Created in COMSOL Multiphysics 6.0

Thin-Film BAW Composite Resonator

Introduction

Bulk acoustic wave (BAW) resonators can be used as narrow band filters in radio-frequency applications. Their chief advantage compared with traditional ceramic electromagnetic resonators is that they can be made smaller in size because they can be designed to have an acoustic wavelength smaller than the electromagnetic wavelength.

In addition to the desired bulk acoustic mode, the resonator structure may have many spurious modes with very narrow spacing. The design goal is usually to maximize the quality of the main component and to reduce the effect of spurious modes.

This tutorial shows how you can model thin-film BAW resonators in 2D using eigenfrequency and frequency-response analyses. The geometry used here is the same as that in Ref. 1 and Ref. 2.

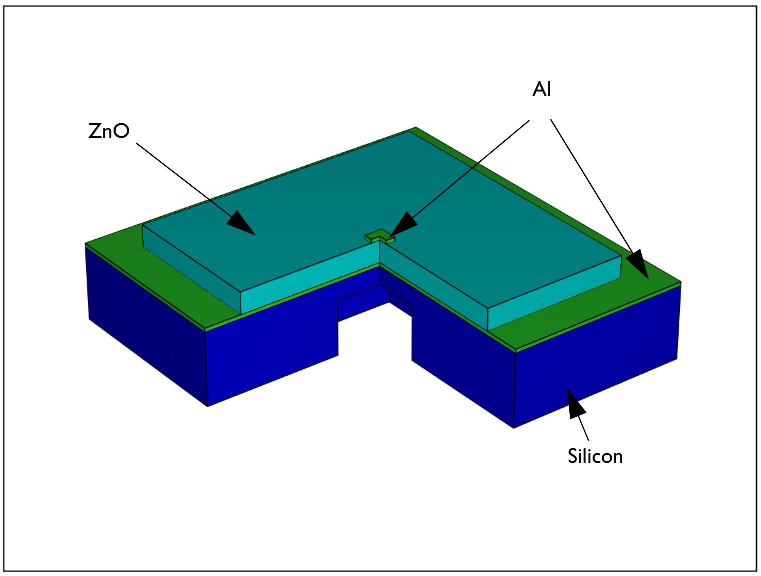


Figure 1: Arbitrarily scaled geometry of a thin film BAW resonator.

Model Definition

Figure 1 shows the geometry of the resonator from Ref. 1. The lowest layer of the resonator is silicon. On top of that, there is an aluminum layer that operates as the ground electrode. Above the aluminum layer is the active piezoelectric layer made of zinc oxide

(ZnO). The topmost layer of the resonator is an aluminum electrode. The material properties used in this model are obtained from the MEMS Module material library.

A large part of the silicon layer is etched away from the lower end of the central region of the resonator structure. This effectively reduces the thickness of the active central region thereby making the device a thin-film composite BAW resonator.

The thickness of the silicon layer at the central region is 7 μm. Both aluminum layers are 0.2 μm thick, and the piezoelectric layer is 9.5 μm thick. The width of the rectangular top electrode is 500 μm. The thin silicon area is roughly 1.7 mm wide.

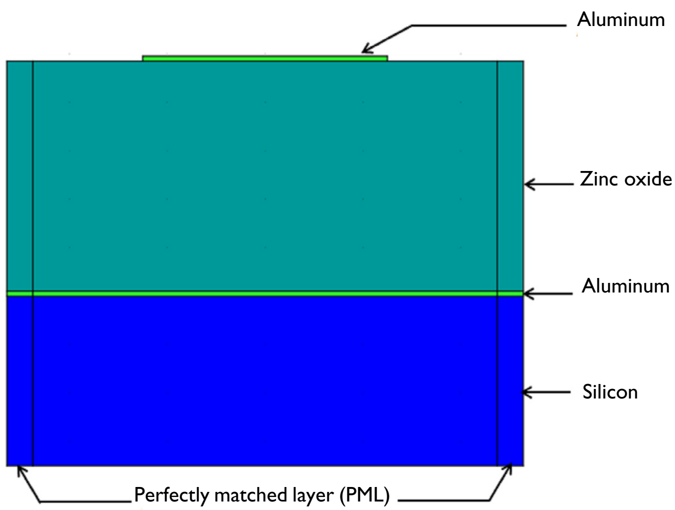


Figure 2: The 2D geometry (not drawn to scale) used in the tutorial.

