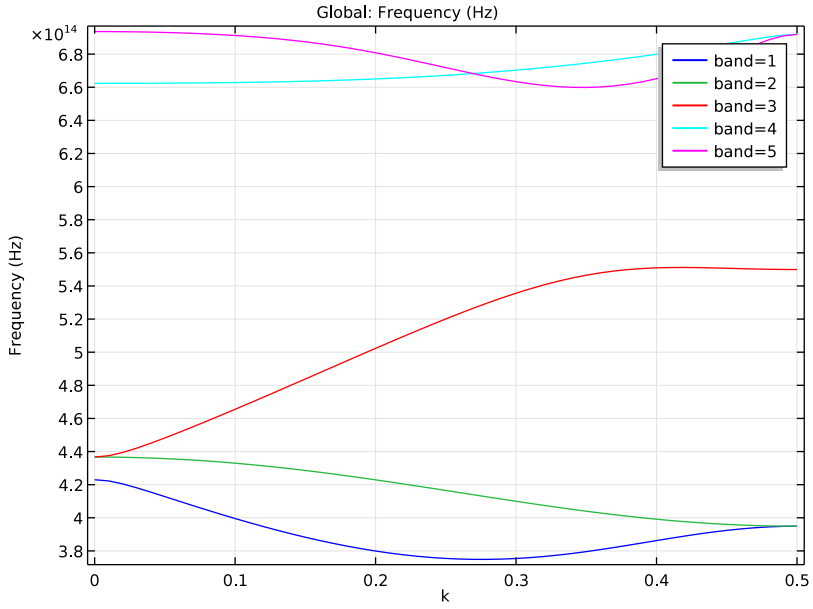


Figure 4: The dispersion relation (frequency versus wave number), when the wave vector is varied in the direction (1,1), for the five lowest bands.

Notes About the COMSOL Implementation

One catch with the nonlinear formulation is that the mode normalization performed by the global equation involves setting the domain integral of Ez*conj(Ez) to unity. However, the conjugate function is non-analytical in complex mathematics sense so a correct Jacobian cannot be obtained by the nonlinear solver.

To obtain a correct Jacobian, COMSOL's complex splitting functionality is used. Thereby COMSOL internally splits complex entities into the constituent real and imaginary parts. Thus, the problem is converted from a complex-valued problem to a real-valued problem that is fully differentiable. After solution, COMSOL translates the solution back into complex form.

The complex splitting makes the problem solve faster and more robustly.

References

1. C. Kittel, *Introduction to Solid State Physics*, 7th ed., John Wiley & Sons, New York, 1996.

2. J. D. Joannopoulus, R. D. Meade, and J. N. Winn, *Photonic Crystals (Modeling the Flow of Light)*, Princeton University Press, 1995.

Application Library path: `Wave_Optics_Module/Gratings_and_Metamaterials/bandgap_photonic_crystal`

Modeling Instructions

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

NEW

1 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 **Preset Studies>Eigenfrequency**.

6 Click **Done**.

GEOMETRY 1

On the **Home** toolbar, click **Parameters**.

GLOBAL DEFINITIONS

Parameters

First add parameters, characterizing the geometry of the periodic cell.

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

2 In the table, enter the following settings:

Name	Expression	Value	Description
a	375[nm]	3.75E-7 m	Primitive cell side length
b	70[nm]	7E-8 m	GaAs pillar radius
k	0	0	Fraction of wave vector magnitude
k1	1	1	First component of wave direction vector
k2	1	1	Second component of wave direction vector
a1x	a	3.75E-7 m	First lattice vector, x-component
a1y	0[nm]	0 m	First lattice vector, y-component
a2x	0[nm]	0 m	Second lattice vector, x-component
a2y	a	3.75E-7 m	Second lattice vector, y-component
band	1	1	Band number

The last parameter, band, will be used for selecting what band to calculate the dispersion relation for.

DEFINITIONS

Variables 1

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

Add variables representing the reciprocal lattice vector and the Floquet wave vector (used later in the periodic boundary condition).

