Residual Stress in a Thin-Film Resonator—3D 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.

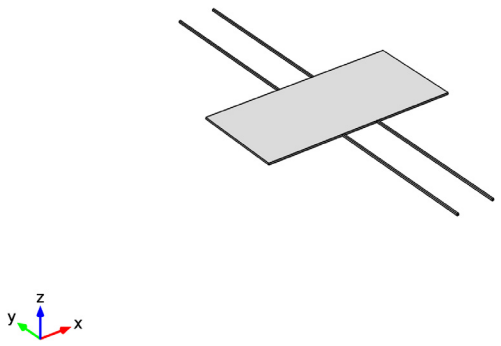

Figure 1: A thin-film resonator with four straight cantilever beam springs.

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 from these 3D

models can be compared with analytical solutions by referring to the Model Library tutorial Residual Stress in a Thin-Film Resonator—2D Model.

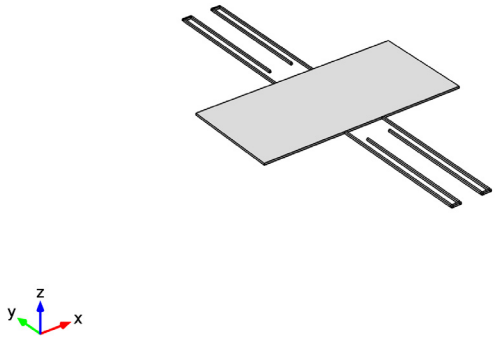

Figure 2: A thin-film resonator with four folded cantilever beam springs.

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. 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.

Results and Discussion

Table 3 summarizes the resonant frequencies for the first in-plane bending eigenmode. The solutions from the 3D models are compared with those obtained from a 2D plane-stress model available in the Model Library tutorial Residual Stress in a Thin-Film Resonator—2D Model. As the table shows, the resonant frequency for the straight cantilevers increases significantly when the model includes residual stress. As expected, the stress sensitivity of the resonant frequency is reduced by folding the cantilevers. The results from the 3D models agree closely with those obtained from the 2D models. This indicates that such thin-film resonators can be efficiently modeled using a 2D plane-stress approach.

TABLE 3: RESONANT FREQUENCIES WITH AND WITHOUT RESIDUAL STRESS.

	STRAIGHT CANTILEVERS		FOLDED CANTILEVERS	
	2D MODEL	3D MODEL	2D MODEL	3D MODEL
Without stress	14.82 kHz	14.91 kHz	14.11 kHz	14.18 kHz
With residual stress	32.05 kHz	32.25 kHz	14.22 kHz	14.29 kHz

Note that for the 2D models, the first (lowest) eigenmode is the in-plane bending mode. However for the 3D models, the first (lowest) eigenmode is an out-of-plane torsional mode that you see in the default plot when you solve the eigenfrequency study. The desired in-plane bending mode is the second eigenmode in the list of

computed solutions. Hence, the main advantage of the 3D model is in finding any eigenmode where the resonator deforms largely in the out-of-plane direction.

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

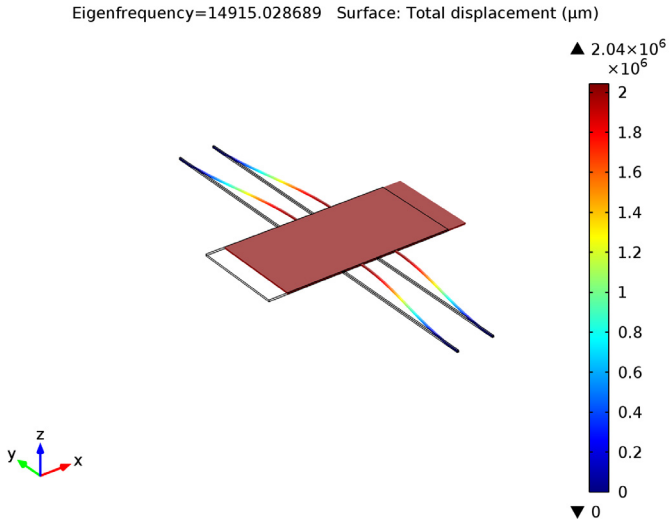

Figure 3: The first in-plane bending eigenmode of the unstressed resonator with straight cantilevers.

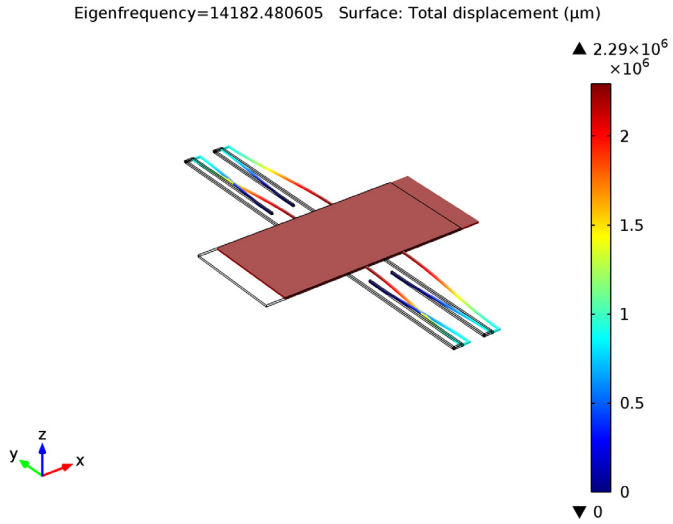

Figure 4: The first in-plane bending eigenmode of the unstressed resonator with folded cantilevers.

