



Dispersion Diagram of a Thin-Film BAW Structure

Introduction

This model shows how to create dispersion diagrams from simulation results by extending the tutorial Thin-Film BAW Composite Resonator. The dispersion curve can be plotted against both real and imaginary values of the wave number, corresponding to the propagating modes and evanescent modes, respectively. Each mode can also be visualized by plotting its displacement field. The consideration about such propagating and evanescent modes is an important part of the process in selecting appropriate design parameters for the layer structure of a BAW resonator.

See the PDF documentation for the tutorial Thin-Film BAW Composite Resonator (`thin_film_baw_resonator.mph`) for a general discussion on BAW resonators and for the specific device structure that the model is based on. ([Ref. 1](#))

Model Definition

This model simulates a uniform layer structure extending horizontally to infinity. The computed dispersion diagram of such an infinite plate can be used to optimize device designs - an example is given in [Ref. 2](#). For this tutorial, we take a thin slice from the center of the device given in [Ref. 1](#) and use the periodic boundary condition to extend it laterally to infinity.

Results and Discussion

[Figure 1](#) shows the computed dispersion curve. The results for the real and imaginary parts of the wave number are combined by taking the positive k -axis for the real part and the negative k -axis for the imaginary part.

[Figure 2](#) through [Figure 4](#) show three typical mode shapes along the dispersion curve shown in [Figure 1](#). They correspond to the lower branch for the TS2 mode (thickness-shear), the upper branch for the TE1 mode (thickness-extension), and the left branch for the evanescent modes.

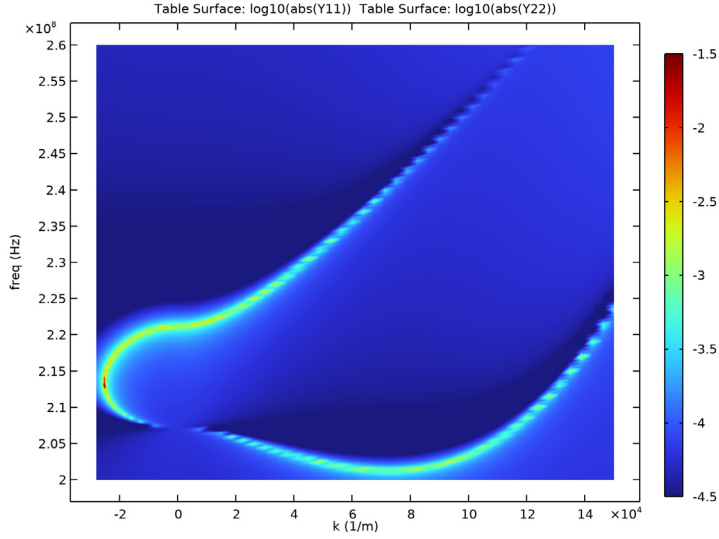


Figure 1: The dispersion diagram covering both real and imaginary parts of the wave number.

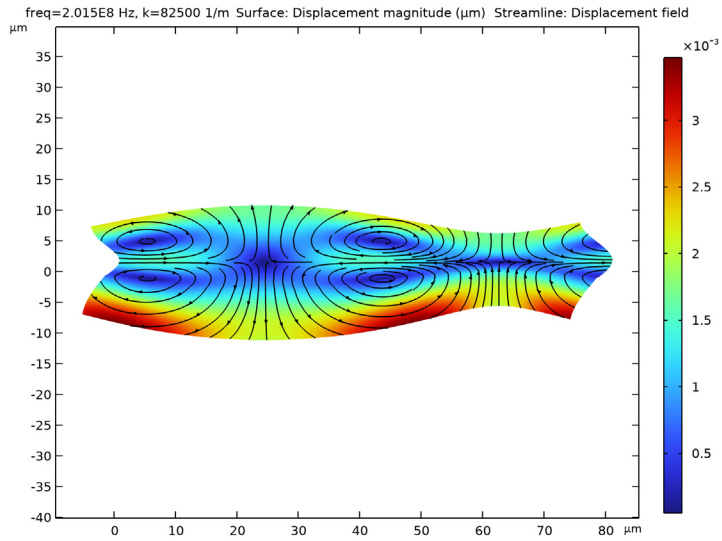


Figure 2: Mode shape of the TS2 mode at the lower branch of the dispersion curve.

