Residual Stress in a Thin-Film Resonator—2D Model

Introduction

Almost all surface-micromachined thin films experience residual stress as a result of the fabrication process. The most common source of residual stress is thermal stress, which is caused by a change in temperature experienced during the fabrication sequence and also due to the difference in the coefficient of thermal expansion between the film and the substrate. This tutorial shows how to model thermal residual stress due to a temperature difference and how it changes the resonant frequency of a thin-film resonator. The substrate is not included in the model and it is also assumed that at a given state (which indicates a particular step of the process sequence), the temperature is uniform throughout the cantilever.

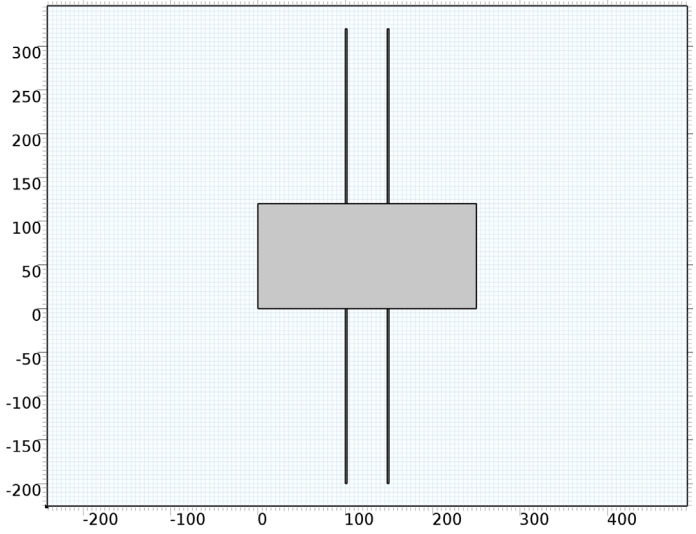

Figure 1: A thin-film resonator with four straight cantilever beam springs.

The tutorial investigates two design choices; a resonator with straight cantilevers (Figure 1) and another one with folded cantilevers (Figure 2). For each of the designs, the resonant frequency is computed for the cases when the structure is unstressed and

when it is subjected to a residual thermal stress. The results obtained are compared with analytical solutions.

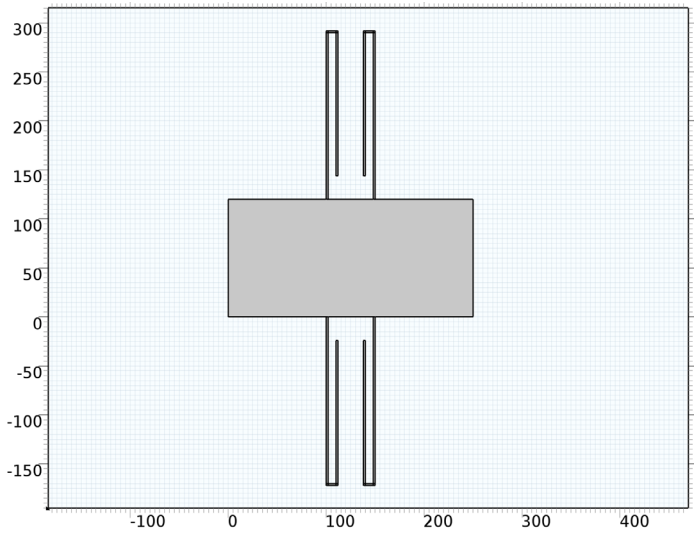

Figure 2: A thin-film resonator with four folded cantilever beam springs.

Model Definition

This tutorial uses the dimensions and material properties presented in Table 1 and Table 2. These values were obtained from the example in Chapter 27.2.5 in Ref. 1. It calculates the length of the folded cantilever using the equivalent spring-constant relationship discussed later.

This simulation models thermal residual stress using the Thermal Expansion feature in the Solid Mechanics physics interface. The coefficient of thermal expansion is computed by assuming a residual stress of 50 MPa in the straight cantilevers, a film deposition temperature of 605 °C (see Chapter 16.13.2.3 in Ref. 1) and a room temperature of 25 °C.

TABLE 1: DIMENSIONS OF THE STRUCTURE.

