Application Note

Defining Anisotropic Materials in TEM

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Version 8.5/PC

Part Number 30-090-101
March 2009

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I IntelliSuite v8.5 and Earlier

Anisotropic materials have different physical properties in different directions relative to the crystal orientation of the materials. For example, the Young's modulus of single crystalline silicon depends on the measurement direction relative to the crystal orientation. Therefore, when designing MEMS structures using anisotropic mechanical materials, the designer should be aware of the orientation relation between the mechanical structure and the material crystals, and specify the relation in the simulation settings.

In the ThermoElectroMechanical analysis module, the user can set a material to be either isotropic or orthotropic in the *Material* menu.

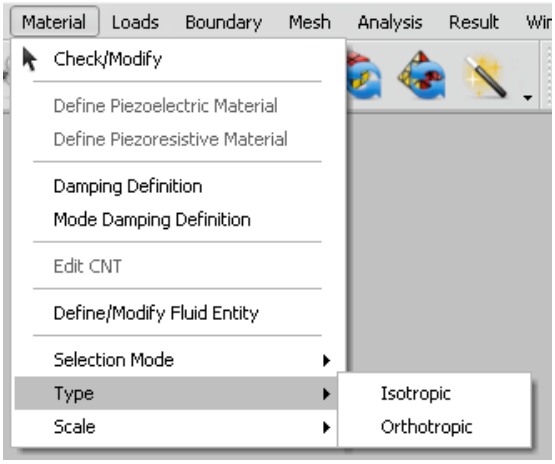


Figure 1: Material Menu

When the *Type* is set to *Orthotropic*, selecting *Material…Check/Modify* and clicking on an entity will bring up the following window.

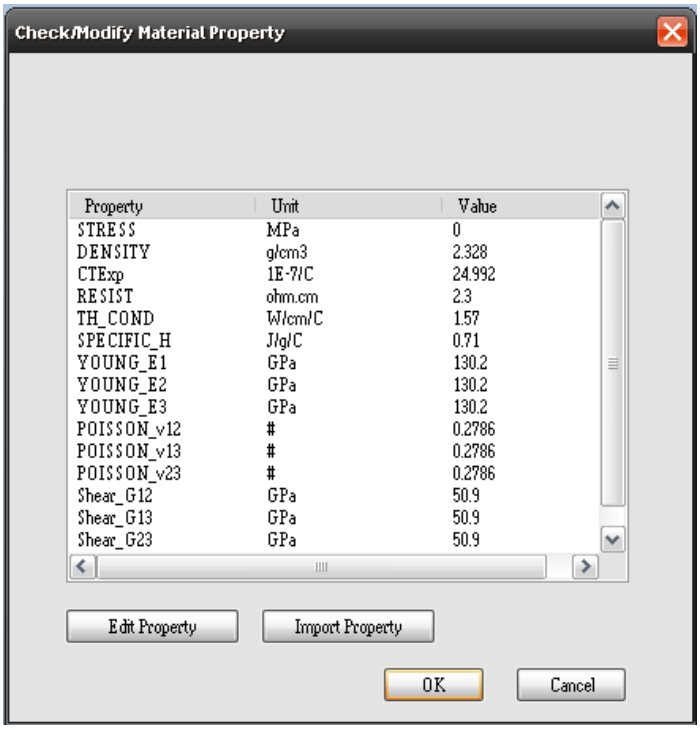


Figure 2: Material Property Settings

1.1 Elastic Parameter Calculator

To determine the values for the Young's modulus, shear modulus, and Poisson ratio, the Elastic Parameter Calculator can be used. Opening *ElasticParameterCalculator.exe* will open the calculator.