Figure 5 and Figure 7 show the first in-plane bending resonance mode for the resonator with straight and folded cantilevers respectively when they have a residual thermal stress.

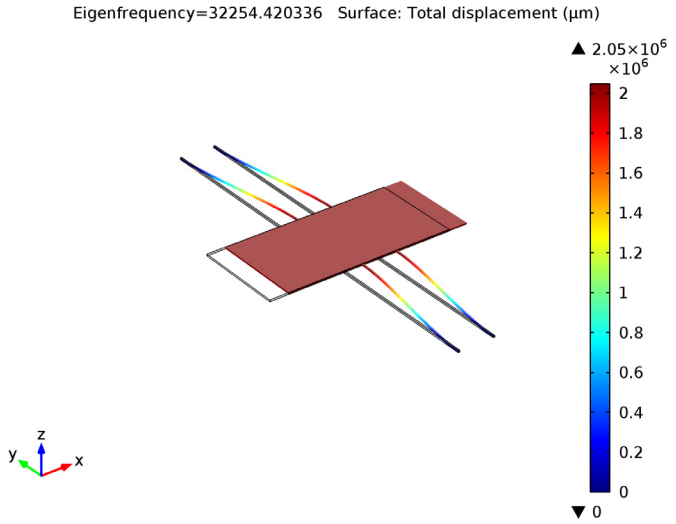

Figure 5: The first in-plane bending eigenmode of the resonator with straight cantilevers having residual thermal stress.

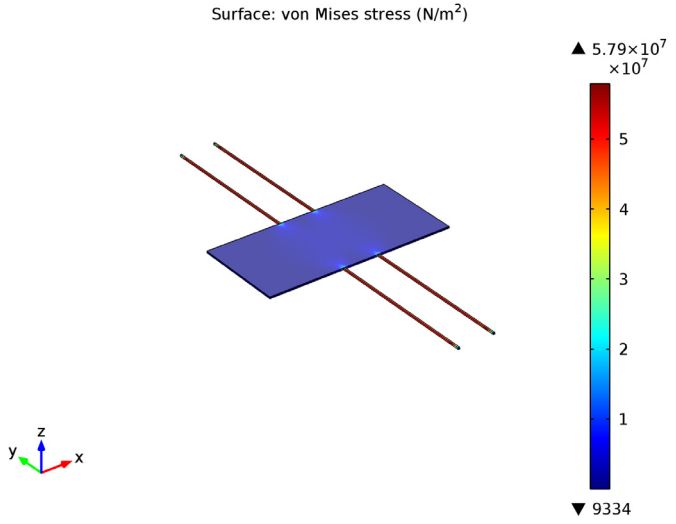

Figure 6: Residual thermal stress in the resonator with straight cantilevers when it is cooled from 605 °*C to* 25 °*C.*

Figure 6 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 6 shows that the residual stress is almost uniform in the straight cantilever and is about 49 MPa. 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 44 MPa.

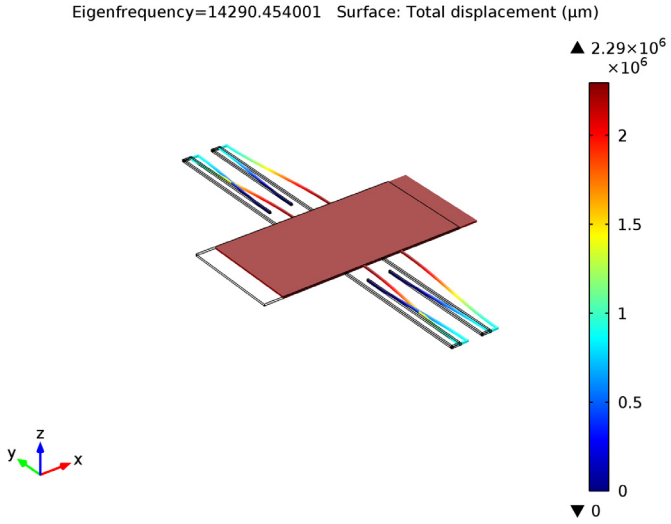

Figure 7: The first in-plane bending eigenmode of the resonator with folded cantilevers having residual thermal stress.