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
b1x	2*pi*a2y/(a1x*a2y-a1y*a2x)	1/m	First reciprocal lattice vector, x-component
b1y	-2*pi*a2x/(a1x*a2y-a1y*a2x)	1/m	First reciprocal lattice vector, y-component
b2x	-2*pi*a1y/(a1x*a2y-a1y*a2x)	1/m	Second reciprocal lattice vector, x-component

Name	Expression	Unit	Description
b2y	2*pi*a1x/(a1x*a2y-a1y*a2x)	1/m	Second reciprocal lattice vector, y-component
kx	k*(k1*b1x+k2*b2x)	1/m	Floquet vector, x-component
ky	k*(k1*b1y+k2*b2y)	1/m	Floquet vector, y-component

GEOMETRY 1

The geometry consists of a square air cell surrounding a circular GaAs pillar.

Square 1 (sq1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Square**.

2 In the **Settings** window for Square, locate the **Size** section.

3 In the **Side length** text field, type a.

4 Locate the **Position** section. From the **Base** list, choose **Center**.

Circle 1 (c1)

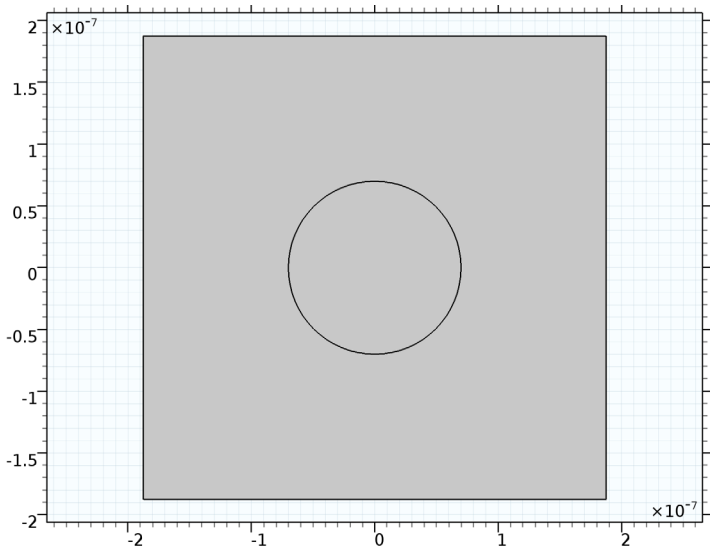
1 On the **Geometry** toolbar, click **Primitives** and choose **Circle**.

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

3 In the **Radius** text field, type b.

4 Click the **Build All Objects** button.

5 Click the **Zoom Extents** button on the **Graphics** toolbar.



ADD MATERIAL

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

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

Define the air, that will surround the GaAs pillar.

3 In the tree, select **Built-In>Air**.

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

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

DEFINITIONS

Analytic 1 (an1)

1 On the **Home** toolbar, click **Functions** and choose **Global>Analytic**.

The dispersion relation for the refractive index of GaAs will be used in more than one place, so it is best to define it as an analytical function.

2 In the **Settings** window for Analytic, type `n_GaAs` in the **Function name** text field.

3 Locate the **Definition** section. In the **Expression** text field, type `3.3285e5[s/m]*c_const/f+3.5031`.

4 In the **Arguments** text field, type `f`.

5 Locate the **Units** section. In the **Arguments** text field, type `Hz`.

6 In the **Function** text field, type `1`.

ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EWFD)

Compute the solution for out-of-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 **Out-of-plane vector**.