This example is modeled in 2D, using the plane strain assumption where the out-of-plane thickness is specified to be 1.7 mm. The modeled geometry (Figure 2) is a symmetric 1-mm section in the center of the resonator. The Perfectly Matched Layer (PML) domains used on the two sides effectively increase the length of the resonator and simulates the effect of propagation and absorption of elastic waves in the adjoining regions which are not resolved in the true geometric scale.

The absorption of elastic waves in the PML domains contribute to the damping of the structure. This is also known as *anchor loss*. Additionally, the model also incorporates mechanical and electrical losses in the piezoelectric zinc oxide layer by means of loss factors. A structural loss factor represents the hysteresis in a stress-strain curve and a dielectric loss factor represents the polarization loss, which manifests itself as the hysteresis in the polarization versus electric field curve of the material. The structural and dielectric loss factors appear as the imaginary components of the mechanical stiffness and relative permittivity, respectively.

Ref. 3 gives the material quality Q_m and the dielectric loss tangent $\tan\delta$ for many materials. The magnitude of Q_m is roughly 100–1000, and the magnitude of $\tan\delta$ is roughly 0.001–0.01. Based on that data, the following values are used:

- Structural loss factor: $\eta_{cE} = 0.001$.
- Dielectric loss factor: $\eta_{\varepsilon S} = 0.01$.

In this model, COMSOL Multiphysics solves for both structural and electrical equations in the piezoelectric layer but only solves for the structural equation in the other layers. The electrical equations are not solved in the metallic aluminum layers because the electrical conductivity of aluminum is several orders of magnitude higher than that of zinc oxide and hence the aluminum layers almost act as equipotential regions allowing extremely small conduction current through them. Therefore the electrical characteristics of aluminum do not have any significant effect on the response of the resonator. The dominant electromechanical coupling is exhibited by the piezoelectric layer only.

This tutorial shows two different analyses. In the first step, you compute and investigate the eigenmodes of the structure, with its lateral ends fixed. In the second step, you analyze the frequency response of the resonator within the desired bandwidth of 215 MHz to 235 MHz.

Results and Discussion

Figure 3 shows the lowest BAW mode of the structure which occurs at 221.4 MHz. This plot was generated from the results of the eigenfrequency analysis. This is the fundamental longitudinal thickness mode. The plot shows scaled deformation only to be used for visualization of the mode shape. Note that COMSOL Multiphysics computes complex-valued eigenfrequencies where the imaginary part gives a measure of the damping due to structural loss, polarization loss and anchor loss.

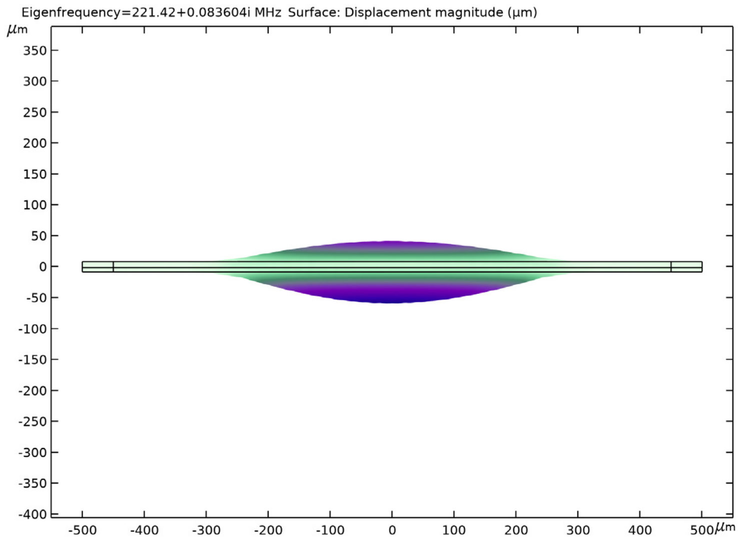


Figure 3: The lowest bulk acoustic mode of the resonator identified from the solutions of the eigenfrequency analysis.