PARAMETER	STRAIGHT CANTILEVERS	FOLDED CANTILEVERS			PLATE
		L1	L2	L3	
Length	200 µm	170 µm	10 µm	146 µm	250 µm
Width	2 µm	2 µm	2 µm	2 µm	120 µm
Thickness	2.25 µm	2.25 µm	2.25 µm	2.25 µm	2.25 µm

TABLE 2: MATERIAL PROPERTIES OF THE STRUCTURE.

PROPERTY	VALUE
Material	polysilicon
Young's modulus	155 GPa
Poisson's ratio	0.23
Density	2330 kg/m^3
T_0	605 °C
T_I	25 °C

In order to determine the eigenfrequencies for the case with residual stress, a Prestressed-Eigenfrequency Study is used. This predefined study type first solves for a static thermal expansion problem to compute the residual stress. The solution of this static problem is then used to create a shift in the linearization point around which the eigenfrequencies are then computed. This approach accurately computes the shift in eigenfrequency by accounting for the stress-stiffening effect.

2D ANALYTICAL MODEL

For a lateral resonator with four cantilever-beam springs, the first in-plane bending resonant frequency is given by Equation 1.

$$f_0 \approx \frac{1}{2\pi}\sqrt{\frac{4Etb^3}{mL^3} + \frac{24\sigma_r tb}{5mL}} \quad (1)$$

Here m is the mass of the resonator plate, E is Young's modulus, L is the length of each cantilever arm, b is its width, t is its thickness, and σ_r is the residual stress in each cantilever. In this tutorial, the stress is assumed to be purely because of temperature difference but in reality it could be a sum of external stresses, the thermal stress, and intrinsic components. Assuming the material is isotropic, the stress is constant through the film thickness, and the stress component in the direction normal to the substrate is zero (i.e. plane stress). The stress-strain relationship is then given by Equation 2. Here ν is the Poisson's ratio.

$$\sigma_r = \left(\frac{E}{1-\nu}\right)\varepsilon \quad (2)$$

The strain comes from $\varepsilon = \alpha\Delta T$ where α is the thermal-expansion coefficient of the cantilever material and ΔT is the difference between the deposition temperature and the normal operating temperature.

Thermal residual stress in thin-film spring structures is typically relieved by folding the flexures as shown in Figure 2. The flexures relieve axial stress because each is free to expand or contract in the axial direction.

The basic folded structure is a U-shaped spring. For springs in series, the equivalent spring constant is given by Equation 3.

$$\frac{1}{k_{\text{eq}}} = \frac{1}{k_1} + \frac{1}{k_2} + \frac{1}{k_3} \tag{3}$$

The first and third springs are cantilever beams. The equivalent spring constant for these can be computed as $k = 3EI/L^3$, where I is the moment of inertia. For a beam with rectangular cross-section and for a rotation about the local y-axis of the beam (the axis parallel to the in-plane width), the moment of inertia is $I = bt^3/12$, where b is the width and t is the structure's thickness. You can treat the second spring as a column with a spring constant of $k = AE/L$, where A is the cross-sectional area $A = bt$. Assuming the spring thickness (t) and width (b) are the same everywhere, Equation 3 can be used to find the equivalent length of each set of folded springs. The equivalent length can be expressed in terms of the out-of-plane thickness (t) and the length of each of the three sections of a folded cantilever as shown in Equation 4.

$$L_{\text{eq}}^3 = L_1^3 + \frac{t^2 L_2}{4} + L_3^3, \tag{4}$$

Using the information provided in Table 1 and Table 2 and by using Equation 1 and Equation 2, one could compute the resonant frequency for the unstressed and stressed thin-film resonator with straight cantilever. Additionally by using Equation 4 along with the other information, one could also find the resonant frequency for the unstressed resonator with folded cantilevers. Note that the residual stress in the folded cantilevers are negligible by design and hence there is no need to compute the resonant frequency for this scenario. A summary of the analytical results are shown in Table 3 where they are compared with the solution obtained from the 2D plane-stress COMSOL model.

Results and Discussion

Table 3 summarizes the resonant frequencies for the first in-plane bending eigenmode. For the 2D COMSOL models this is the lowest (first) eigenmode. As the table shows, the resonant frequency for the straight cantilevers increases significantly when the model includes residual stress. The model results agree closely with the analytical

estimates. As expected, the stress sensitivity of the resonant frequency is reduced by folding the cantilevers.

TABLE 3: RESONANT FREQUENCIES WITH AND WITHOUT RESIDUAL STRESS.