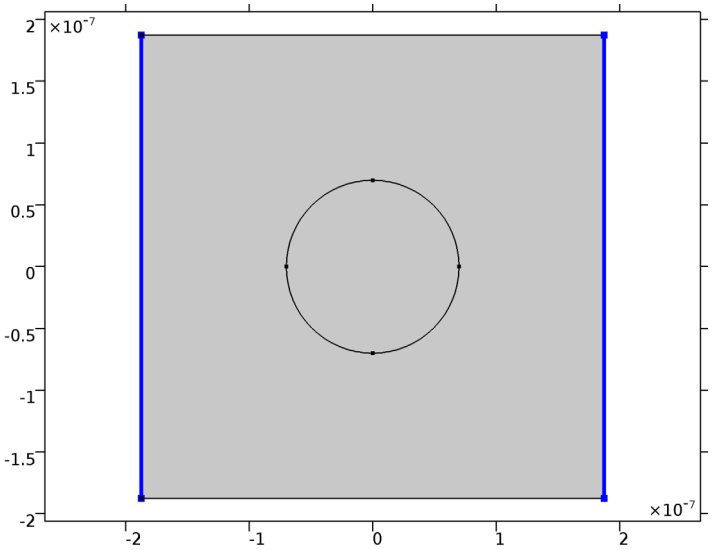
Periodic Condition 1

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

Define the periodic boundary conditions, using the Floquet wave vector.

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

3 Select Boundaries 1 and 4 only.



4 In the **Settings** window for Periodic Condition, locate the **Periodicity Settings** section.

5 From the **Type of periodicity** list, choose **Floquet periodicity**.

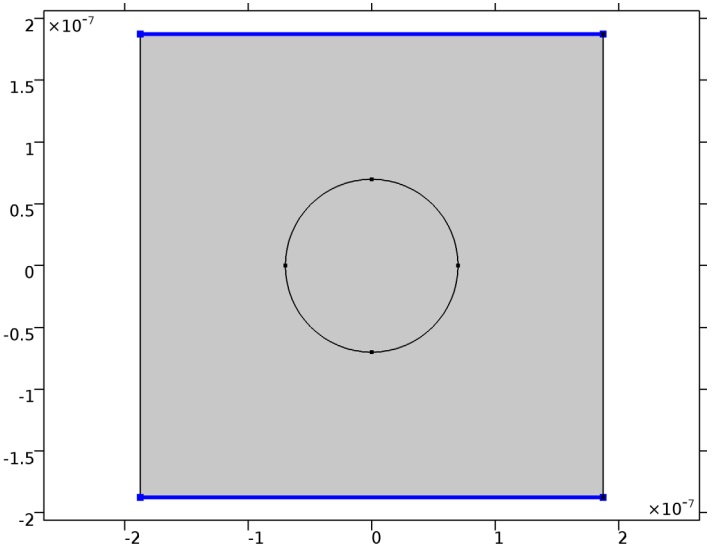
6 Specify the $\mathbf{k}_F$ vector as

kx	x
ky	y

Periodic Condition 2

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

2 Select Boundaries 2 and 3 only.



3 In the **Settings** window for Periodic Condition, locate the **Periodicity Settings** section.

4 From the **Type of periodicity** list, choose **Floquet periodicity**.

5 Specify the $\mathbf{k}_F$ vector as

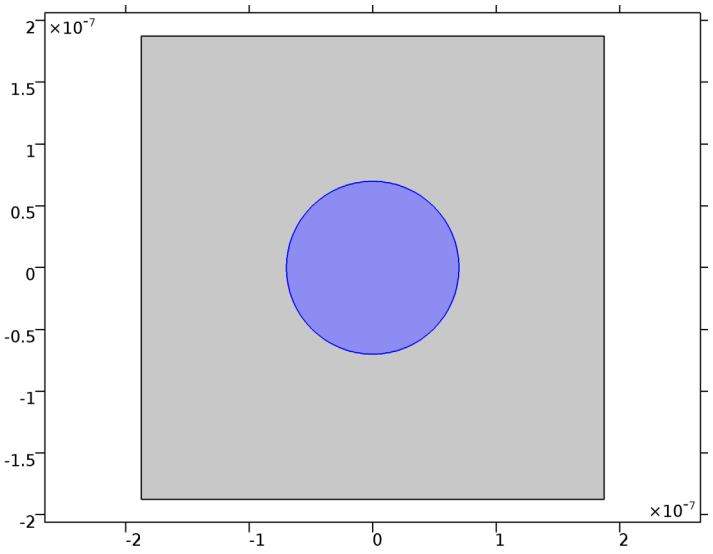
kx	x
ky	y

Add a wave equation feature, representing the GaAs pillar.