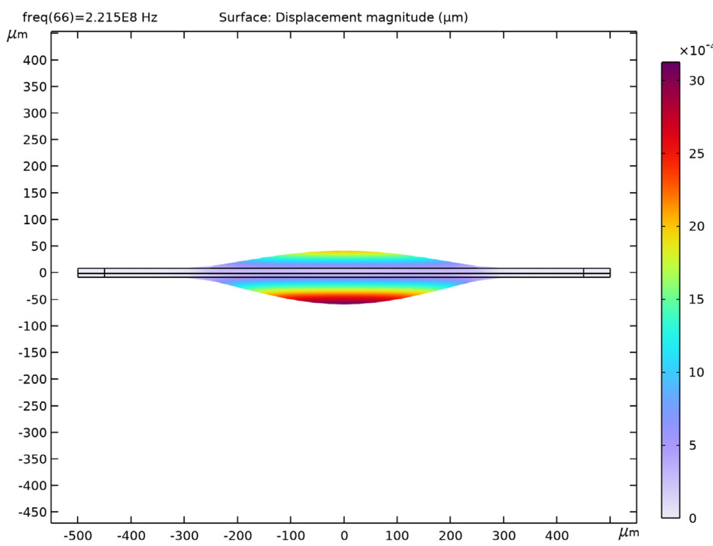


Figure 4: The lowest bulk acoustic mode of the resonator identified from the solutions of the frequency domain analysis.

Figure 4 shows the deformation of the resonator obtained from the frequency response analysis when the zinc oxide layer is excited with 1 volt (zero-to-peak voltage) at 221.5 MHz. The maximum deflection is about 3 nm.

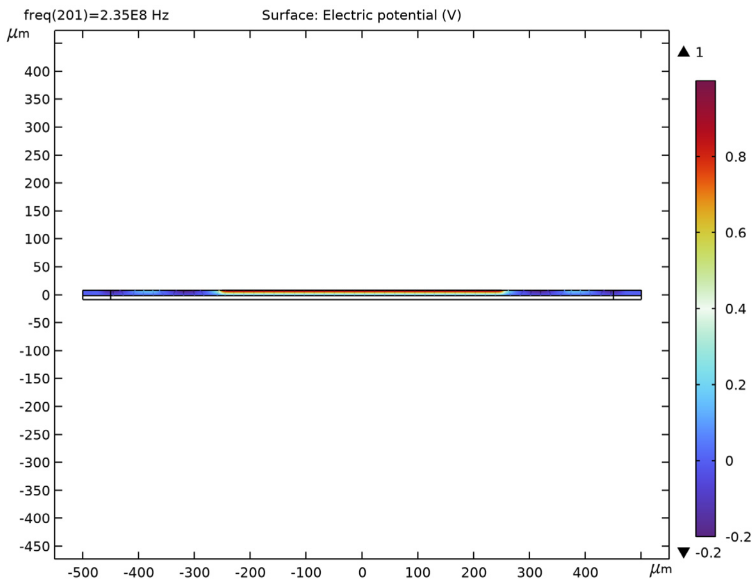


Figure 5: Electric potential distribution in the zinc oxide layer at 235 MHz excitation.

Figure 5 shows the voltage distribution in the piezoelectric layer when excited at 235 MHz.

COMSOL Multiphysics' Terminal boundary condition which is used to specify the voltage on the piezoelectric material also automatically computes the admittance. The admittance is the ratio of the total current flowing through the piezoelectric material to the voltage across it. It is a complex-valued quantity for a lossy material. Typically the imaginary part reflects the displacement current and the real part reflects the conduction current as well as other losses in the structure. Figure 6 shows the absolute value of admittance as a function of frequency. Within the investigated range of 215 MHz to 235 MHz, the admittance is very similar to that shown in Ref. 2. Note that the highest peak in admittance occurs at the lowest BAW mode of 221 MHz.