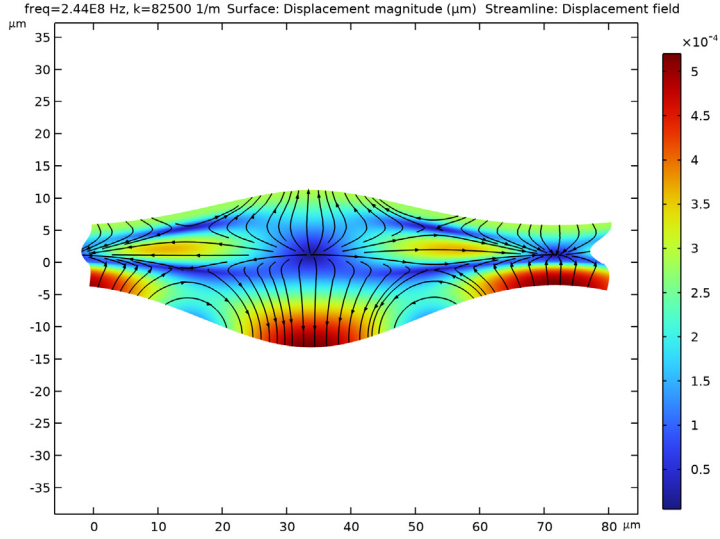


Figure 3: Mode shape of the TE1 mode at the upper branch of the dispersion curve.

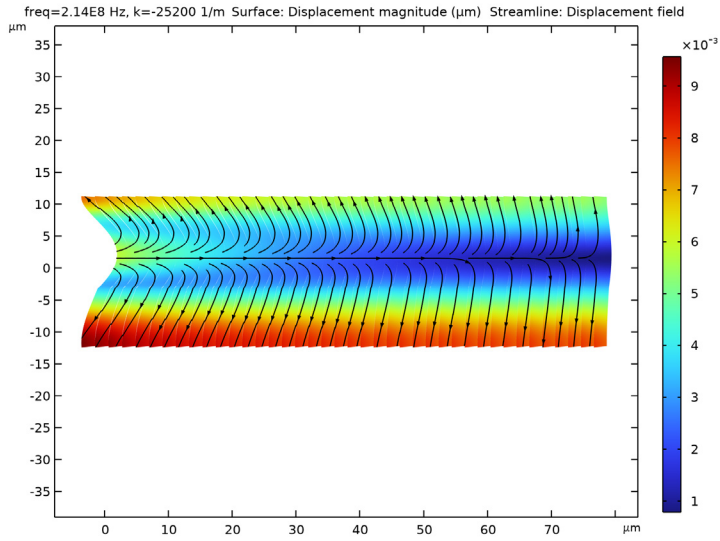


Figure 4: Mode shape of the evanescent mode at the left branch of the dispersion curve.

References

1. See the PDF documentation for the original tutorial under MEMS_Module/Piezoelectric_Devices/thin_film_baw_resonator.
2. United States Patent US9294069B2.


Application Library path: MEMS_Module/Piezoelectric_Devices/
thin_film_baw_resonator_dispersion_diagram

Modeling Instructions

ROOT

Open the tutorial model Thin-Film BAW Composite Resonator (filename: thin_film_baw_resonator.mph).

APPLICATION LIBRARIES

- 1 From the **File** menu, choose **Application Libraries**.
- 2 In the **Application Libraries** window, select **MEMS Module>Piezoelectric Devices>thin_film_baw_resonator** in the tree.
- 3 Click  **Open**.

Make a thin slice at the center of the device to simulate a uniform layer structure extending horizontally to infinity.

COMPONENT 1 (COMPI)

In the **Model Builder** window, expand the **Component 1 (comp1)** node.

GEOMETRY 1

Rectangle 1 (r1)



- 1 In the **Model Builder** window, expand the **Component 1 (comp1)>Geometry 1** node, then click **Rectangle 1 (r1)**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type 2.
- 4 Click to expand the **Layers** section. Clear the **Layers to the left** check box.

- 5 Clear the **Layers to the right** check box.

