Model created in COMSOL Multiphysics 6.4

Band-Gap Analysis of a Photonic Crystal

This application performs a band-gap 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 from propagating inside the crystal structure. This frequency range is called the photonic band gap (Ref. 2). There are several band gaps for a certain structure, and this application extracts the band gaps for the lowest bands of the crystal.

Model Definition

This model is similar to the Photonic Crystal waveguide model. The difference is that in this model 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 band-gap analysis. Firstly, the refractive index of GaAs is frequency dependent, creating a nonlinear eigenfrequency problem. Secondly, the wave vector must be ramped for the band diagram. The first complication can be handled with the use of a nonlinear eigenfrequency solver. The second complication is addressed by adding a parametric sweep to the solver to ramp over the relevant values of the wave vector, k. Furthermore, mode following can be used to automatically group the found eigenfrequencies into the correct bands.

The wave vector for the propagating wave, 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.

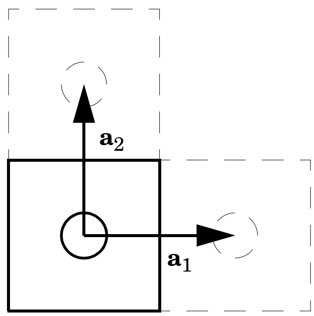


Figure 1: Definition of the square primitive cells and the lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$.

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 for $k = 0$.

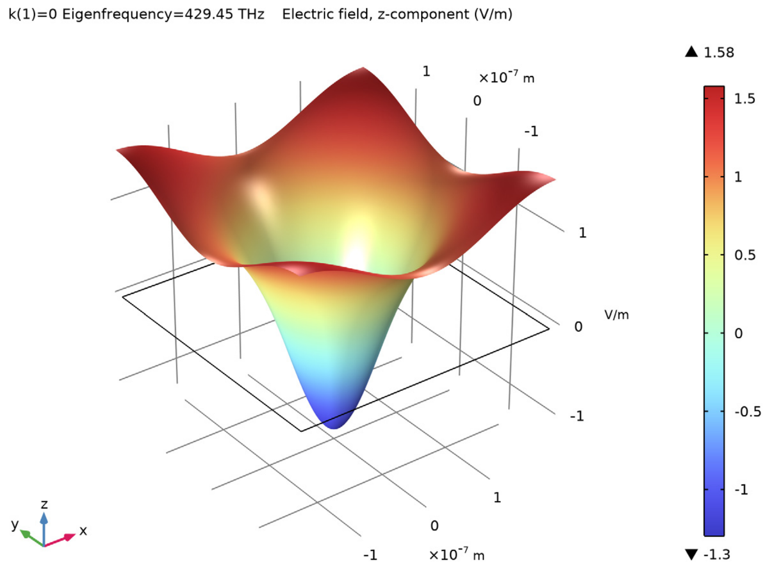


Figure 2: z-component of the electric field for k = 0.

[Figure 3](#) shows the *z*-component of the electric field for k = 0.5 for the fifth band.

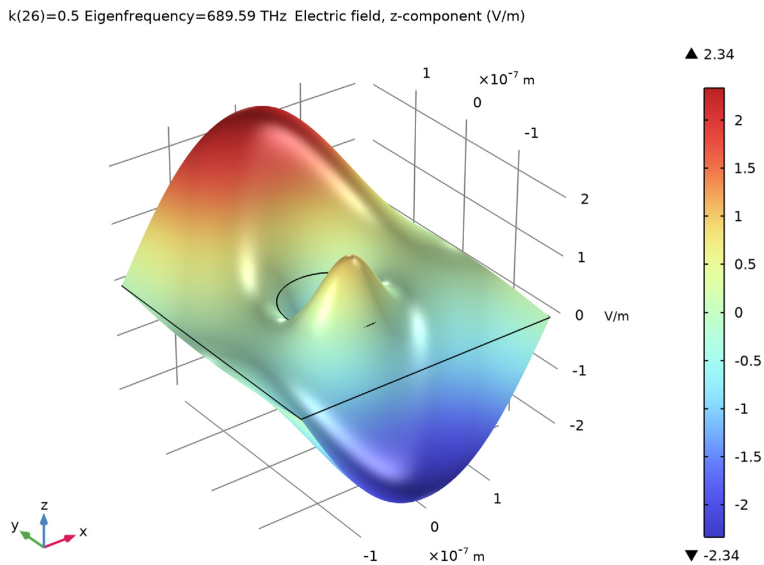


Figure 3: z-component of the electric field for the fifth band and k = 0.5.