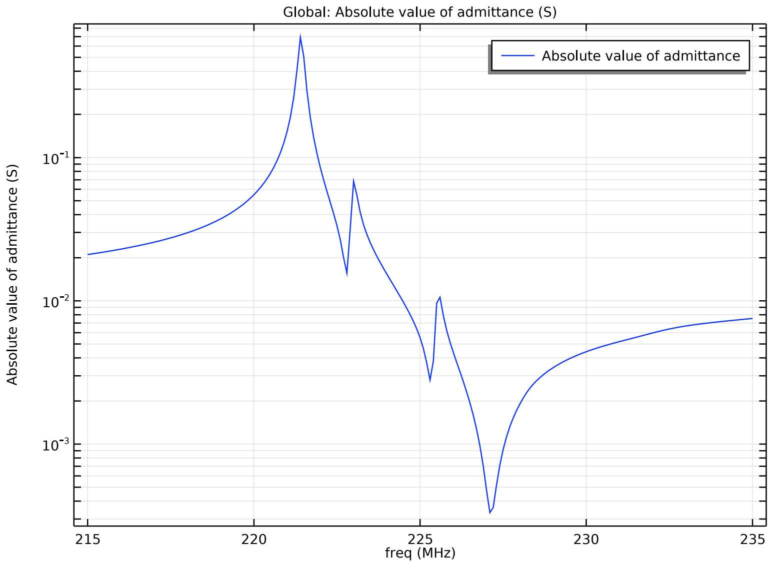


Figure 6: Absolute value of the admittance vs. frequency.

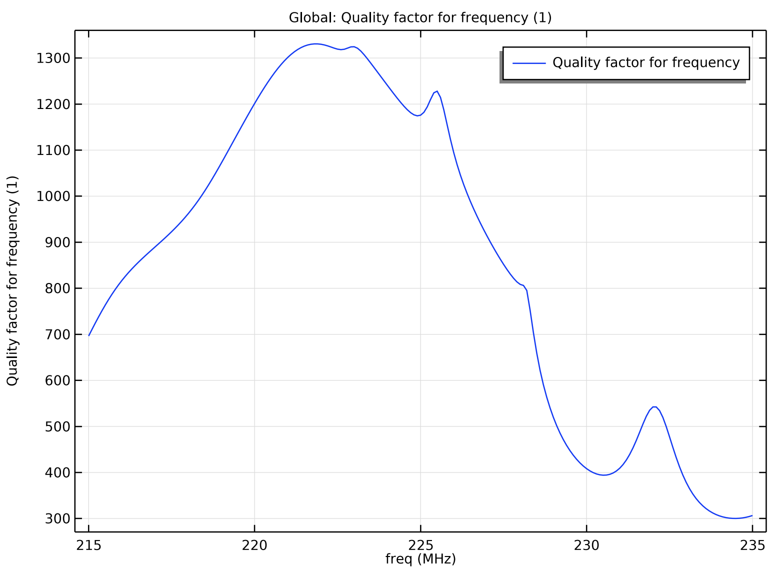


Figure 7: Quality factor vs. frequency.

Figure 7 shows the quality factor of the device as a function of frequency. The quality factor or Q-factor indicates the number of cycles (at the given frequency) in which the total energy of the system decreases by a factor of $e^{2\pi}$. This is also automatically computed by COMSOL Multiphysics. Figure 7 shows that the maximum value of Q ~ 1300 is obtained at around 221 MHz. This value obtained from the frequency-response analysis agrees well with the Q-factor computed by the eigenfrequency analysis. The results from the eigenfrequency analysis shows the Q-factor at 221.4 MHz to be 1326.

The eigenfrequency analysis also automatically computes the decay factor for each eigenfrequency. The inverse of the decay factor is the time required for the amplitude of a damped signal to reduce to e^{-1} of its initial amplitude. The decay factor at 221.4 MHz was computed to be $5.25 \cdot 10^5\ \mathrm{s}^{-1}$.

References

1. R.F. Milsom, J.E., Curran, S.L. Murray, S. Terry-Wood, and M. Redwood, "Effect of Mesa-Shaping on Spurious Modes in ZnO/Si Bulk-Wave Composite Resonators," *Proc. IEEE Ultrason. Symp.*, pp. 498–503, 1983.

2. T. Makkonen, A. Holappa, J. Ellä, and M.M. Salomaa, "Finite element simulations of thin-film composite BAW resonators," *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, vol. 48, no. 5, 2001.

3. Morgan Advanced Materials, http://www.morganelectroceramics.com

Application Library path: `MEMS_Module/Piezoelectric_Devices/thin_film_baw_resonator`

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 **Structural Mechanics>Electromagnetics-Structure Interaction>Piezoelectricity>Piezoelectricity, Solid**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Multiphysics>Eigenfrequency**.

6 Click **Done**.

GEOMETRY 1

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 **µm**.