Rectangle 2 (r2)

- 1 In the **Model Builder** window, click **Rectangle 2 (r2)**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type 2.
- 4 Locate the **Layers** section. Clear the **Layers to the left** check box.
- 5 Clear the **Layers to the right** check box.

Rectangle 3 (r3)

- 1 In the **Model Builder** window, click **Rectangle 3 (r3)**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type 2.
- 4 Click  **Build All Objects**.
- 5 Click the  **Zoom Extents** button in the **Graphics** toolbar.



Make sure the Materials and physics setup have not changed after the change in the geometry. Click on each existing node in the Model Builder tree structure to check the domain or boundary **Selection**. The automatically generated instruction below does not include the nodes where no change is made in their Settings window, for example, all the nodes under **Materials**. So remember to click each node to check the selection by comparing with the original model. The first material **Si - Silicon (single-crystal, anisotropic)** appears to have missing material properties. The reason is that the physics node **Linear Elastic Material 2** under Solid Mechanics has lost its domain selection. To extend the thin slice into an infinite plate, replace the Fixed Constraint boundary condition with a Periodic Condition with **Floquet periodicity**.

DEFINITIONS

In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions** node.

ARTIFICIAL DOMAINS

Perfectly Matched Layer 1 (pml1)

- 1 In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions>Artificial Domains** node, then click **Perfectly Matched Layer 1 (pml1)**.
- 2 In the **Settings** window for **Perfectly Matched Layer**, locate the **Domain Selection** section.
- 3 Click  **Clear Selection**.
- 4 Click to clear the  **Activate Selection** toggle button.

SOLID MECHANICS (SOLID)

In the **Model Builder** window, expand the **Component 1 (comp1)>Materials** node.


Linear Elastic Material 2

- 1 In the **Model Builder** window, expand the **Solid Mechanics (solid)** node, then click **Linear Elastic Material 2**.
- 2 Select Domain 1 only.

Fixed Constraint 1

In the **Model Builder** window, right-click **Fixed Constraint 1** and choose **Delete**.

Periodic Condition 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Periodic Condition**.
- 2 Select Boundaries 1, 3, 5, 7, and 10–13 only.
- 3 In the **Settings** window for **Periodic Condition**, locate the **Periodicity Settings** section.
- 4 From the **Type of periodicity** list, choose **Floquet periodicity**.

Create a global parameter for the wave number and enter it into the Settings window for the Periodic Condition. This one will be for real wave numbers (propagating modes). Rename the title to reflect this. Then duplicate the Periodic Condition to make one for imaginary wave numbers (evanescent modes).

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 In the table, enter the following settings:

Name	Expression	Value	Description
k	0 [1/m]	0 1/m	wave number

SOLID MECHANICS (SOLID)

Periodic Condition 1: real k

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Solid Mechanics (solid)** click **Periodic Condition 1**.
- 2 In the **Settings** window for **Periodic Condition**, locate the **Periodicity Settings** section.

3 Specify the \mathbf{k}_F vector as

k	X
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4 In the **Label** text field, type Periodic Condition 1: real k.

5 Right-click **Component 1 (comp1)>Solid Mechanics (solid)>Periodic Condition 1: real k** and choose **Duplicate**.

Periodic Condition 2: imag k

1 In the **Model Builder** window, under **Component 1 (comp1)>Solid Mechanics (solid)** click **Periodic Condition 1: real k 1**.

2 In the **Settings** window for **Periodic Condition**, type Periodic Condition 2: imag k in the **Label** text field.

3 Locate the **Periodicity Settings** section. Specify the \mathbf{k}_F vector as

i*k	X
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Continue checking the selection for each Electrostatics physics node. Then create Periodic Conditions for the real and imaginary wave numbers in a similar procedure.

ELECTROSTATICS (ES)

In the **Model Builder** window, expand the **Component 1 (comp1)>Electrostatics (es)** node, then click **Electrostatics (es)**.

Periodic Condition 1: real k

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

2 In the **Settings** window for **Periodic Condition**, type Periodic Condition 1: real k in the **Label** text field.

3 Select Boundaries 5 and 12 only.

4 Locate the **Periodic Condition** section. From the **Type of periodicity** list, choose **Floquet periodicity**.

5 Specify the \mathbf{k}_F vector as

k	x
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6 Right-click **Periodic Condition 1: real k** and choose **Duplicate**.