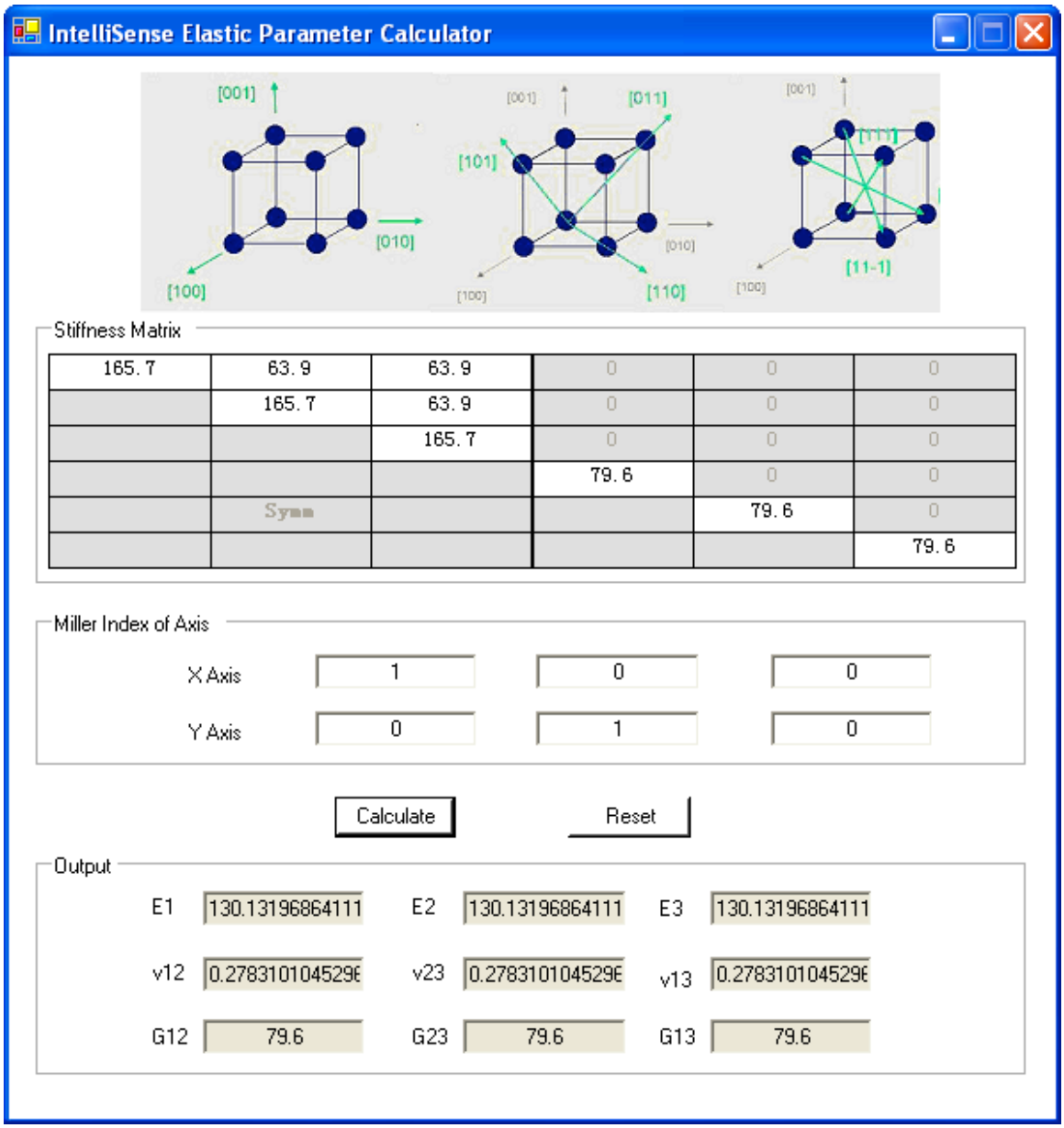


Figure 3: Elastic Parameter Calculator

The first step is to complete the stiffness matrix for the material. The default stiffness matrix for silicon is already loaded into the calculator and has units of GPa.

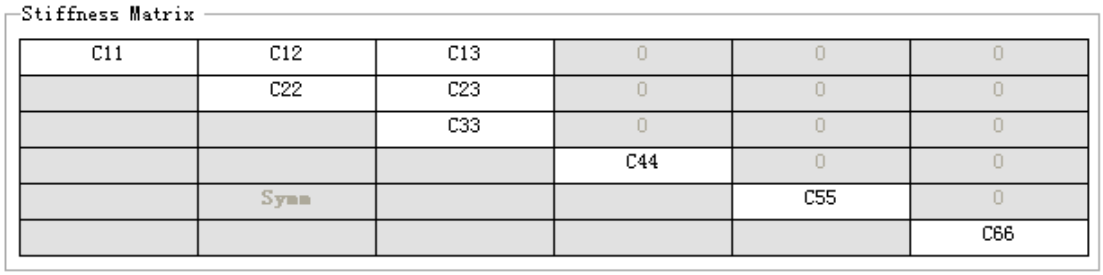


Figure 4: Stiffness Matrix

The second step is to input the wafer orientation. Find the relation between the coordinate axes of the mechanical structure and the material crystal orientation. Edit the Miller Indices of the mechanical structure using the crystal orientation as the reference axes. For example, assuming you want to align the x- and y-axes of the mechanical structure along the [100] and [010] crystalline orientations of silicon, you should enter (1, 0, 0) for the x-axis and (0, 1, 0) for the y-axis. The anisotropic elasticity calculation is similar to geometric coordinate system transformation. The Miller Indices of the z-axis do not need to be specified, as they are automatically obtained by cross-multiplying the x- and y-axes.