Rectangle 1 (r1)

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

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

3 In the **Width** text field, type `1000`.

4 In the **Height** text field, type `16.7`.

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

6 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (µm)
Layer 1	50

7 Select the **Layers to the left** check box.

8 Select the **Layers to the right** check box.

9 Clear the **Layers on bottom** check box.

10 Click **Build Selected**.

Rectangle 2 (r2)

1 Right-click **Rectangle 1 (r1)** and choose **Duplicate**.

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

3 In the **Height** text field, type `0.2`.

4 Locate the **Position** section. In the **y** text field, type `-1.25`.

5 Click **Build Selected**.

Rectangle 3 (r3)

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

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

3 In the **Width** text field, type `500`.

4 In the **Height** text field, type `0.2`.

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

6 In the **y** text field, type `8.45`.

7 Click **Build All Objects**.

DEFINITIONS

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

Axis

Change the aspect ratio to have a better view of the model, and make the domain selections easier.

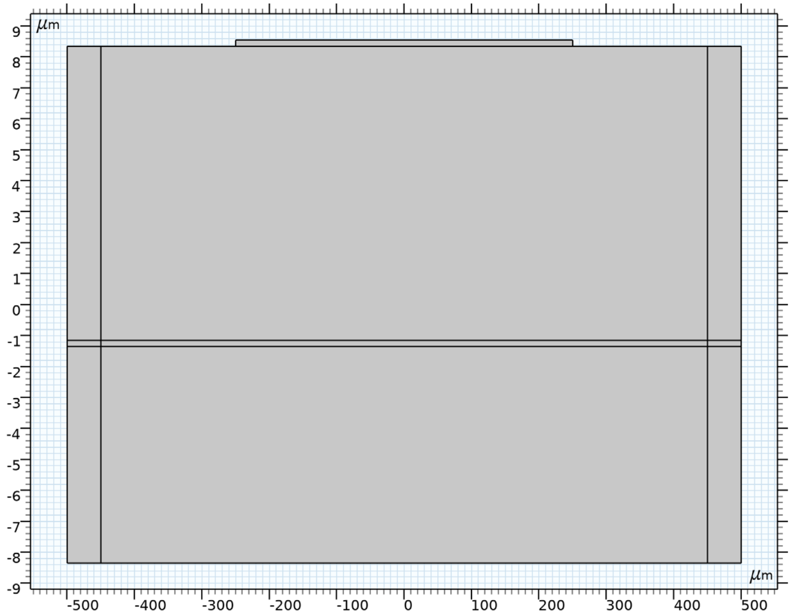
1 In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions>View 1** node, then click **Axis**.

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

3 From the **View scale** list, choose **Automatic**.

4 Click **Update**.

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



Perfectly Matched Layer 1 (pml1)

1 In the **Definitions** toolbar, click **Perfectly Matched Layer**.

2 In the **Settings** window for **Perfectly Matched Layer**, locate the **Domain Selection** section.

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `1-3,8-10` in the **Selection** text field.

5 Click **OK**.

In this way you specify that the layers on the two sides of the geometry form a perfectly matched layer.

Use the scaling settings to help cover longer wavelength waves.

6 In the **Settings** window for **Perfectly Matched Layer**, locate the **Scaling** section.

7 In the **PML scaling factor** text field, type `5`.

8 In the **PML scaling curvature parameter** text field, type `2`.

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 **MEMS>Semiconductors>Si - Silicon (single-crystal, anisotropic)**.

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

5 In the tree, select **MEMS>Metals>Al - Aluminum**.

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

7 In the tree, select **Piezoelectric>Zinc Oxide**.

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

9 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

Al - Aluminum (mat2)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Al - Aluminum (mat2)**.

2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `2 5 7 9` in the **Selection** text field.

5 Click **OK**.

Zinc Oxide (mat3)

1 In the **Model Builder** window, click **Zinc Oxide (mat3)**.

2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `3 6 10` in the **Selection** text field.

5 Click **OK**.

SOLID MECHANICS (SOLID)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Solid Mechanics (solid)**.

2 In the **Settings** window for **Solid Mechanics**, locate the **Thickness** section.

3 In the d text field, type `1.7[mm]`.

Use a fixed wave speed to avoid inconsistent PML geometry due to the discontinuity in sound speed across material boundaries.

4 Click to expand the **Typical Wave Speed for Perfectly Matched Layers** section. In the c_{ref} text field, type `9000[m/s]`.

Piezoelectric Material 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Solid Mechanics (solid)** click **Piezoelectric Material 1**.