Wave Equation, Electric 2

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

2 Select Domain 2 only.



3 In the **Settings** window for Wave Equation, Electric, locate the **Electric Displacement Field** section.

4 From the *n* list, choose **User defined**. In the associated text field, type `n_GaAs(freq)`.

5 From the *k* list, choose **User defined**.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

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

3 From the **Element size** list, choose **Finer**.

STUDY 1

Step 1: Eigenfrequency

Find the initial eigenfrequency, for k = 0, around 400 THz.

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

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

3 In the **Desired number of eigenfrequencies** text field, type `5`.

4 In the **Search for eigenfrequencies around** text field, type `4e14`.

Solution 1

1 On the **Study** toolbar, click **Show Default Solver**.

Define the Transform point to the initial eigenfrequency guess, to make sure that a zero frequency will not be assigned to the denominator in any expression.

2 In the **Model Builder** window, expand the **Solution 1** node, then click **Eigenvalue Solver 1**.

3 In the **Settings** window for Eigenvalue Solver, locate the **Values of Linearization Point** section.

4 Find the **Value of eigenvalue linearization point** subsection. In the **Point** text field, type `4e14`.

5 On the **Study** toolbar, click **Compute**.

RESULTS

Electric Field (ewfd)

Visualize the z-component of the electric field, deforming the surface using a height expression.

1 In the **Model Builder** window, expand the **Electric Field (ewfd)** node, then click **Surface 1**.

2 In the **Settings** window for Surface, locate the **Expression** section.

3 In the **Expression** text field, type `ewfd.Ez`.

4 Right-click **Results>Electric Field (ewfd)>Surface 1** and choose **Height Expression**.

5 Click the **Zoom Extents** button on the **Graphics** toolbar. Compare the results with Figure 2.

COMPONENT 1 (COMP1)

To find the frequencies for the non-zero wave vectors, solve for the frequency using a nonlinear state equation, requiring the field to be normalized in the unit cell, and a second wave equation.The solution from the first wave equation is used as the initial value for the second wave equation.

ADD PHYSICS

1 On the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.

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

3 In the **Add physics** tree, select **Mathematics>ODE and DAE Interfaces>Global ODEs and DAEs (ge)**.

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

GLOBAL ODES AND DAES (GE)

Global Equations 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Global ODEs and DAEs (ge)** click **Global Equations 1**.

2 In the **Settings** window for Global Equations, locate the **Global Equations** section.

3 In the table, enter the following settings:

Name	f(u,ut,utt,t) (1)	Initial value (u_0) (1)	Initial value (u_t0) (1/s)	Description
freq1	1[V^2/m^2]-nEz	-imag(lambda)/(2*pi)	0	Frequency

Calculate the initial value for the frequency from the eigenvalue from the eigenfrequency analysis.

4 Locate the **Units** section. Find the **Dependent variable quantity** subsection. From the list, choose **Frequency (Hz)**.

5 Find the **Source term quantity** subsection. From the list, choose **None**.

6 In the **Unit** text field, type `V^2/m^2`.

ADD PHYSICS

1 Go to the **Add Physics** window.

2 In the **Add physics** tree, select **Recently Used>Electromagnetic Waves, Frequency Domain (ewfd)**.

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

4 On the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN 2 (EWFD2)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Electromagnetic Waves, Frequency Domain 2 (ewfd2)**.

2 In the **Settings** window for Electromagnetic Waves, Frequency Domain, click to expand the **Equation** section.

The frequency used by this interface is the one solved for with the state equation, `freq1`.

3 From the **Equation form** list, choose **Frequency domain**.

4 From the **Frequency** list, choose **User defined**. In the *f* text field, type `freq1`.

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

Initial Values 1

Assign the initial value to the solution from the initial eigenfrequency analysis. As more than one eigenfrequency solution was found, you will later specify, for the Stationary study step, which of the eigenfrequency solutions to select for the initial value.