Periodic Condition 2: imag k

1 In the **Model Builder** window, under **Component 1 (comp1)>Electrostatics (es)** click **Periodic Condition 1: real k 1**.

- 2 In the **Settings** window for **Periodic Condition**, type Periodic Condition 2: $\text{imag } k$ in the **Label** text field.
- 3 Locate the **Periodic Condition** section. Specify the \mathbf{k}_F vector as

$i*k$	x
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Make the electric potential on the terminal boundary consistent with the Floquet periodic condition.

Terminal 1: real k

- 1 In the **Model Builder** window, click **Terminal 1**.
- 2 In the **Settings** window for **Terminal**, type Terminal 1: $\text{real } k$ in the **Label** text field.
- 3 Locate the **Terminal** section. In the V_0 text field, type $1[V]*\exp(-i*k*x)$.
Create another terminal boundary condition for the case of imaginary wave number. Note that the terminal number automatically increments from 1 to 2. Later on when we evaluate the admittance of the terminal we will also change the expression from Y11 to Y22.
- 4 Right-click **Terminal 1: real k** and choose **Duplicate**.

Terminal 2: $\text{imag } k$

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Electrostatics (es)** click **Terminal 1: real k 1**.
- 2 In the **Settings** window for **Terminal**, type Terminal 2: $\text{imag } k$ in the **Label** text field.
- 3 Locate the **Terminal** section. In the V_0 text field, type $1[V]*\exp(-i*i*k*x)$.

Continue checking the selection for the Piezoelectricity multiphysics coupling node. Then adjust the mesh - use a coarse mesh to save time - mesh refinement study is always recommended.

MESH 1

In the **Model Builder** window, expand the **Component 1 (comp1)>Mesh 1** node.

Distribution 1

- 1 In the **Model Builder** window, expand the **Component 1 (comp1)>Mesh 1>Mapped 1** node, then click **Distribution 1**.
- 2 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 3 In the **Number of elements** text field, type 1.

Distribution 2

In the **Model Builder** window, right-click **Distribution 2** and choose **Delete**.

Distribution 3



In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1>Mapped 1** right-click **Distribution 3** and choose **Delete**.

Distribution 4

In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1>Mapped 1** right-click **Distribution 4** and choose **Delete**.




Add a frequency domain study with auxiliary sweep to sweep through a list of real wave numbers. Disable the physics nodes for imaginary wave numbers in the study step settings.

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 **General Studies>Frequency Domain**.
- 4 Click **Add Study** in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.

STUDY 3

Step 1: Frequency Domain

- 1 In the **Settings** window for **Frequency Domain**, locate the **Study Settings** section.
- 2 In the **Frequencies** text field, type range(200,0.5,260) [MHz].
- 3 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** check box.
- 4 In the tree, select **Component 1 (comp1)>Solid Mechanics (solid)>Periodic Condition 2: imag k**.
- 5 Click  **Disable**.
- 6 In the tree, select **Component 1 (comp1)>Electrostatics (es)>Periodic Condition 2: imag k**.
- 7 Click  **Disable**.
- 8 In the tree, select **Component 1 (comp1)>Electrostatics (es)>Terminal 2: imag k**.
- 9 Click  **Disable**.
- 10 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

11 Click  **Add**.

12 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
k (wave number)	range(0,0.025,1)*1.5e5	1/m

13 In the **Model Builder** window, click **Study 3**.

14 In the **Settings** window for **Study**, type Study 3: Freq domain, real k in the **Label** text field.

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

Similarly add a frequency domain study for the case of imaginary wave numbers.

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 **General Studies>Frequency Domain**.

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

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

STUDY 4: FREQ DOMAIN, IMAG K

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

2 In the **Frequencies** text field, type range(200,0.5,260) [MHz].

3 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** check box.

4 In the tree, select **Component 1 (comp1)>Solid Mechanics (solid)>Periodic Condition 1: real k**.

5 Click  **Disable**.

6 In the tree, select **Component 1 (comp1)>Electrostatics (es)>Terminal 1: real k**.

7 Click  **Disable**.

8 In the tree, select **Component 1 (comp1)>Electrostatics (es)>Periodic Condition 1: real k**.

9 Click  **Disable**.

10 Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.