2 In the **Settings** window for **Piezoelectric Material**, locate the **Domain Selection** section.

3 Click **Clear Selection**.

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog box, type `3 6 10` in the **Selection** text field.

6 Click **OK**.

These are piezoelectric domains.

Mechanical Damping 1

1 In the **Physics** toolbar, click **Attributes** and choose **Mechanical Damping**.

2 In the **Settings** window for **Mechanical Damping**, locate the **Damping Settings** section.

3 From the **Damping type** list, choose **Isotropic loss factor**.

4 From the η_s list, choose **User defined**. In the associated text field, type `0.001`.

Piezoelectric Material 1

In the **Model Builder** window, click **Piezoelectric Material 1**.

Dielectric Loss 1

1 In the **Physics** toolbar, click **Attributes** and choose **Dielectric Loss**.

2 In the **Settings** window for **Dielectric Loss**, locate the **Dielectric Loss Settings** section.

3 From the $\eta_{\varepsilon S}$ list, choose **User defined**. In the associated text field, type `0.01`.

Linear Elastic Material 2

1 In the **Physics** toolbar, click **Domains** and choose **Linear Elastic Material**.

2 In the **Settings** window for **Linear Elastic Material**, locate the **Domain Selection** section.

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `1 4 8` in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Linear Elastic Material**, locate the **Linear Elastic Material** section.

7 From the **Solid model** list, choose **Anisotropic**.

These are the silicon domains that are modeled as an anisotropic linear elastic material.

The remaining domains are the aluminum domains that are modeled as an isotropic linear elastic material.

Fixed Constraint 1

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

2 In the **Settings** window for **Fixed Constraint**, locate the **Boundary Selection** section.

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `1 3 5 27-29` in the **Selection** text field.

5 Click **OK**.

These are the boundaries of the perfectly matched layers. In this way you indicate that the device is fixed on its sides that are far away from the region that you are modeling.

ELECTROSTATICS (ES)

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

2 In the **Settings** window for **Electrostatics**, locate the **Domain Selection** section.

3 Click **Clear Selection**.

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog box, type `3 6 10` in the **Selection** text field.

6 Click **OK**.

7 In the **Settings** window for **Electrostatics**, locate the **Thickness** section.

8 In the d text field, type `1.7[mm]`.

Ground 1

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

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `6 13 25` in the **Selection** text field.

5 Click **OK**.

Terminal 1

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

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `16` in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Terminal**, locate the **Terminal** section.

7 From the **Terminal type** list, choose **Voltage**.

MESH 1

Mapped 1

In the **Mesh** toolbar, click **Mapped**.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type 2 21 in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Distribution**, locate the **Distribution** section.

7 In the **Number of elements** text field, type 10.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type 9 in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Distribution**, locate the **Distribution** section.

7 In the **Number of elements** text field, type 100.

Distribution 3

1 Right-click **Mapped 1** and choose **Distribution**.

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type 8 in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Distribution**, locate the **Distribution** section.

7 In the **Number of elements** text field, type 2.

Distribution 4

1 Right-click **Mapped 1** and choose **Distribution**.

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type 12 in the **Selection** text field.

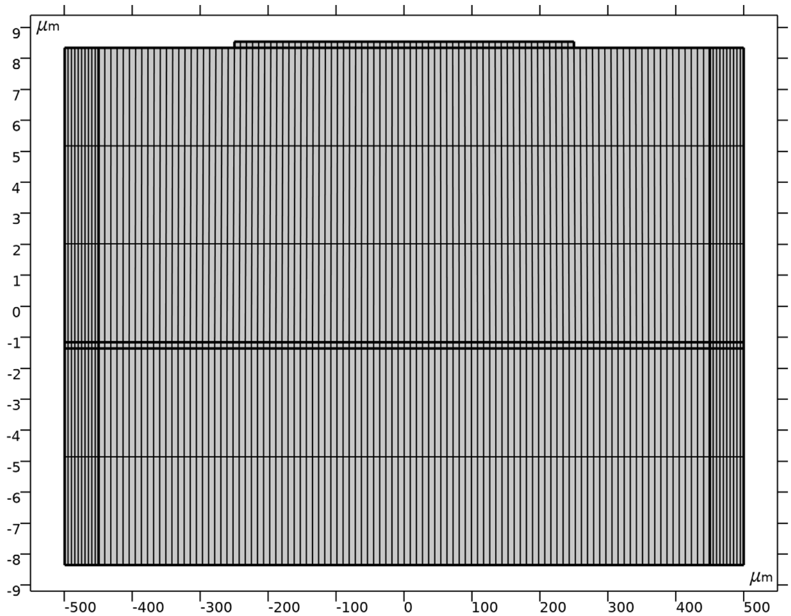
5 Click **OK**.