	STRAIGHT CANTILEVERS		FOLDED CANTILEVERS	
	ANALYTICAL	2D MODEL	ANALYTICAL	2D MODEL
Without stress	14.99 kHz	14.82 kHz	14.97 kHz	14.11 kHz
With residual stress	33.08 kHz	32.05 kHz	-	14.22 kHz

Figure 3 and Figure 4 show the first in-plane bending resonance mode for the unstressed resonator with straight and folded cantilevers respectively.

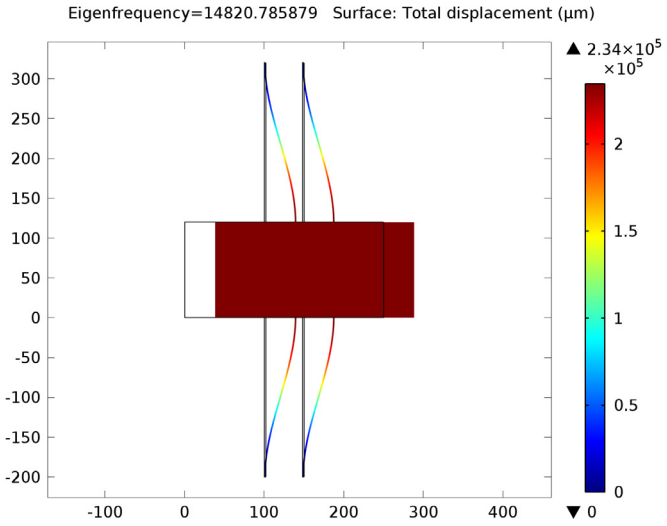

Figure 3: The first in-plane bending eigenmode of the unstressed resonator with straight cantilevers.

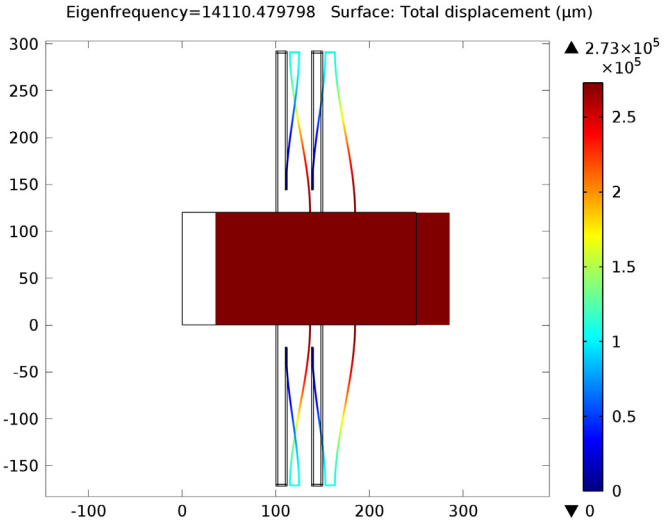

Figure 4: The first in-plane bending eigenmode of the unstressed resonator with folded cantilevers.

Figure 5 and Figure 6 show the first in-plane bending resonance mode for the resonator with straight and folded cantilevers respectively when they have a residual thermal stress.

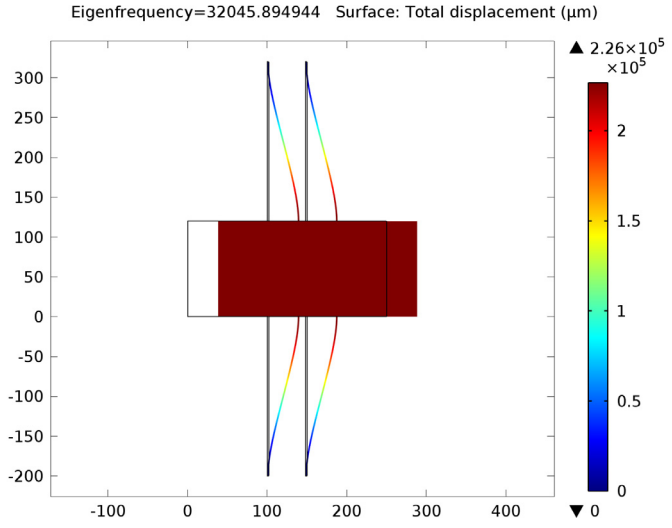

Figure 5: The first in-plane bending eigenmode of the resonator with straight cantilevers having residual thermal stress.