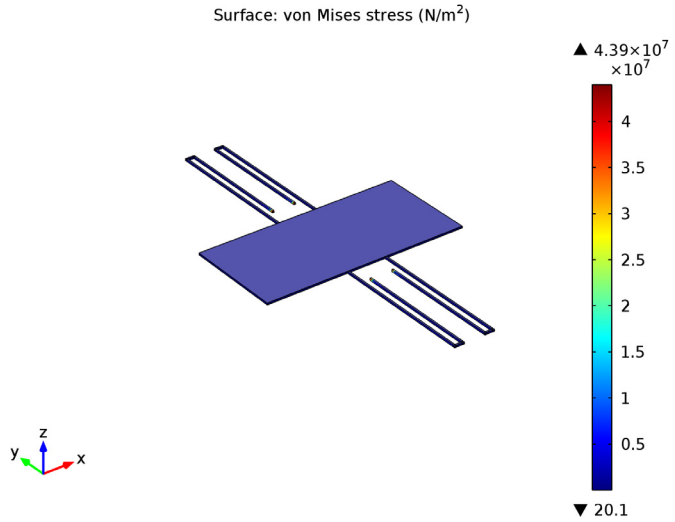

Figure 8: Residual thermal stress in the resonator with folded cantilevers when it is cooled from 605 °C *to* 25 °C.

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_3d`

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 **3D** 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 Browse to the model's Model Library folder and double-click the file `residual_stress_resonator_3d_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_3d_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)

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 `7,15,21,29` in the **Selection** edit field.

5 Click **OK**.

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

MATERIALS

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 and swept mesh is appropriate for this device geometry.

Mapped 1

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

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `4,9,14,23,28` in the **Selection** edit field.

5 Click **OK**.

Distribution 1

1 Right-click **Component 1 (comp1)>Mesh 1>Mapped 1** and choose **Distribution**.

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `16,21,44,49` 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**.

Swept 1

In the **Model Builder** window, right-click **Mesh 1** and choose **Swept**.

Distribution 1

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

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

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

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 inserted for convenience.

ROOT

On the **Home** toolbar, click **Add Component** and choose **3D**.

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_3d_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)

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 `46,48,68,70` 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

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

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `4,9,13,18,22,27,36,41,45,50,54,63,67,72,76,81,88,93,97,102,106` in the **Selection** edit field.

5 Click **OK**.

Distribution 1

1 Right-click **Component 2 (comp2)>Mesh 2>Mapped 1** and choose **Distribution**.

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `12,21,26,30,73,78,104,113,118,122,161,166` 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.

Swept 1

In the **Model Builder** window, right-click **Mesh 2** and choose **Swept**.

Distribution 1

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

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

3 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 **Model Builder** window, expand the **Study 1 - Straight Cantilever, No Stress** node, then 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 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, right-click **Study 2** and choose **Rename**.

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

3 Click **OK**.

STUDY 2 - FOLDED 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 (solid)	×	physics

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 linearization point around which the eigenfrequencies 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, right-click **Study 3** and choose **Rename**.

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

3 Click **OK**.

STUDY 3 - STRAIGHT CANTILEVER, RESIDUAL STRESS

Step 1: Stationary

1 In the **Stationary** 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

Step 2: Eigenfrequency

1 In the **Model Builder** window, under **Study 3 - Straight Cantilever, Residual Stress** 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

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, right-click **Study 4** and choose **Rename**.

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

3 Click **OK**.

STUDY 4 - FOLDED CANTILEVER, RESIDUAL STRESS

Step 1: Stationary

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

2 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 - Folded Cantilever, Residual Stress** 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

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 3D Plot Group** dialog box, type `Straight Cantilever, No Stress` in the **New name** edit field.

3 Click **OK**.

4 In the **3D Plot Group** settings window, locate the **Data** section.

5 From the **Eigenfrequency** list, choose **14915.028904**.

6 On the **3D plot group** toolbar, click **Plot**.

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 3D Plot Group** dialog box, type `Folded Cantilever, No Stress` in the **New name** edit field.

3 Click **OK**.

4 In the **3D Plot Group** settings window, locate the **Data** section.

5 From the **Eigenfrequency** list, choose **14182.479798**.

6 On the **3D plot group** toolbar, click **Plot**.

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

3 Click **OK**.

4 In the **3D Plot Group** settings window, locate the **Data** section.

5 From the **Eigenfrequency** list, choose **32254.424256**.

6 On the **3D plot group** toolbar, click **Plot**.

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

3 Click **OK**.

4 In the **3D Plot Group** settings window, locate the **Data** section.

5 From the **Eigenfrequency** list, choose **14290.453766**.

6 On the **3D plot group** toolbar, click **Plot**.

3D Plot Group 5

1 On the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Model Builder** window, under **Results** right-click **3D Plot Group 5** and choose **Rename**.

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

4 Click **OK**.

5 In the **3D 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 **3D plot group** toolbar, click **Plot**.

3D Plot Group 6

1 On the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Model Builder** window, under **Results** right-click **3D Plot Group 6** and choose **Rename**.

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

4 Click **OK**.

5 In the **3D 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 **3D plot group** toolbar, click **Plot**.