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

Between bands 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 the lowest band in Figure 4. However, the frequencies in this band are so small 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.

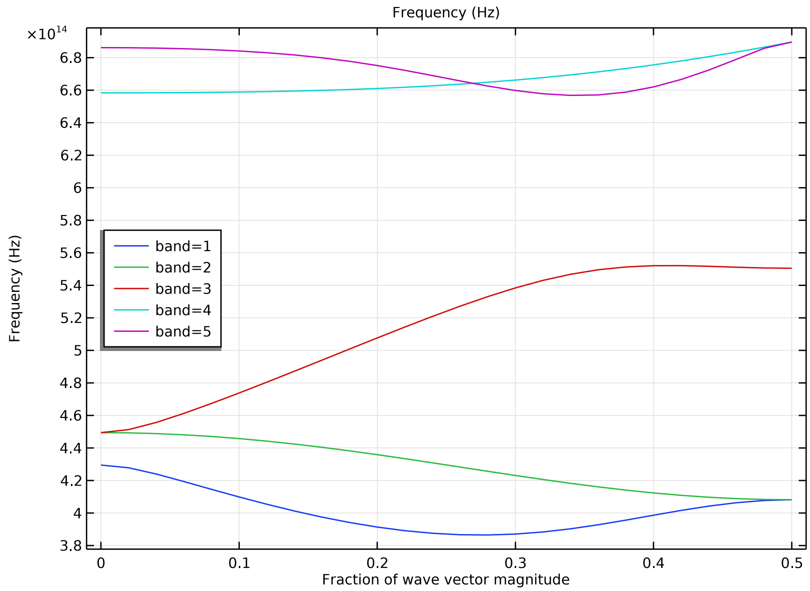


Figure 4: The dispersion relation (frequency versus wave number), when the wave vector is varied in the direction (1,1), for five bands.

References

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

2. J.D. Joannopoulos, 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

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

MODEL WIZARD

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

2 In the **Select Physics** tree, select **Optics** > **Wave Optics** > **Electromagnetic Waves, Frequency Domain (ewfd)**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

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

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
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

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
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 In the **Geometry** toolbar, click **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)

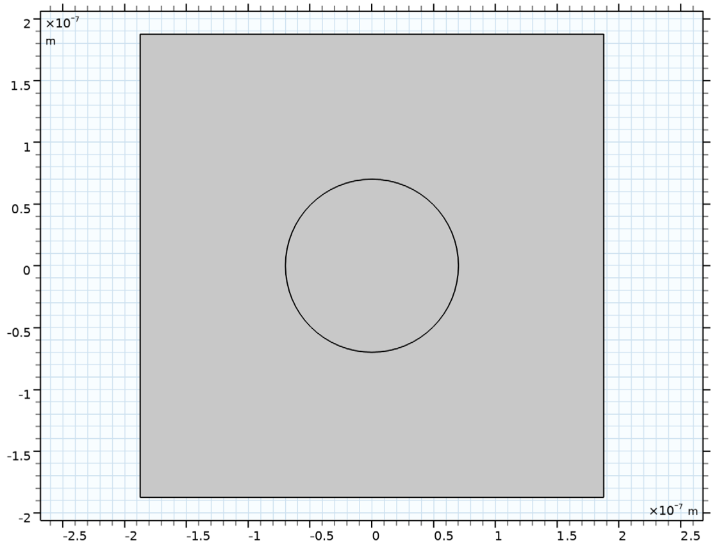
1 In the **Geometry** toolbar, click **Circle**.