11 Click  **Add**.

12 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
k (wave number)	-range(0,0.025,1)*2.8e4	1/m

13 In the **Model Builder** window, click **Study 4**.


14 In the **Settings** window for **Study**, type Study 4: Freq domain, imag k in the **Label** text field.

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

To plot the dispersion curve from the previous two studies, evaluate the log of the absolute value of the admittance as a function of frequency and wave number using an **Evaluation Group**. Remember to change the expression from Y11 to Y22 for the second terminal as discussed earlier.

RESULTS

Evaluation Group 1: Dispersion diagram

- 1 In the **Results** toolbar, click  **Evaluation Group**.
- 2 In the **Settings** window for **Evaluation Group**, type Evaluation Group 1: Dispersion diagram in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **None**.

Global Evaluation 1: real k

- 1 Right-click **Evaluation Group 1: Dispersion diagram** and choose **Global Evaluation**.
- 2 In the **Settings** window for **Global Evaluation**, type Global Evaluation 1: real k in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 3: Freq domain, real k/ Solution 3 (sol3)**.
- 4 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
$\log_{10}(\text{abs}(\text{es.Y11})/1[\text{S}])$		$\log_{10}(\text{abs}(\text{Y11}))$

- 5 Right-click **Global Evaluation 1: real k** and choose **Duplicate**.


Global Evaluation 2: imag k

- 1 In the **Model Builder** window, under **Results>Evaluation Group 1: Dispersion diagram** click **Global Evaluation 1: real k 1**.

- 2 In the **Settings** window for **Global Evaluation**, type Global Evaluation 2: imag k in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 4: Freq domain, imag k/ Solution 4 (sol4)**.
- 4 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
$\log_{10}(\text{abs}(\text{es.Y22})/1[\text{S}])$		$\log_{10}(\text{abs}(\text{Y22}))$

Evaluation Group 1: Dispersion diagram

- 1 In the **Model Builder** window, click **Evaluation Group 1: Dispersion diagram**.
- 2 In the **Evaluation Group 1: Dispersion diagram** toolbar, click  **Evaluate**.

EVALUATION GROUP 1: DISPERSION DIAGRAM

- 1 Go to the **Evaluation Group 1: Dispersion diagram** window.
The result of evaluating the Evaluation Group appears in a table with the same title as the evaluation group. Click on the **Table Surface** button to create a surface plot for the real wave numbers. Then duplicate it for the imaginary wave numbers.
- 2 Click **Table Surface** in the window toolbar.

RESULTS

Table Surface 1: real k


- 1 In the **Model Builder** window, under **Results>2D Plot Group 15** click **Table Surface 1**.
- 2 In the **Settings** window for **Table Surface**, locate the **Data** section.
- 3 From the **x-axis column** list, choose **k (1/m)**.
- 4 From the **y-axis column** list, choose **freq (Hz)**.
- 5 Click to expand the **Range** section. Select the **Manual color range** check box.
- 6 In the **Minimum** text field, type -4.5.
- 7 In the **Maximum** text field, type -1.5.
- 8 In the **Label** text field, type Table Surface 1: real k.
- 9 Right-click **Results>2D Plot Group 15>Table Surface 1: real k** and choose **Duplicate**.

