Model created in COMSOL Multiphysics 6.4

# Micromechanical Model of a Triply-Periodic-Minimal-Surface-Based Composite

## *Introduction*

The use of composites in various industries like automotive, aerospace, infrastructure, and many others has been rising over last few decades. Ever-increasing advancement of the technology demands advancements in the materials. Triply-periodic-minimal-surface-based (TPMS-based) composites are finding increasing use in various applications due to their outstanding mechanical and thermal properties; see Ref. 1. The accuracy of structural and thermal analyses relies on an accurate estimation of the mechanical and thermal properties of the composite material. At global scale, the composite needs to be treated as a homogeneous material in the continuum mechanics, which needs homogenization techniques to get the effective properties for such materials based on the material properties of the constituents.

In this example, the homogenized elastic and thermal properties of a composite material based on a TPMS are computed and the results are compared to those presented in Ref. 1. A gyroid TPMS-based unit cell is subjected to periodic boundary conditions to get the homogenized material properties. The effects of a negative Poisson's ratio and different volume fractions on the homogenized properties are analyzed.

## *Model Definition*

A unit cell of a gyroid TPMS is shown in Figure 1. The size of unit cell is 100 mm. The TPMS volume fraction is computed from the wall thickness of the TPMS.

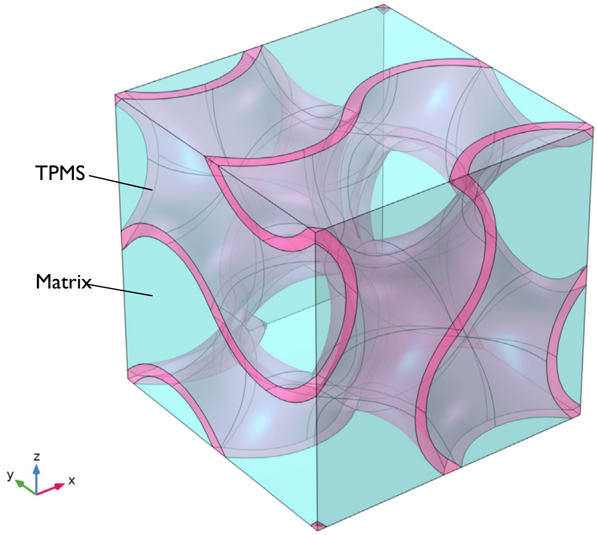


*Figure 1: Geometry of the gyroid unit cell.*

*TPMS and Matrix Properties*

The material properties are taken from Ref. 1. The elastic moduli of TPMS and matrix are not explicitly given in Ref. 1; rather a ratio of 20 is given. This example assumes the elastic moduli 200 GPa and 10 GPa of the TPMS and matrix, respectively. The Poisson's ratio of the TPMS and matrix in Ref. 1 are taken from a set of [0.3, –0.3, –0.5, –0.75]. For this example, we vary the Poisson's ratio of the TPMS from the above set but keep the Poisson's ratio of the matrix fixed to 0.3. The coefficient of thermal expansion for the TMPS and matrix are given as $0.8 \times 10^{-6}$ 1/K and $44 \times 10^{-6}$ 1/K, respectively.

## Results and Discussion

Figure 2, Figure 3, and Figure 4 show the variation of the effective Young's modulus, Poisson's ratio, and shear modulus with different Poisson's ratio and volume fractions of the TPMS. The variation of the effective coefficient of thermal expansion is shown in Figure 5. The result matches closely with results presented in Ref. 1 (see figure 5).

The authors in Ref. 1 investigated the effect of a negative Poisson's ratio of the TPMS on the effective properties of the composite. As reported in Ref. 1, with negative Poisson's ratio of the TPMS, the effective Young's modulus, shear modulus, and coefficient of thermal expansion increase, while the effective Poisson's ratio decreases. An increasing fiber volume fraction of the TPMS increases the effective Young's modulus and shear modulus. The coefficient of thermal expansion and effective Poisson's ratio decrease with increases in the TPMS fiber volume fraction.