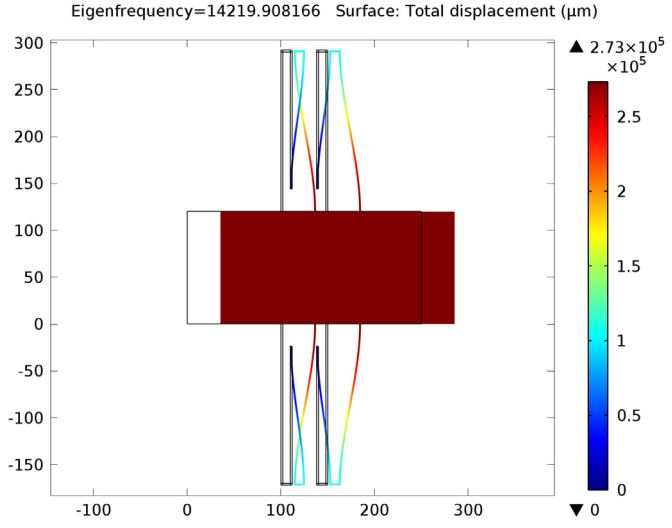

Figure 6: The first in-plane bending eigenmode of the resonator with folded cantilevers having residual thermal stress.

Figure 7 and Figure 8 show the residual thermal stress (von Mises stress) distribution in the resonator with straight and folded cantilevers respectively when they are cooled from 605 °C to 25 °C. Figure 7 shows that the residual stress is almost uniform in the straight cantilever and is about 49 MPa. The maximum stress is about 55 MPa at the two ends of the cantilevers. Figure 8 shows that the folded configuration significantly reduces the residual stress build-up. In this case the residual stress is around 2 MPa in most part of the cantilever except near the fixed end where it is close to 39 MPa.

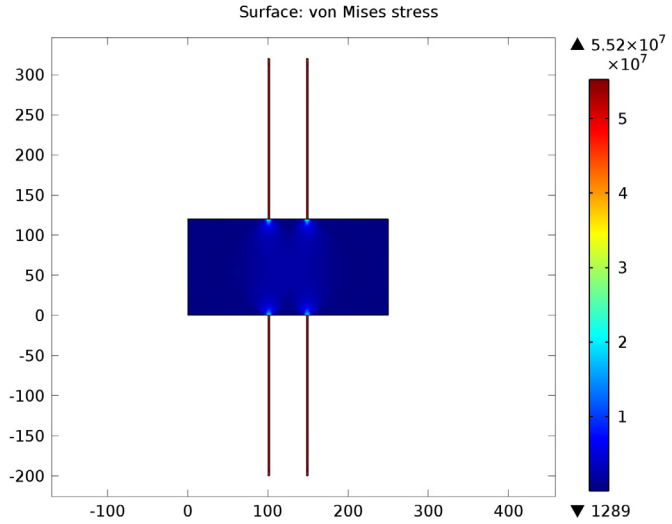

Figure 7: Residual thermal stress in the resonator with straight cantilevers when it is cooled from 605 °C *to* 25 °C.

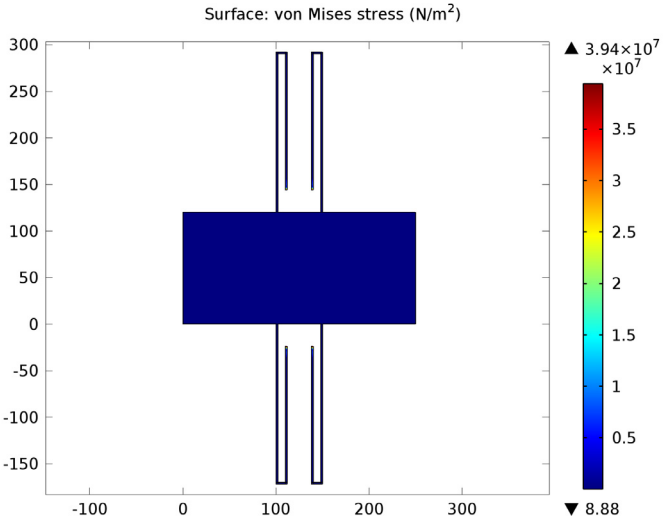

Figure 8: Residual thermal stress in the resonator with folded cantilevers when it is cooled from 605 °*C to* 25 °*C.*

Reference

1. M. Gad-el-Hak, ed., *The MEMS Handbook*, CRC Press, London, 2002, ch. 16.12 and 27.2.5.

Model Library path: `MEMS_Module/Actuators/residual_stress_resonator_2d`

Modeling Instructions

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

NEW

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

MODEL WIZARD

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

2 In the **Select physics** tree, select **Structural Mechanics>Solid Mechanics (solid)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select study** tree, select **Preset Studies>Eigenfrequency**.