6 In the **Settings** window for **Distribution**, locate the **Distribution** section.

7 In the **Number of elements** text field, type 3.

8 Click **Build All**.

The mesh should look as shown in this figure.



STUDY 1

Step 1: Eigenfrequency

Use the **Region** search method to avoid spurious solutions.

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 search method** list, choose **Region**.

4 In the **Approximate number of eigenfrequencies** text field, type 6.

5 Find the **Search region** subsection. From the **Unit** list, choose **MHz**.

6 In the **Smallest real part** text field, type 220.

7 In the **Largest real part** text field, type 230.

8 In the **Largest imaginary part** text field, type `0.1`.

Solution 1 (sol1)

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

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Eigenvalue Solver 1**.

3 In the **Settings** window for **Eigenvalue Solver**, locate the **General** section.

4 In the **Value of eigenvalue linearization point** text field, type `2e8`.

5 Click **Compute**.

DEFINITIONS

Axis

Set the view to the default scale type for the result plots.

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

2 From the **View scale** list, choose **None**.

3 Click **Update**.

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

RESULTS

Mode Shape (solid)

1 In the **Model Builder** window, under **Results** click **Mode Shape (solid)**.

2 In the **Mode Shape (solid)** toolbar, click **Plot**.

Compare this plot with Figure 3.

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 2

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(215,0.1,235)[MHz]`.

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

RESULTS

Displacement (solid)

1 In the **Settings** window for **2D Plot Group**, type `Displacement (solid)` in the **Label** text field.

2 Locate the **Data** section. From the **Parameter value (freq (Hz))** list, choose **2.215E8**.

Surface 1

1 In the **Model Builder** window, expand the **Displacement (solid)** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Solid Mechanics>Displacement>solid.disp - Displacement magnitude - m**.

3 In the **Displacement (solid)** toolbar, click **Plot**.

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

Compare this plot with Figure 4.

Electric Potential (es) 1

1 In the **Model Builder** window, under **Results** click **Electric Potential (es) 1**.

2 In the **Electric Potential (es) 1** toolbar, click **Plot**.

Compare this plot with Figure 5.

Admittance

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

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

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

Global 1

1 Right-click **Admittance** 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
abs(es.Y11)	S	Absolute value of admittance

4 Locate the **x-Axis Data** section. From the **Unit** list, choose **MHz**.

5 In the **Admittance** toolbar, click **Plot**.

6 Click the **y-Axis Log Scale** button in the **Graphics** toolbar.

Compare this plot with Figure 6.

Quality Factor

1 In the **Model Builder** window, right-click **Admittance** and choose **Duplicate**.

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

Global 1

1 In the **Model Builder** window, expand the **Quality Factor** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Solid Mechanics>Global>solid.Q_freq - Quality factor for frequency**.

3 Click the **y-Axis Log Scale** button in the **Graphics** toolbar.

4 In the **Quality Factor** toolbar, click **Plot**.

Compare this plot with Figure 7.

The following steps show how to compute the quality factor and the decay factor for the resonance at 221.4 MHz from the eigenfrequency study. You will see that the value for the quality factor agrees well with that obtained from the frequency domain study at the same frequency.

Q-Factor

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, type `Q-Factor` in the **Label** text field.

3 Locate the **Data** section. From the **Eigenfrequency selection** list, choose **From list**.

4 In the **Eigenfrequency (MHz)** list, select **221.42+0.083604i**.

5 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)>Solid Mechanics>Global>solid.Q_eig - Quality factor for eigenvalue**.

6 Click **Evaluate**.

Decay Factor

1 Right-click **Q-Factor** and choose **Duplicate**.

2 In the **Settings** window for **Global Evaluation**, click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)>Solid Mechanics>Global>solid.decay - Exponential decay factor**.

3 In the **Label** text field, type `Decay Factor`.

4 Click **Evaluate**.