The study indicates that the properties of the gyroid-based composite can be customized by changing the Poisson's ratio or fiber volume fraction of the TPMS.

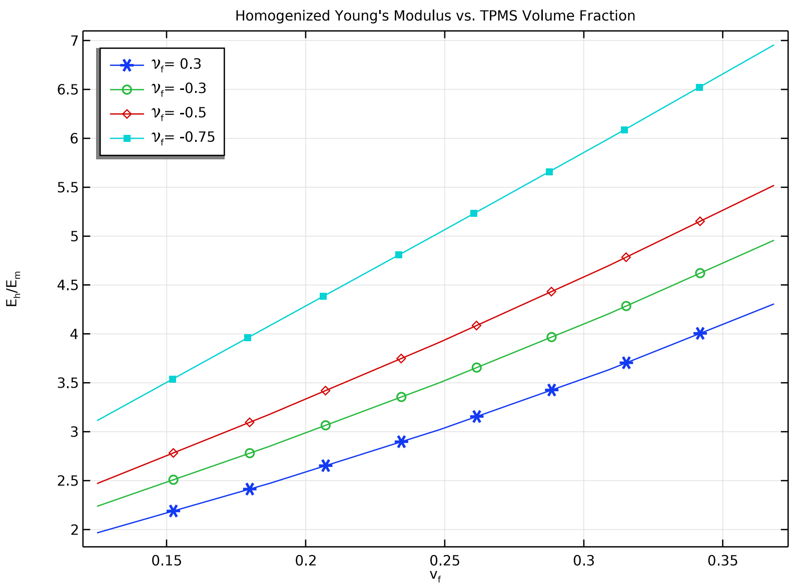


*Figure 2: Effective Young's modulus versus TPMS volume fraction.*

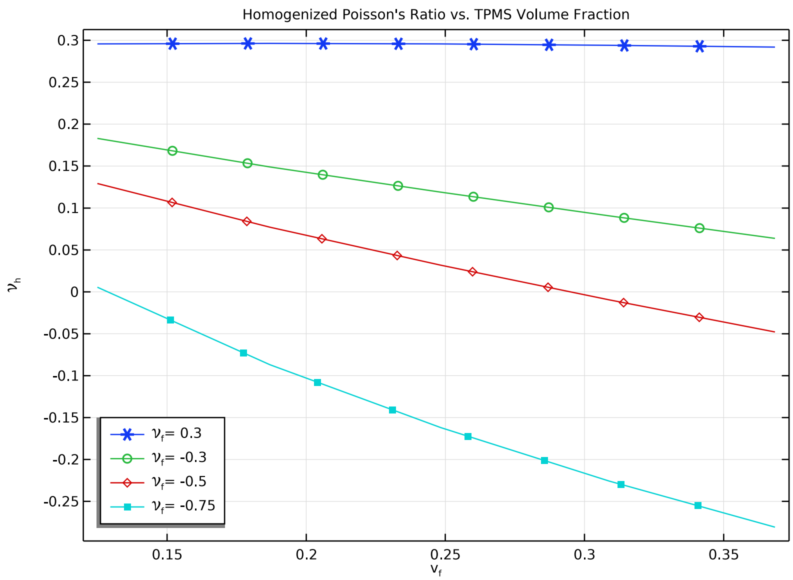


*Figure 3: Effective Poisson's ratio versus TPMS volume fraction.*

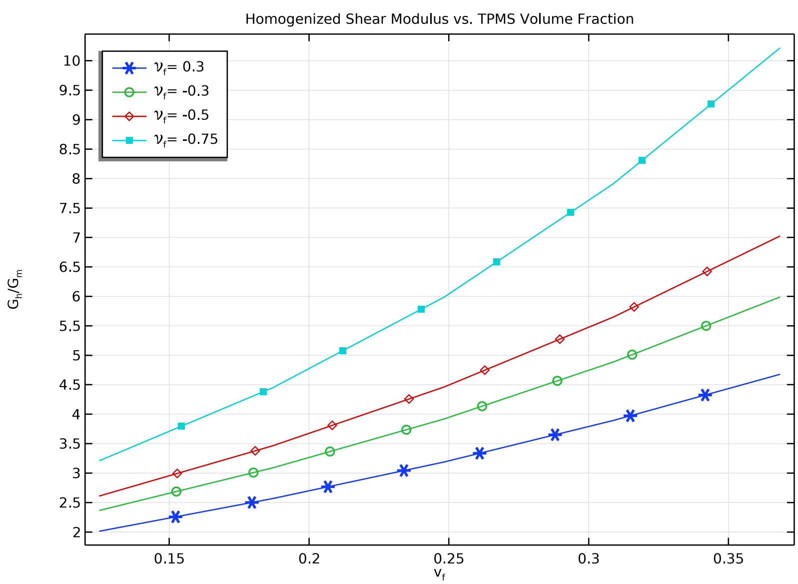


*Figure 4: Effective shear modulus versus TPMS volume fraction.*

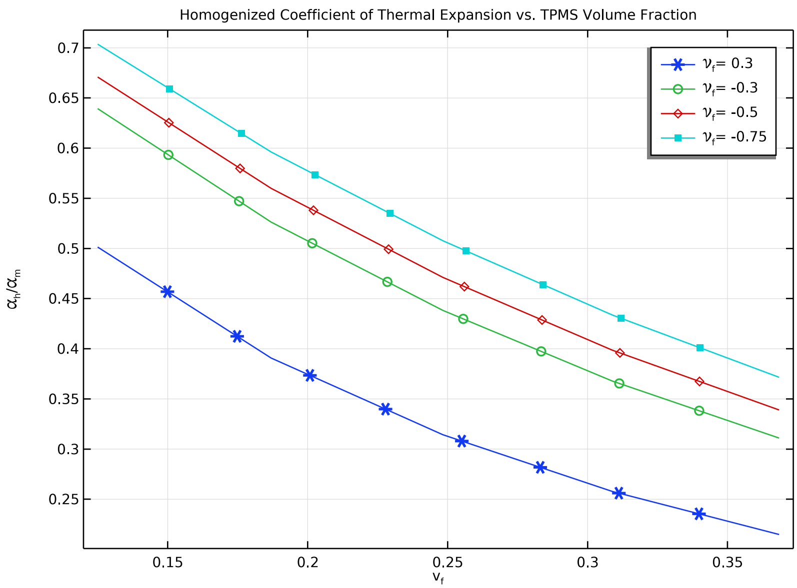


*Figure 5: Effective coefficient of thermal expansion versus TPMS volume fraction.*

## *Notes About the COMSOL Implementation*

- In order to perform a micromechanical analysis, the **Cell Periodicity** node in the **Solid Mechanics** interface is used. The **Cell Periodicity** node is used to apply periodic boundary conditions to the three (two) pairs of faces of the unit cell in 3D (2D).
- The **Cell Periodicity** node has three action buttons in the toolbar of the **Periodicity Type** section: **Create Load Groups and Study**, **Create Material by Value**, and **Create Material by Reference**. The action button **Create Load Groups and Study** generates load groups and a stationary study with load cases. The action button **Create Material by Value** generates a **Global Material** with homogenized material properties, with material properties as numbers. The action button **Create Material by Reference** generates a **Global Material** with homogenized material properties, with material properties as variables. The action buttons are active depending on the choices in the **Periodicity Type** and **Calculate Average Properties** lists.
- The **Create Load Groups and Study** button does not generate a parametric study by default. In many situations, a parametric study is needed and the homogenized elasticity

matrix **D** needs to be based on the tag of the parametric solution. To do this, use the given options in the **Advanced** section of the feature.

- Use the **Free Expansion** option with **Coefficient of thermal expansion** to extract the homogenized coefficient of thermal expansions.