1 In the **Model Builder** window, under **Component 1 (comp1)>Electromagnetic Waves, Frequency Domain 2 (ewfd2)** click **Initial Values 1**.

2 In the **Settings** window for Initial Values, locate the **Initial Values** section.

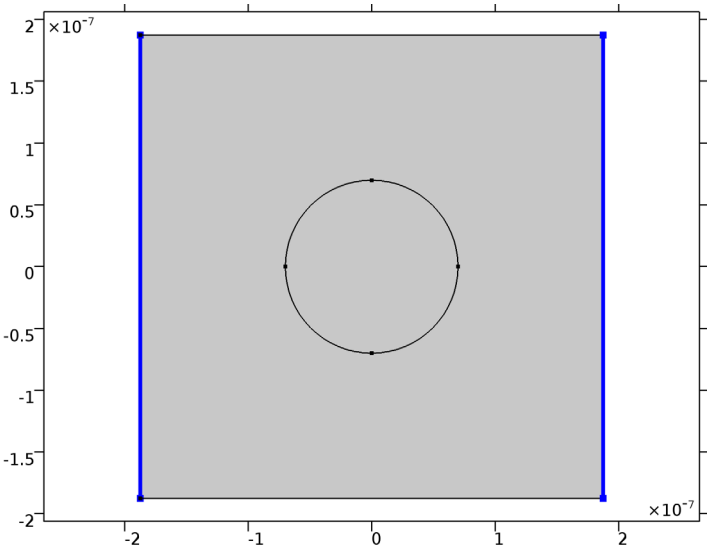
3 Specify the $\mathbf{E}2$ vector as

0	x
0	y
ewfd.Ez	z

Periodic Condition 1

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

2 Select Boundaries 1 and 4 only.



3 In the **Settings** window for Periodic Condition, locate the **Periodicity Settings** section.

4 From the **Type of periodicity** list, choose **Floquet periodicity**.

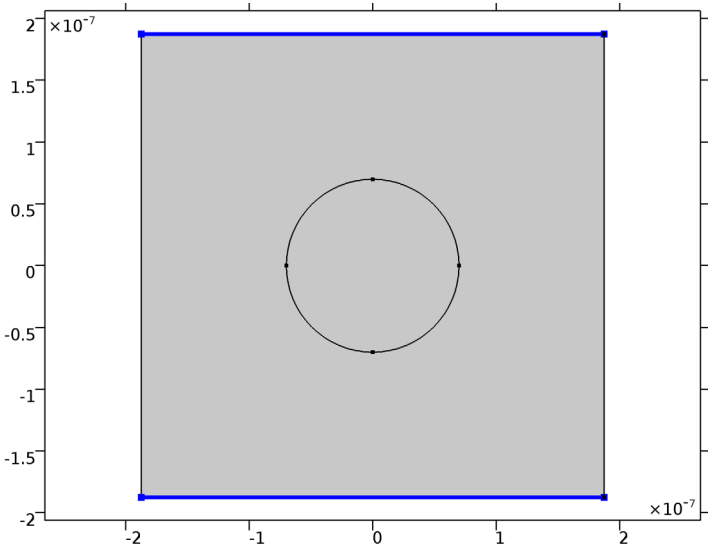
5 Specify the $\mathbf{k}_F$ vector as

kx	x
ky	y

Periodic Condition 2

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

2 Select Boundaries 2 and 3 only.



3 In the **Settings** window for Periodic Condition, locate the **Periodicity Settings** section.

4 From the **Type of periodicity** list, choose **Floquet periodicity**.

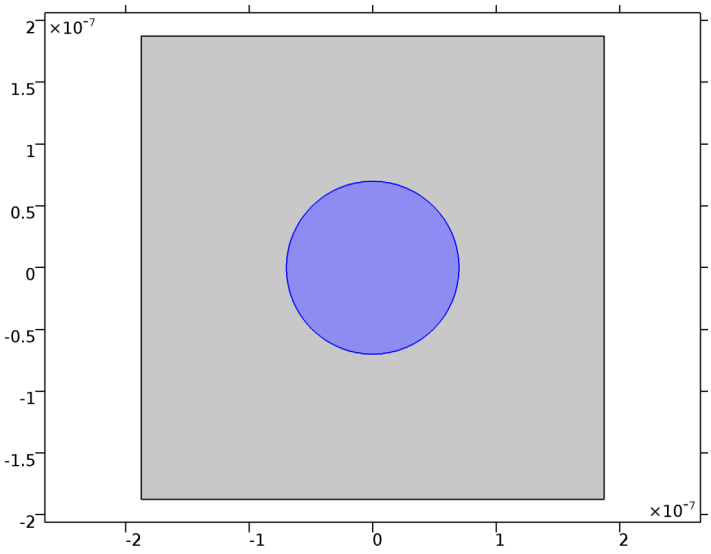
5 Specify the $\mathbf{k}_F$ vector as

kx	x
ky	y

Wave Equation, Electric 2

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

2 Select Domain 2 only.



3 In the **Settings** window for Wave Equation, Electric, locate the **Electric Displacement Field** section.

4 From the *n* list, choose **User defined**. In the associated text field, type `n_GaAs(freq1)`. Notice that it must be the frequency `freq1` that is used here.