Figure 5: Miller Index Settings

Clicking the *Calculate button* will output Young's modulus, Poisson ratio, and shear modulus values that can be entered into the Material Property window in TEM.

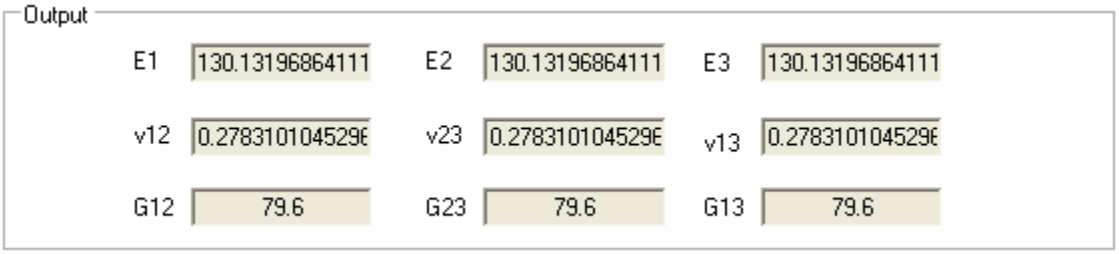


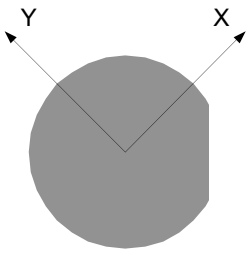
Figure 6: Material Property Outputs

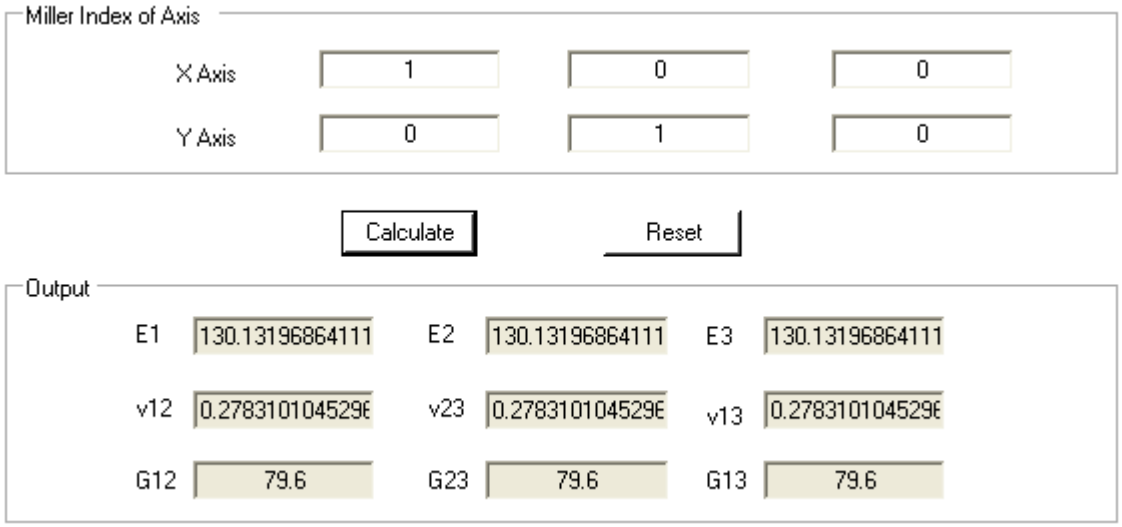
1.2 Settings for Common MEMS Wafers

Below are listed a few common wafer orientations and the corresponding Miller index inputs and resulting material property outputs from the Elastic Parameter Calculator.