## *Reference*


1. K. Chawla and R. Kiran, "Numerical predictions for the effect of negative Poisson's ratio on thermoelastic properties of triply periodic minimal surface-based composites," *Results Mater.*, vol. 14, p. 100273, 2022.


**Application Library path:** `Structural_Mechanics_Module/Material_Models/micromechanical_model_of_a_tpms_composite`

## *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 **3D**.

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

3 Click **Add**.

4 Click **Done**.

### 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 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `micromechanical_model_of_a_tpms_composite_parameters.txt`.

### GEOMETRY 1

Next, create a unit cell for a gyroid (TPMS) based composite. This unit cell like many others can be found in the built-in **Part Libraries**.

### PART LIBRARIES

1 In the **Geometry** toolbar, click **Part Libraries**.

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

3 In the **Part Libraries** window, select **Design Module** > **Unit Cells and RVEs** > **gyroid** in the tree.

*Gyroid 1 (pi1)*

1 Right-click **Component 1 (comp1)** > **Geometry 1** and choose **Add to Geometry**.

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

3 In the table, enter the following settings:

| Name | Expression | Value | Description |
|---|---|---|---|
| lm | L | lm | Cell length |
| th | th | th | Wall thickness |

Use **Remove Details** to automatically fix small issues in the geometry. This will improve meshing and computation.

*Remove Details 1 (rmd1)*

1 In the **Geometry** toolbar, click **Virtual Operations** and choose **Remove Details**.

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

3 In the **Continuous tangent tolerance** text field, type 10.

4 Click **Build Selected**.

*Form Union (fin)*

In the **Geometry** toolbar, click **Build All**.

### DEFINITIONS

*Integration 1 (intop1)*

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, locate the **Source Selection** section.

3 From the **Selection** list, choose **Gyroid domain (Gyroid 1)**.

*Variables 1*

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

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

3 In the table, enter the following settings:

| Name | Expression | Unit | Description |
|---|---|---|---|
| `v_f` | `intop1(1)/L^3` | | `Volume fraction of tpms` |
| `E_h` | `1/solid.cp1.Dinv11` | | `Homogenized Young's modulus` |
| `nu_h` | `-E_h*solid.cp1.Dinv12` | | `Homogenized Poisson's ratio` |
| `G_h` | `1/solid.cp1.Dinv55` | | `Homogenized shear modulus` |
| `alpha_h` | `solid.cp2.alphaXX` | | `Homogenized coefficient of thermal expansion` |

## SOLID MECHANICS (SOLID)

*Linear Elastic Material 1*

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

*Thermal Expansion 1*

1 In the **Physics** toolbar, click **Attributes** and choose **Thermal Expansion**.

2 In the **Settings** window for **Thermal Expansion**, locate the **Model Input** section.

3 From the $T$ list, choose **User defined**. In the associated text field, type `294.15[K]`.

*Cell Periodicity for Elastic Properties*

1 In the **Physics** toolbar, click **Domains** and choose **Cell Periodicity**.

2 In the **Settings** window for **Cell Periodicity**, type `Cell Periodicity for Elastic Properties` in the **Label** text field.

3 Locate the **Periodicity Settings** section. From the **Boundary conditions** list, choose **Average strain**.

4 Locate the **Effective Properties** section. Select the **Compute elasticity matrix, standard notation** checkbox.

*Boundary Pair 1*

1 In the **Physics** toolbar, click **Attributes** and choose **Boundary Pair**.

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

**3** From the **Selection** list, choose **Pair 1 (Gyroid 1)**.

**4** Right-click **Boundary Pair 1** and choose **Manual Destination Selection**.

**5** Locate the **Destination Selection** section. From the **Selection** list, choose **Pair 1, Destination (Gyroid 1)**.

*Boundary Pair 2*

**1** Right-click **Boundary Pair 1** and choose **Duplicate**.

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

**3** From the **Selection** list, choose **Pair 2 (Gyroid 1)**.

**4** Locate the **Destination Selection** section. From the **Selection** list, choose **Pair 2, Destination (Gyroid 1)**.