6 Click **Done**.

GLOBAL DEFINITIONS

Load in the required global parameters. These values are used later for comparison between the model and the analytical solution.

Parameters

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

2 In the **Parameters** settings window, locate the **Parameters** section.

3 Click **Load from File**.

4 Under the Model Library root, browse to the folder `MEMS_Module/Actuators` and double-click the file `residual_stress_resonator_2d_parameters.txt`.

GEOMETRY 1

First create a component to model the resonator with straight cantilevers. For convenience, the device geometry will be inserted from an existing file.

1 On the **Geometry** toolbar, click **Insert Sequence**.

2 Browse to the model's Model Library folder and double-click the file `residual_stress_resonator_2d_geom_sequence.mph`.

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

4 In the **Insert Sequence from File** dialog box, click the **OK** button.

5 On the **Home** toolbar, click **Build All**.

Next set up the required solid mechanics physics for the problem by adding a thermal expansion feature and specifying the fixed boundaries.

SOLID MECHANICS (SOLID)

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

2 In the **Solid Mechanics** settings window, locate the **2D Approximation** section.

3 From the **2D approximation** list, choose **Plane stress**.

4 Locate the **Thickness** section. In the d edit field, type `thickness`.

Thermal Expansion 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Solid Mechanics (solid)** right-click **Linear Elastic Material 1** and choose **Thermal Expansion**.

2 In the **Thermal Expansion** settings window, locate the **Model Inputs** section.

3 In the T edit field, type `T0`.

4 Locate the **Thermal Expansion Properties** section. In the T_{ref} edit field, type `T1`.

Fixed Constraint 1

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

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `5,9,15,19` in the **Selection** edit field.

5 Click **OK**.

MATERIALS

Now add a new material to the component in order to define the required physical properties of the device.

Material 1 (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **New Material**.

2 In the **Material** settings window, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Young's modulus	E	`E1`	Pa	Basic
Poisson's ratio	nu	`nu1`	1	Basic
Density	rho	`rho1`	kg/m³	Basic
Coefficient of thermal expansion	alpha	`daT`	1/K	Basic

MESH 1

Configure a suitable mesh, a mapped mesh is appropriate for this device geometry.

Mapped 1

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

Distribution 1

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

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `6,8,16,18` in the **Selection** edit field.

5 Click **OK**.

6 In the **Distribution** settings window, locate the **Distribution** section.

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

Size

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

2 In the **Size** settings window, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extra fine**.

4 Click the **Build All** button.

Add a second component to model the resonator with folded cantilevers. As with the first component, the device geometry will be imported for convenience.

ROOT

On the **Home** toolbar, click **Add Component** and choose **2D**.

GEOMETRY 2

1 On the **Geometry** toolbar, click **Insert Sequence**.

2 Browse to the model's Model Library folder and double-click the file `residual_stress_resonator_2d_geom_sequence.mph`.

3 In the **Model Builder** window, under **Component 2 (comp2)** click **Geometry 2**.

4 In the **Insert Sequence from File** dialog box, In the **Select geometry sequence to insert** list, select **Geometry 2**.

5 click the **OK** button.

6 On the **Home** toolbar, click **Build All**.

Now the solid mechanics physics can be configured, as with the first component. In addition, a material will be added to define the required properties of the second device and an appropriate mesh will be created.

ADD PHYSICS

1 On the **Home** toolbar, click **Add Physics**.

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

3 In the **Add physics** tree, select **Structural Mechanics>Solid Mechanics (solid)**.

4 In the **Add physics** window, click **Add to Component**.

5 On the **Home** toolbar, click **Add Physics**.

SOLID MECHANICS 2 (SOLID2)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Solid Mechanics 2 (solid2)**.

2 In the **Solid Mechanics** settings window, locate the **2D Approximation** section.

3 From the **2D approximation** list, choose **Plane stress**.

4 Locate the **Thickness** section. In the d edit field, type `thickness`.

Thermal Expansion 1

1 In the **Model Builder** window, under **Component 2 (comp2)>Solid Mechanics 2 (solid2)** right-click **Linear Elastic Material 1** and choose **Thermal Expansion**.