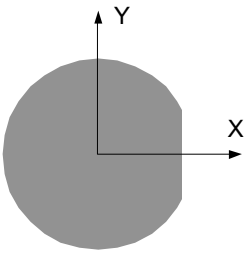
1.2.1 <100> wafer

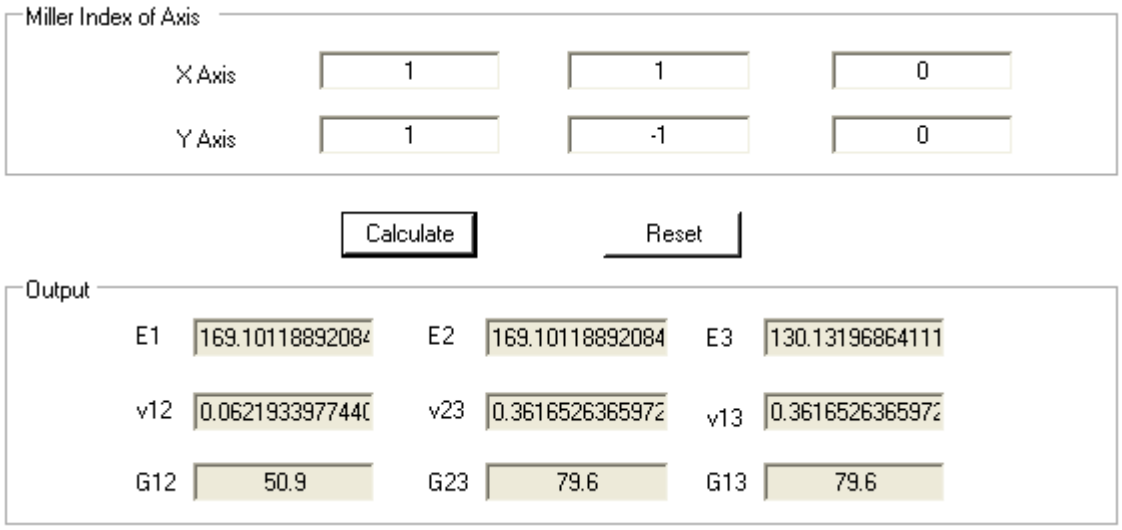
1. The x-axis is at a 45 degree diagonal to the wafer flat and the wafer surface is parallel to the z-axis. This is the default case.





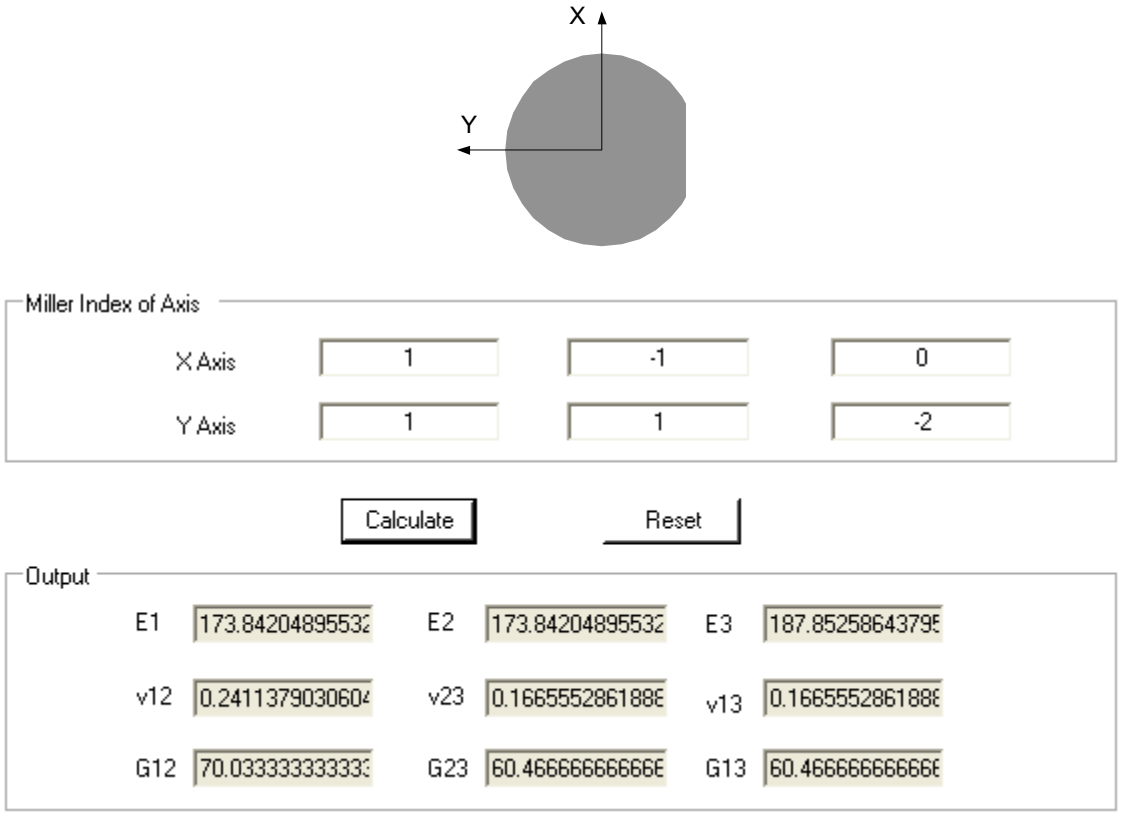
2. The normal vector of the wafer flat is parallel to the x-axis and the wafer surface is parallel to the z-axis.