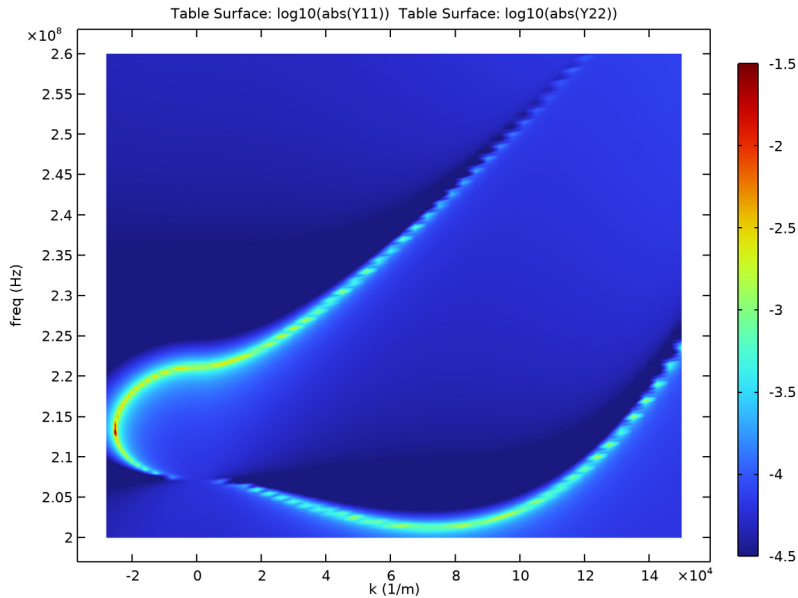
Table Surface 2: imag k

- 1 In the **Model Builder** window, under **Results>2D Plot Group 15** click **Table Surface 1: real k 1**.

- 2 In the **Settings** window for **Table Surface**, type Table Surface 2: imag k in the **Label** text field.
- 3 Locate the **Data** section. From the **x-axis column** list, choose **k (1/m)**.
- 4 From the **y-axis column** list, choose **freq (Hz)**.
- 5 From the **Data column** list, choose **log10(abs(Y22))**.
- 6 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Table Surface 1: real k**.

Dispersion Diagram

- 1 In the **Model Builder** window, under **Results** click **2D Plot Group 15**.
- 2 In the **Settings** window for **2D Plot Group**, type Dispersion Diagram in the **Label** text field.
- 3 In the **Dispersion Diagram** toolbar, click  **Plot**.




Plot a few mode shapes along the dispersion curve. Even though we only solved a thin slice of the infinite plate, we can still plot a wider section using the **Array 2D** dataset, with the Floquet wave number parameterized.

Array 2D 1: real k

- 1 In the **Results** toolbar, click  **More Datasets** and choose **Array 2D**.

- 2 In the **Settings** window for **Array 2D**, type `Array 2D 1: real k` in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 3: Freq domain, real k/ Solution 3 (sol3)**.
- 4 Locate the **Array Size** section. In the **x size** text field, type 40.
- 5 Click to expand the **Advanced** section. Select the **Floquet-Bloch periodicity** check box.
- 6 Find the **Wave vector** subsection. In the **x** text field, type k .

TS2 Mode

- 1 In the **Results** toolbar, click  **2D Plot Group**.
- 2 In the **Settings** window for **2D Plot Group**, type *TS2 Mode* in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Array 2D 1: real k**.
- 4 From the **Parameter value (freq (Hz))** list, choose **2.015E8**.
- 5 From the **Parameter value (k (1/m))** list, choose **82500**.
- 6 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

Surface 1

Right-click **TS2 Mode** and choose **Surface**.



Deformation 1

In the **Model Builder** window, right-click **Surface 1** and choose **Deformation**.

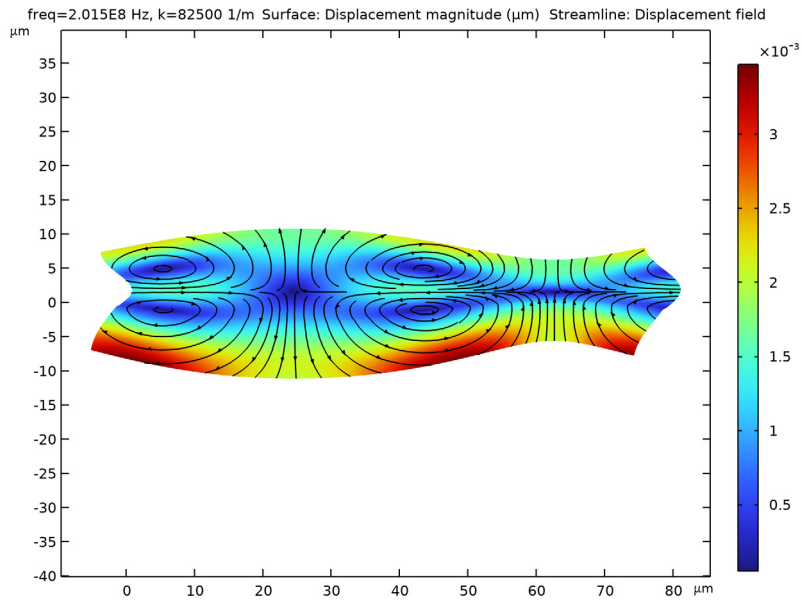
Streamline 1

- 1 In the **Model Builder** window, right-click **TS2 Mode** and choose **Streamline**.
- 2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.
- 3 From the **Positioning** list, choose **Uniform density**.
- 4 In the **Separating distance** text field, type 0.025.
- 5 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Type** list, choose **Arrow**.
- 6 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Surface 1**.
- 7 Clear the **Color** check box.