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

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

4 Click **Build All Objects**.

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



ADD MATERIAL

1 In the **Materials** 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 the **Add to Component** button in the window toolbar.

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

DEFINITIONS

Analytic 1 (an1)

1 In the **Definitions** toolbar, click **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[1/m]*c_const/f+3.8359`.

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

5 Locate the **Units** section. In the table, enter the following settings:

Argument	Unit
f	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**.

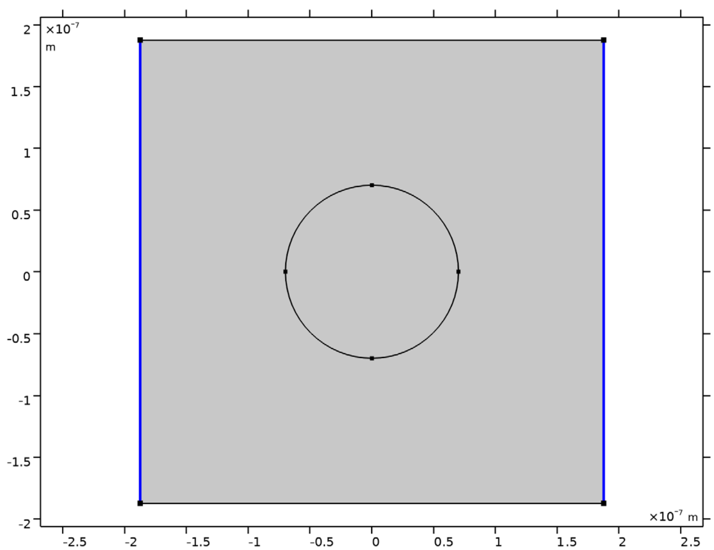
Periodic Condition 1

1 In 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 in 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**.

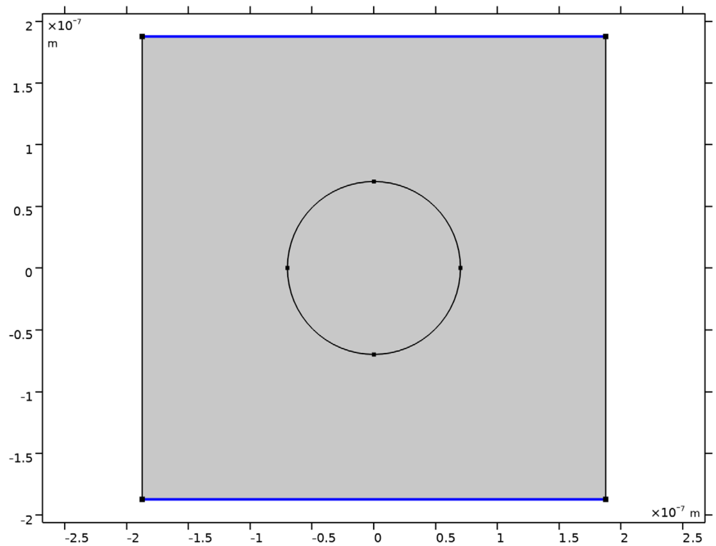
6 Specify the $\mathbf{k}_F$ vector as

kx	x
ky	y

Periodic Condition 2

1 In 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

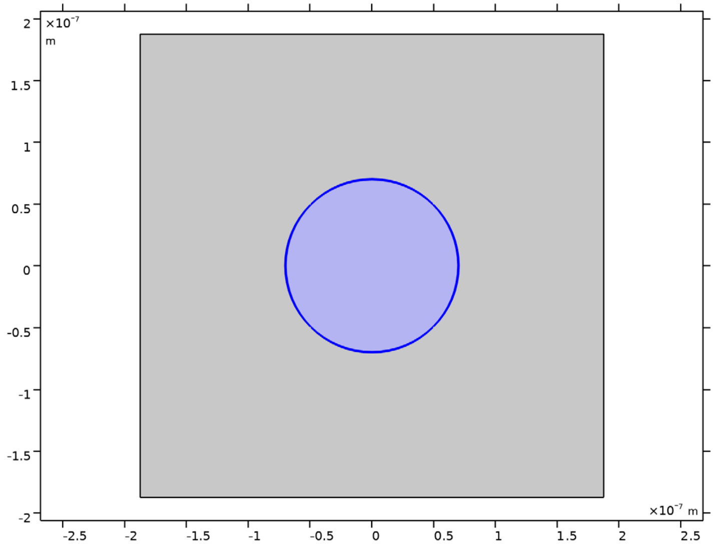
kx	x
ky	y

Add a wave equation feature, representing the GaAs pillar.

Wave Equation, Electric 2

1 In 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**. To set the imaginary part of the refractive index to the default value of 0.

MESH 1

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

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

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

Define the mesh so that the meshes on opposite edges are identical. This is important for the periodic boundary conditions, so that the source and destination meshes are the same.

Edge 1

1 In the **Mesh** toolbar, click **More Generators** and choose **Edge**.

2 Select Boundaries 1 and 2 only.

Copy Edge 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Copying Operations** > **Copy Edge**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Copy Edge**, locate the **Destination Boundaries** section.

4 Click to select the **Activate Selection** toggle button.

5 Select Boundary 4 only.

Copy Edge 2

1 Right-click **Mesh 1** and choose **Copying Operations** > **Copy Edge**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Copy Edge**, locate the **Destination Boundaries** section.

4 Click to select the **Activate Selection** toggle button.

5 Select Boundary 3 only.

Free Triangular 1

1 In the **Mesh** toolbar, click **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, click **Build All**.

STUDY 1

Step 1: Eigenfrequency

The ARPACK nonlinear solver is used to handle the nonlinear eigenvalue problem posed by the frequency dependence of the refractive index.