*Boundary Pair 3*

**1** Right-click **Boundary Pair 2** and choose **Duplicate**.

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

**3** From the **Selection** list, choose **Pair 3 (Gyroid 1)**.

**4** Locate the **Destination Selection** section. From the **Selection** list, choose **Pair 3, Destination (Gyroid 1)**.

With the **Average strain** option in the **Cell Periodicity** feature, appropriate load groups, a study and a material with computed elastic properties can be generated automatically. To create load groups and a study node, click the **Create Load Groups and Study** button in the section toolbar.

*Cell Periodicity for Elastic Properties*

To create a parametric study, use the options in the **Advanced** section of the feature. To see the section, activate the **Advanced Physics** option from **Show** button.

**1** Click the **Show More Options** button in the **Model Builder** toolbar.

**2** In the **Show More Options** dialog, in the tree, select the checkbox for the node **Physics** > **Advanced Physics Options**.

**3** Click **OK**.

**4** In the **Model Builder** window, click **Cell Periodicity for Elastic Properties**.

**5** In the **Settings** window for **Cell Periodicity**, click to expand the **Advanced** section.

**6** From the **Add parametric sweep** list, choose **Yes**.

**7** From the **Sweep type** list, choose **All combinations**.

**8** Click **Add**.

9 In the **Parameters** table, enter the following settings:

| Index | Parameter name | Parameter value list | Parameter unit |
|---|---|---|---|
| 1 | th | range(4,2,12) | mm |
| 2 | nu_f | 0.3 -0.3 -0.5 -0.75 | 1 |

10 Locate the **Periodicity Settings** section. Click **Create Load Groups and Study** in the upper-right corner of the section.

*Cell Periodicity for Thermal Properties*

1 Right-click **Cell Periodicity for Elastic Properties** and choose **Duplicate**.

2 In the **Settings** window for **Cell Periodicity**, type `Cell Periodicity for Thermal Properties` in the **Label** text field.

3 Locate the **Periodicity Settings** section. From the **Boundary conditions** list, choose **Free expansion**.

4 Locate the **Effective Properties** section. Select the **Compute coefficient of thermal expansion** checkbox.

## MATERIALS

*Material 1: Matrix*

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

2 In the **Settings** window for **Material**, type `Material 1: Matrix` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Selection** list, choose **Matrix (Gyroid 1)**.

4 Locate the **Material Contents** section. In the table, enter the following settings:

| Property | Variable | Value | Unit | Property group |
|---|---|---|---|---|
| Young's modulus | E | E_m | Pa | Young's modulus and Poisson's ratio |
| Poisson's ratio | nu | nu_m | 1 | Young's modulus and Poisson's ratio |

| Property | Variable | Value | Unit | Property group |
|---|---|---|---|---|
| Density | rho | `rho_m` | kg/m³ | Basic |
| Coefficient of thermal expansion | alpha_iso ; alphaii = alpha_iso, alphaij = 0 | `alpha_m` | 1/K | Basic |

*Material 2: TPMS*

1 Right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for **Material**, type `Material 2: TPMS` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Selection** list, choose **Gyroid domain (Gyroid 1)**.

4 Locate the **Material Contents** section. In the table, enter the following settings:

| Property | Variable | Value | Unit | Property group |
|---|---|---|---|---|
| Young's modulus | E | `E_f` | Pa | Young's modulus and Poisson's ratio |
| Poisson's ratio | nu | `nu_f` | 1 | Young's modulus and Poisson's ratio |
| Density | rho | `rho_f` | kg/m³ | Basic |
| Coefficient of thermal expansion | alpha_iso ; alphaii = alpha_iso, alphaij = 0 | `alpha_f` | 1/K | Basic |

## MESH 1

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

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

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

4 In the table, clear the **Use** checkbox for **Geometric Analysis, Detail Size**.

5 Click **Build All**.

For this study, disable the thermal expansion node and the cell periodicity feature for thermal expansion.