1.2.2 <111> wafer

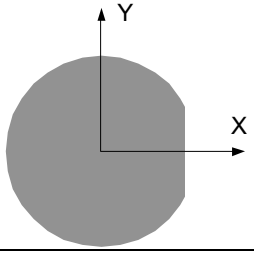
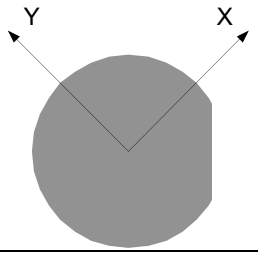
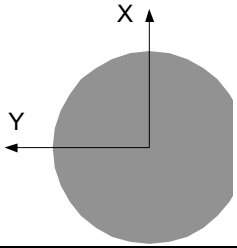
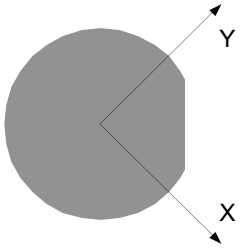
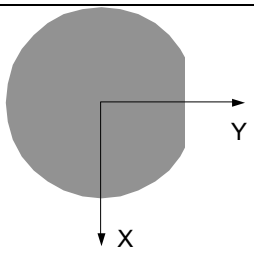
The z-axis is normal to the wafer surface and the x-axis lies parallel to the wafer flat in the plane of the wafer.



1.2.3 List of possible orientations

Below is a table listing the Miller Index values for various orientations of the mechanical structure. Only the primary flat is shown for wafers; the secondary flat is omitted. The X and Y axes are the axes designers

use to draw the mechanical structures. The Z axis can be obtained by cross multiplying the X and Y axes. Designers only need to specify the orientation relation between the flat of a wafer and the coordinate system of the designed mechanical structure by entering the corresponding Miller indices. The aforementioned 3 examples can also be found in the table.

Orientation relation	Axis	Miller indices of wafers					
		{100}			{111}		
	X	1	-1	0	-1	1	0
	Y	1	1	0	-1	-1	2
	X	1	0	0	-2	0	2
	Y	0	1	0	0	-2	2
	X	1	1	0	-1	-1	1
	Y	-1	1	0	1	-1	1
	X	0	-1	0	0	1	1
	Y	1	0	0	-1	0	1
	X	-1	-1	0	1	1	1
	Y	1	-1	0	-1	1	1

2 IntelliSuite v8.6 and Later

In IntelliSuite v8.6 and later, a separate calculator does not need to be used. Users can input the stiffness matrix directly into the Material Property window in TEM and the resulting material properties will be automatically taken into account.

2.1 Isotropic Materials

The stress-strain relation of an isotropic elastic material is given by

$$\begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \gamma_{23} \\ \gamma_{13} \\ \gamma_{12} \end{Bmatrix} = \begin{bmatrix} 1/E & -\nu/E & -\nu/E & 0 & 0 & 0 \\ -\nu/E & 1/E & -\nu/E & 0 & 0 & 0 \\ -\nu/E & -\nu/E & 1/E & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix}$$

The elasticity is determined by the Young's modulus, E, and the Poisson's ratio, ν. The shear modulus, G, is expressed in terms of E and ν as $G = E/2(1+\nu)$. When the *Elastic Parameter* option is set to *Isotropic, t*he elasticity settings can be specified as in the figure below.