2 In the **Thermal Expansion** settings window, locate the **Model Inputs** section.

3 In the T edit field, type `T0`.

4 Locate the **Thermal Expansion Properties** section. In the T_{ref} edit field, type `T1`.

Fixed Constraint 1

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

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `28,30,42,44` in the **Selection** edit field.

5 Click **OK**.

MATERIALS

Material 2 (mat2)

1 In the **Model Builder** window, under **Component 2 (comp2)** right-click **Materials** and choose **New Material**.

2 In the **Material** settings window, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Young's modulus	E	E1	Pa	Basic
Poisson's ratio	nu	nu1	1	Basic
Density	rho	rho1	kg/m³	Basic
Coefficient of thermal expansion	alpha	daT	1/K	Basic

MESH 2

Mapped 1

In the **Model Builder** window, under **Component 2 (comp2)** right-click **Mesh 2** and choose **Mapped**.

Distribution 1

1 In the **Model Builder** window, under **Component 2 (comp2)>Mesh 2** right-click **Mapped 1** and choose **Distribution**.

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `4,8,10,11,28,30,38,42,44,45,60,62` in the **Selection** edit field.

5 Click **OK**.

6 In the **Distribution** settings window, locate the **Distribution** section.

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

Size

1 In the **Model Builder** window, under **Component 2 (comp2)>Mesh 2** click **Size**.

2 In the **Size** settings window, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extra fine**.

4 Click the **Build All** button.

In order to perform the required computations four studies are required. The first two studies, one for each of the components, are for the case of zero-stress. These studies require one **Eigenfrequency** solver step, which will be used to calculate the eigenfrequency and mode of each resonator.

STUDY 1

1 In the **Model Builder** window, right-click **Study 1** and choose **Rename**.

2 In the **Rename Study** dialog box, type `Study 1 - Straight Cantilever, No Stress` in the **New name** edit field.

3 Click **OK**.

STUDY 1 - STRAIGHT CANTILEVER, NO STRESS

Step 1: Eigenfrequency

1 In the **Eigenfrequency** settings window, locate the **Physics and Variables Selection** section.

2 In the table, enter the following settings:

Physics	Solve for	Discretization
Solid Mechanics 2 (solid2)	×	physics

ADD STUDY

1 On the **Home** toolbar, click **Add Study**.

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

3 Find the **Studies** subsection. In the **Select study** tree, select **Preset Studies>Eigenfrequency**.

4 In the **Add study** window, click **Add Study**.

5 On the **Home** toolbar, click **Add Study**.

STUDY 2

Step 1: Eigenfrequency

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

2 In the **Eigenfrequency** settings window, locate the **Physics and Variables Selection** section.

3 In the table, enter the following settings:

Physics	Solve for	Discretization
Solid Mechanics (solid)	×	physics

4 In the **Model Builder** window, right-click **Study 2** and choose **Rename**.

5 In the **Rename Study** dialog box, type `Study 2 - Folded Cantilever, No Stress` in the **New name** edit field.

6 Click **OK**.

The second two studies require two study steps: an initial **Stationary** study step is used to calculate the residual thermal stress due to the difference between the fabrication and operation temperatures; the solution to this step is then used to shift the linerization point around which the eigenfrequenies are computed in a subsequent **Eigenfrequency** study step. **Prestressed Analysis, Eigenfrequency** studies are used as this study type contains the required study steps by default.

ADD STUDY

1 On the **Home** toolbar, click **Add Study**.

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

3 Find the **Studies** subsection. In the **Select study** tree, select **Preset Studies>Prestressed Analysis, Eigenfrequency**.

4 In the **Add study** window, click **Add Study**.

5 On the **Home** toolbar, click **Add Study**.

STUDY 3

Step 1: Stationary

1 In the **Model Builder** window, under **Study 3** click **Step 1: Stationary**.

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

3 In the table, enter the following settings:

Physics	Solve for	Discretization
Solid Mechanics 2 (solid2)	×	physics

Step 2: Eigenfrequency

1 In the **Model Builder** window, under **Study 3** click **Step 2: Eigenfrequency**.

2 In the **Eigenfrequency** settings window, locate the **Physics and Variables Selection** section.

3 In the table, enter the following settings:

Physics	Solve for	Discretization
Solid Mechanics 2 (solid2)	×	physics

4 In the **Model Builder** window, right-click **Study 3** and choose **Rename**.

5 In the **Rename Study** dialog box, type `Study 3 - Straight Cantilever, Residual Stress` in the **New name** edit field.