Deformation 1

- 1 Right-click **Streamline 1** and choose **Deformation**.
- 2 In the **TS2 Mode** toolbar, click  **Plot**.
- 3 Click the  **Zoom Extents** button in the **Graphics** toolbar.

4 In the **Model Builder** window, click **Deformation 1**.



TS2 Mode

In the **Model Builder** window, under **Results** right-click **TS2 Mode** and choose **Duplicate**.


TE1 Mode

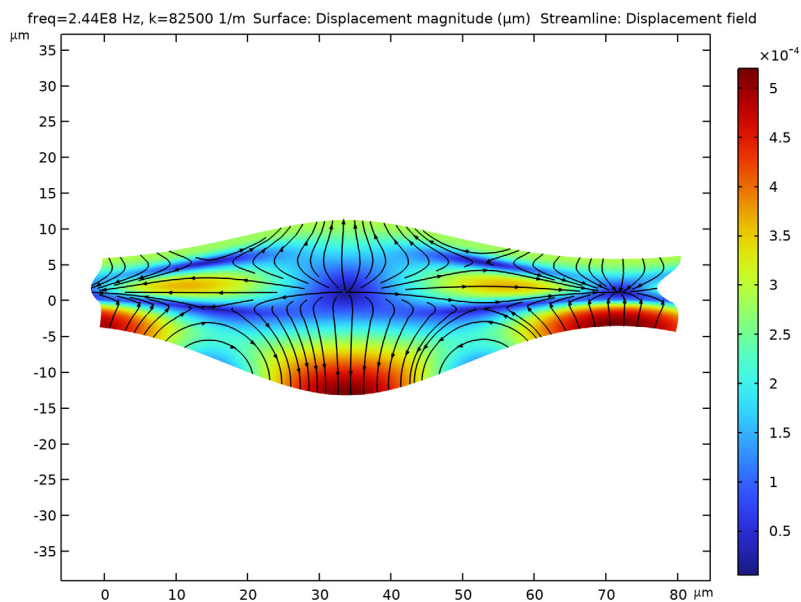
1 In the **Model Builder** window, under **Results** click **TS2 Mode 1**.

2 In the **Settings** window for **2D Plot Group**, type TE1 Mode in the **Label** text field.

3 Locate the **Data** section. From the **Parameter value (freq (Hz))** list, choose **2.44E8**.

4 In the **TE1 Mode** toolbar, click  **Plot**.

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



Array 2D 1: real k

In the **Model Builder** window, under **Results>Datasets** right-click **Array 2D 1: real k** and choose **Duplicate**.

Array 2D 1: imag k



- 1 In the **Model Builder** window, under **Results>Datasets** click **Array 2D 1: real k 1**.
- 2 In the **Settings** window for **Array 2D**, type Array 2D 1: imag k in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 4: Freq domain, imag k/ Solution 4 (sol4)**.
- 4 Locate the **Advanced** section. Find the **Wave vector** subsection. In the **x** text field, type $i*k$.

TEI Mode

In the **Model Builder** window, under **Results** right-click **TEI Mode** and choose **Duplicate**.

Evanescence Mode

- 1 In the **Model Builder** window, under **Results** click **TEI Mode 1**.
- 2 In the **Settings** window for **2D Plot Group**, type Evanescence Mode in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Array 2D 1: imag k**.

- 4 From the **Parameter value (freq (Hz))** list, choose **2.14E8**.
- 5 From the **Parameter value (k (1/m))** list, choose **-25200**.
- 6 In the **Evanescent Mode** toolbar, click  **Plot**.
- 7 Click the  **Zoom Extents** button in the **Graphics** toolbar.