5 From the *k* list, choose **User defined**.

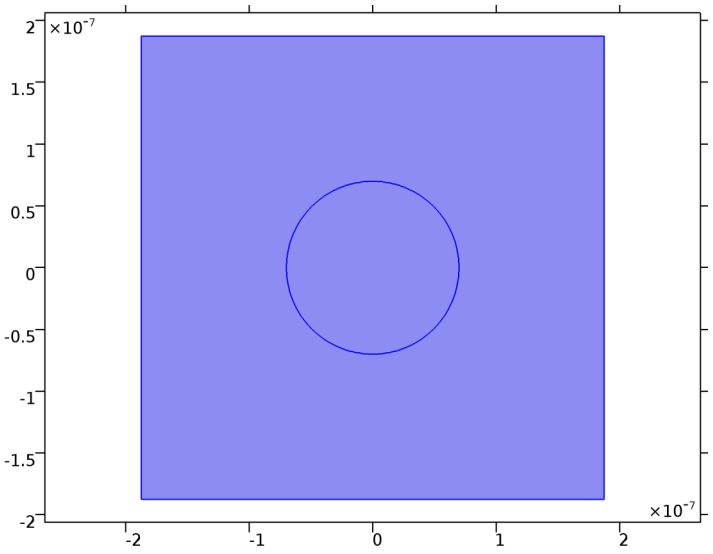
DEFINITIONS

Define the integration operator, used for the normalization of the field.

Integration 1 (intop1)

1 On the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.

2 Select Domains 1 and 2 only.



Variables 1

Add the variables that define the normalization of the field.

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** click **Variables 1**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
A	`intop1(1)`	m^2	Area
nEz	`intop1(realdot(ewfd2.Ez,ewfd2.Ez))/A`	$kg^2 \cdot m^2/(s^6 \cdot A^2)$	Normalization integral

ADD STUDY

1 On 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 **Custom Studies>Preset Studies for Some Physics Interfaces>Stationary**.

4 Click **Add Study** in the window toolbar.

5 On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

Step 1: Stationary

The stationary study will not include the first interface (ewfd).

1 In the **Model Builder** window, under **Study 2** click **Step 1: Stationary**.

2 In the **Settings** window for Stationary, locate the **Physics and Variables Selection** section.

3 In the table, enter the following settings:

Physics interface	Solve for	Discretization
Electromagnetic Waves, Frequency Domain		physics

Select what eigenfrequency solution for the first Electromagnetic Waves, Frequency Domain interface (ewfd) that will be used as the initial value to the second Electromagnetic Waves, Frequency Domain (ewfd2) interface.