6 Click **OK**.

ADD STUDY

1 On the **Home** toolbar, click **Add Study**.

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

3 Find the **Studies** subsection. In the **Select study** tree, select **Preset Studies>Prestressed Analysis, Eigenfrequency**.

4 In the **Add study** window, click **Add Study**.

5 On the **Home** toolbar, click **Add Study**.

STUDY 4

Step 1: Stationary

1 In the **Model Builder** window, under **Study 4** click **Step 1: Stationary**.

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

3 In the table, enter the following settings:

Physics	Solve for	Discretization
Solid Mechanics (solid)	×	physics

Step 2: Eigenfrequency

1 In the **Model Builder** window, under **Study 4** click **Step 2: Eigenfrequency**.

2 In the **Eigenfrequency** settings window, locate the **Physics and Variables Selection** section.

3 In the table, enter the following settings:

Physics	Solve for	Discretization
Solid Mechanics (solid)	×	physics

4 In the **Model Builder** window, right-click **Study 4** and choose **Rename**.

5 In the **Rename Study** dialog box, type `Study 4 - Folded Cantilever, Residual Stress` in the **New name** edit field.

6 Click **OK**.

The studies can now be solved and the results visualized.

STUDY 1 - STRAIGHT CANTILEVER, NO STRESS

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

RESULTS

Mode Shape (solid)

1 In the **Model Builder** window, under **Results** right-click **Mode Shape (solid)** and choose **Rename**.

2 In the **Rename 2D Plot Group** dialog box, type `Straight Cantilever, No Stress` in the **New name** edit field.

3 Click **OK**.

STUDY 2 - FOLDED CANTILEVER, NO STRESS

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

RESULTS

Mode Shape (solid2)

1 In the **Model Builder** window, under **Results** right-click **Mode Shape (solid2)** and choose **Rename**.

2 In the **Rename 2D Plot Group** dialog box, type `Folded Cantilever, No Stress` in the **New name** edit field.

3 Click **OK**.

STUDY 3 - STRAIGHT CANTILEVER, RESIDUAL STRESS

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

RESULTS

Mode Shape (solid)

1 In the **Model Builder** window, under **Results** right-click **Mode Shape (solid)** and choose **Rename**.

2 In the **Rename 2D Plot Group** dialog box, type `Straight Cantilever, Residual Stress` in the **New name** edit field.

3 Click **OK**.

STUDY 4 - FOLDED CANTILEVER, RESIDUAL STRESS

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

RESULTS

Mode Shape (solid2)

1 In the **Model Builder** window, under **Results** right-click **Mode Shape (solid2)** and choose **Rename**.

2 In the **Rename 2D Plot Group** dialog box, type `Folded Cantilever, Residual Stress` in the **New name** edit field.

3 Click **OK**.

2D Plot Group 5

1 On the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Model Builder** window, under **Results** right-click **2D Plot Group 5** and choose **Rename**.

3 In the **Rename 2D Plot Group** dialog box, type `Residual Stress in Straight Cantilever` in the **New name** edit field.

4 Click **OK**.

5 In the **2D Plot Group** settings window, locate the **Data** section.

6 From the **Data set** list, choose **Solution 7**.

Residual Stress in Straight Cantilever

1 Right-click **Results>Residual Stress in Straight Cantilever** and choose **Surface**.

2 In the **Surface** settings window, locate the **Expression** section.

3 In the **Expression** edit field, type `solid.mises`.

4 On the **2D plot group** toolbar, click **Plot**.

2D Plot Group 6

1 On the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Model Builder** window, under **Results** right-click **2D Plot Group 6** and choose **Rename**.

3 In the **Rename 2D Plot Group** dialog box, type `Residual Stress in Folded Cantilever` in the **New name** edit field.

4 Click **OK**.

5 In the **2D Plot Group** settings window, locate the **Data** section.

6 From the **Data set** list, choose **Solution 12**.

Residual Stress in Folded Cantilever

1 Right-click **Results>Residual Stress in Folded Cantilever** and choose **Surface**.

2 In the **Surface** settings window, locate the **Expression** section.

3 In the **Expression** edit field, type `solid2.mises`.

4 On the **2D plot group** toolbar, click **Plot**.