### CELL PERIODICITY STUDY FOR ELASTIC PROPERTIES

1 In the **Model Builder** window, click **Cell Periodicity Study**.

2 In the **Settings** window for **Study**, type `Cell Periodicity Study for Elastic Properties` in the **Label** text field.

#### *Step 1: Stationary*

1 In the **Model Builder** window, expand the **Cell Periodicity Study for Elastic Properties** node, then click **Step 1: Stationary**.

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

3 Select the **Modify model configuration for study step** checkbox.

4 In the tree, select **Component 1 (comp1)** > **Solid Mechanics (solid)** > **Linear Elastic Material 1** > **Thermal Expansion 1**.

5 Right-click and choose **Disable**.

6 In the tree, select **Component 1 (comp1)** > **Solid Mechanics (solid)** > **Cell Periodicity for Thermal Properties**.

7 Right-click and choose **Disable**.

#### *Solution (solidcp1sol)*

1 In the **Model Builder** window, right-click **Solver Configurations** and choose **Show Default Solver**.

The iterative solver is lean on memory usage. Enable the default iterative solver.

2 In the **Model Builder** window, expand the **Solution (solidcp1sol)** node.

3 In the **Model Builder** window, expand the **Cell Periodicity Study for Elastic Properties** > **Solver Configurations** > **Solution (solidcp1sol)** > **Stationary Solver 1** node.

4 Right-click **Suggested Iterative Solver (solid)** and choose **Enable**.

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

Add a separate study to compute the homogeneous thermal properties. For this study, disable the cell periodicity feature for elastic properties.

### 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** > **Stationary**.

4 Right-click and choose **Add Study**.

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

### CELL PERIODICITY STUDY FOR THERMAL PROPERTIES

In the **Settings** window for **Study**, type `Cell Periodicity Study for Thermal Properties` in the **Label** text field.

*Parametric Sweep*

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

This study computes the homogenized thermal properties for varying volume fraction and Poisson's ratio. Therefore, use a parametric sweep for the parameter `th` along with `nu_f`.

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

3 From the **Sweep type** list, choose **All combinations**.

4 Click **Add**.

5 In the table, enter the following settings:

| Parameter name | Parameter value list | Parameter unit |
|---|---|---|
| th (Wall thickness) | `range(4,2,12)` | `mm` |

6 Click **Add**.

7 In the table, enter the following settings:

| Parameter name | Parameter value list | Parameter unit |
|---|---|---|
| nu_f (Poisson's ratio, TPMS) | `0.3 -0.3 -0.5 -0.75` | 1 |

*Step 1: Stationary*

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

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

3 Select the **Modify model configuration for study step** checkbox.

4 In the tree, select **Component 1 (comp1)** > **Solid Mechanics (solid)** > **Cell Periodicity for Elastic Properties**.

5 Right-click and choose **Disable**.

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

## RESULTS

*Stress (solid)*

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

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Parameter value (th (mm))** list, choose **4**.

4 From the **Load case** list, choose **Load case 1**.

5 From the **Parameter value (nu_f)** list, choose **0.3**.

6 In the **Stress (solid)** toolbar, click **Plot**.

*Stress (solid) 1*

1 In the **Model Builder** window, click **Stress (solid) 1**.

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Parameter value (th (mm))** list, choose **4**.

4 From the **Parameter value (nu_f)** list, choose **0.3**.

5 In the **Stress (solid) 1** toolbar, click **Plot**.

*Homogenized Young's Modulus vs. TPMS Volume Fraction*

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

2 In the **Settings** window for **1D Plot Group**, type `Homogenized Young's Modulus vs. TPMS Volume Fraction` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cell Periodicity Study for Elastic Properties/Solution 2 (solidcp1solp)**.