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 From the **Eigenfrequency solver** list, choose **ARPACK nonlinear**.

4 In the **Eigenvalue scaling factor** text field, type `1e9`.

Find the eigenfrequencies, for $k = 0$, around 540 THz.

5 Select the **Desired number of eigenfrequencies** checkbox. In the associated text field, type `5`.

6 In the **Search for eigenfrequencies around shift** text field, type `540[THz]`.

7 Click to expand the **Filtering and Sorting** section. Find the **Sorting** subsection. Select the **Mode following** checkbox. The Mode following functionality sorts the found eigenfrequencies into the appropriate bands.

Parametric Sweep

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

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

3 Click Add.

4 From the list in the **Parameter name** column, choose **k (Fraction of wave vector magnitude)**.

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

RESULTS

Electric Field (ewfd)

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

2 From the **Parameter value (k)** list, choose **0**. To select the results for the center of the Brillouin zone.

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

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

Surface 1

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`.

Height Expression 1

1 Right-click **Surface 1** and choose **Height Expression**.

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

Electric Field (ewfd)

1 In the **Model Builder** window, under **Results** click **Electric Field (ewfd)**.

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

3 From the **Parameter value (k)** list, choose **0.5**.

4 From the **Eigenfrequency (THz)** list, choose **689.59**. To select the result for the Brillouin zone boundary.

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

6 Click the **Zoom Extents** button in the **Graphics** toolbar. Compare the results with Figure 3.

Band Diagram

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

2 In the **Settings** window for **1D Plot Group**, type `Band Diagram` in the **Label** text field.

3 Locate the **Legend** section. From the **Position** list, choose **Middle left**.

Global 1

1 Right-click **Band Diagram** and choose **Global**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
`freq`	`Hz`	`Frequency`

4 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol2)**.

5 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **Outer solutions**.

6 From the **Parameter** list, choose **Expression**.

7 In the **Expression** text field, type `k`.

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

9 In the table, enter the following settings:

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

10 In the **Band Diagram** toolbar, click **Plot**. Compare the results with Figure 4.