4 Click to expand the **Values of dependent variables** section. Locate the **Values of Dependent Variables** section. Select the **Initial values of variables solved for** check box.

5 From the **Study** list, choose **Study 1, Eigenfrequency**.

6 From the **Eigenfrequency** list, choose **Manual**.

7 In the **Index** text field, type `band`.

8 Click to expand the **Study extensions** section. Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

9 Click **Add**.

Scan the fraction of the wave vector magnitude from 0 to 0.5 (half the Brillouin zone).

10 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
k		

11 Click **Range**.

12 In the **Range** dialog box, type `0` in the **Start** text field.

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

14 In the **Stop** text field, type `0.5`.

15 Click **Replace**.

Solution 2

1 On the **Study** toolbar, click **Show Default Solver**.

Solve the stationary problem using complex splitting, to split the complex expressions into their real and imaginary parts. Thereby the expressions become analytical and an exact Jacobian can be calculated.

2 In the **Model Builder** window, expand the **Solution 2** node, then click **Compile Equations: Stationary**.

3 In the **Settings** window for Compile Equations, locate the **Study and Step** section.

4 Select the **Split complex variables in real and imaginary parts** check box.

GLOBAL ODES AND DAES (GE)

On the **Physics** toolbar, click **Electromagnetic Waves, Frequency Domain 2 (ewfd2)** and choose **Global ODEs and DAEs (ge)**.

Global Equations 1

1 In the **Model Builder** window's toolbar, click the **Show** button and select **Discretization** in the menu.

2 In the **Model Builder** window, under **Component 1 (comp1)>Global ODEs and DAEs (ge)** click **Global Equations 1**.

3 In the **Settings** window for Global Equations, click to expand the **Discretization** section.

4 From the **Value type when using splitting of complex variables** list, choose **Real**, as the frequency `freq1` has no imaginary part.

STUDY 2

Add a parametric sweep to calculate the dispersion relations for the five lowest bands.

Parametric Sweep

1 On the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for Parametric Sweep, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
band		

5 Click **Range**.

6 In the **Range** dialog box, type 1 in the **Start** text field.

7 In the **Step** text field, type 1.

8 In the **Stop** text field, type 5.

9 Click **Replace**.

Solution 2

1 In the **Model Builder** window, expand the **Study 2>Solver Configurations>Solution 2>Stationary Solver 1** node, then click **Parametric 1**.

2 In the **Settings** window for Parametric, click to expand the **Continuation** section.

3 Select the **Tuning of step size** check box, to make sure the solver takes small enough steps when starting the sweep.

4 In the **Initial step size** text field, type `0.0001`.

5 In the **Minimum step size** text field, type `0.0001`.

6 In the **Maximum step size** text field, type `0.01`.

7 From the **Predictor** list, choose **Constant**. This makes the solver first try with the solution found for the previously calculated `k` value. This is preferred, as even though the states can be degenerate, the field solutions are orthogonal. Thus, the solver is forced to follow the right band.

8 On the **Study** toolbar, click **Compute**.

RESULTS

Electric Field (ewfd2)

1 In the **Model Builder** window, expand the **Electric Field (ewfd2)** node, then click **Surface 1**.

2 In the **Settings** window for Surface, locate the **Expression** section.

3 In the **Expression** text field, type `ewfd2.Ez`.

4 Right-click **Results>Electric Field (ewfd2)>Surface 1** and choose **Height Expression**.

5 Click the **Zoom Extents** button on the **Graphics** toolbar. Compare the results with Figure 3.

1D Plot Group 3

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

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

3 From the **Data set** list, choose **Study 2/Parametric Solutions 1**.

4 On the **1D Plot Group 3** toolbar, click **Global**.

5 In the **Settings** window for Global, click to expand the **Legends** section.

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

7 In the table, enter the following settings:

Legends
band=1
band=2
band=3
band=4
band=5

8 On the **1D Plot Group 3** toolbar, click **Plot**. Compare the results with Figure 4.