4 From the **Parameter selection (Load case)** list, choose **First**.

5 Click to expand the **Title** section. From the **Title type** list, choose **Label**.

6 Locate the **Plot Settings** section.

7 Select the **x-axis label** checkbox. In the associated text field, type `v<sub>f</sub>`.

8 Select the **y-axis label** checkbox. In the associated text field, type `E<sub>h</sub>/E<sub>m</sub>`.

9 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

*Global 1*

1 Right-click **Homogenized Young's Modulus vs. TPMS Volume Fraction** 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 |
|---|---|---|
| E_h/E_m | 1 | |

4 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **th**.

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

6 In the **Expression** text field, type v_f.

7 Click to expand the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

8 From the **Positioning** list, choose **Interpolated**.

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

10 In the table, enter the following settings:

| Legends |
|---|
| \nu<sub>f</sub>= 0.3 |
| \nu<sub>f</sub>= -0.3 |
| \nu<sub>f</sub>= -0.5 |
| \nu<sub>f</sub>= -0.75 |

11 In the **Homogenized Young's Modulus vs. TPMS Volume Fraction** toolbar, click **Plot**.

*Homogenized Poisson's Ratio vs. TPMS Volume Fraction*

1 In the **Model Builder** window, right-click **Homogenized Young's Modulus vs. TPMS Volume Fraction** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type Homogenized Poisson's Ratio vs. TPMS Volume Fraction in the **Label** text field.

3 Locate the **Plot Settings** section. In the **y-axis label** text field, type \nu<sub>h</sub>.

4 Locate the **Legend** section. From the **Position** list, choose **Lower left**.

*Global 1*

1 In the **Model Builder** window, expand the **Homogenized Poisson's Ratio vs. TPMS Volume Fraction** node, then click **Global 1**.

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

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| nu_h | 1 | |

4 In the **Homogenized Poisson's Ratio vs. TPMS Volume Fraction** toolbar, click **Plot**.

*Homogenized Shear Modulus vs. TPMS Volume Fraction*

1 In the **Model Builder** window, right-click **Homogenized Young's Modulus vs. TPMS Volume Fraction** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type Homogenized Shear Modulus vs. TPMS Volume Fraction in the **Label** text field.

3 Locate the **Plot Settings** section. In the **y-axis label** text field, type G<sub>h</sub>/G<sub>m</sub>.

*Global 1*

1 In the **Model Builder** window, expand the **Homogenized Shear Modulus vs. TPMS Volume Fraction** node, then click **Global 1**.

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

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| G_h/G_m | 1 | |

4 In the **Homogenized Shear Modulus vs. TPMS Volume Fraction** toolbar, click **Plot**.

*Homogenized Coefficient of Thermal Expansion vs. TPMS Volume Fraction*

1 In the **Model Builder** window, right-click **Homogenized Young's Modulus vs. TPMS Volume Fraction** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type Homogenized Coefficient of Thermal Expansion vs. TPMS Volume Fraction in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **None**.

4 Locate the **Plot Settings** section. In the **y-axis label** text field, type \alpha<sub>h</sub>/\alpha<sub>m</sub>.

5 Locate the **Legend** section. From the **Position** list, choose **Upper right**.

*Global 1*

1 In the **Model Builder** window, expand the **Homogenized Coefficient of Thermal Expansion vs. TPMS Volume Fraction** node, then click **Global 1**.

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

**3** In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| alpha_h/alpha_m | | |

*Homogenized Coefficient of Thermal Expansion vs. TPMS Volume Fraction*

**1** In the **Model Builder** window, click **Homogenized Coefficient of Thermal Expansion vs. TPMS Volume Fraction**.

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

**3** From the **Dataset** list, choose **Cell Periodicity Study for Thermal Properties/ Parametric Solutions 1 (sol22)**.

*Global 1*

**1** In the **Model Builder** window, click **Global 1**.

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

**3** From the **Axis source data** list, choose **th**.

**4** In the **Homogenized Coefficient of Thermal Expansion vs. TPMS Volume Fraction** toolbar, click **Plot**.