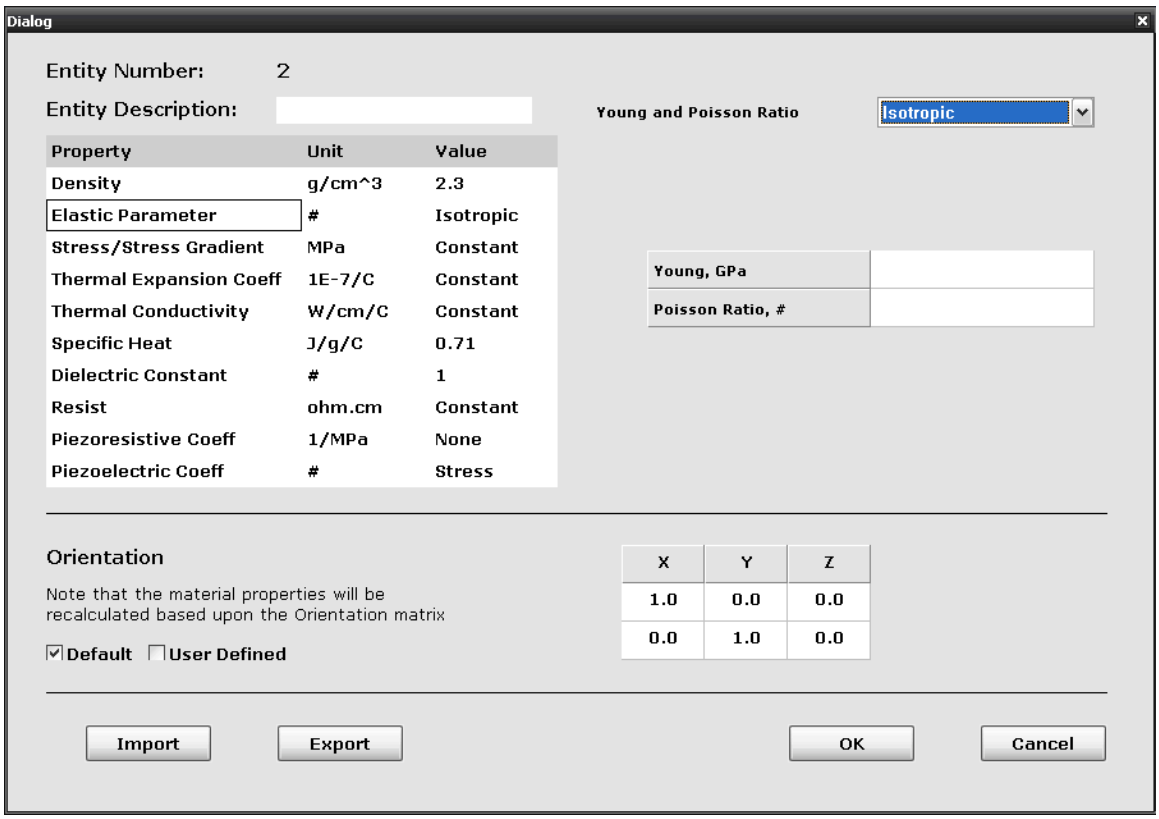


Figure 7: Isotropic material settings

2.2 Orthotropic Materials

The elasticity of an orthotropic material can be set in two ways. One way is specifying the "engineering constants": three Young's moduli E_1, E_2, E_3, Poisson's ratios ν_{12}, ν_{13}, ν_{23}, and shear moduli G_{12}, G_{13}, and G_{23}, shown as in the figure below. These moduli enter the elastic compliance matrix as

$$\begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \gamma_{23} \\ \gamma_{13} \\ \gamma_{12} \end{Bmatrix} = \begin{bmatrix} 1/E_1 & -\nu_{21}/E_2 & -\nu_{31}/E_3 & 0 & 0 & 0 \\ -\nu_{12}/E_1 & 1/E_2 & -\nu_{32}/E_3 & 0 & 0 & 0 \\ -\nu_{13}/E_1 & -\nu_{23}/E_2 & 1/E_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G_{23} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G_{13} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G_{12} \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix}$$

Here, ν_{ij} is the Poisson's ratio that represents the strain in the j-direction when the stress is in the *i*-direction. In general, ν_{ij} is not equal to ν_{ji}. Instead, they are related by $\nu_{ij}/E_i = \nu_{ji}/E_j$. When the *Elastic Parameter* option is set to *Engineering,* the values for *E*,ν, and *G* can be input in the fields on the right side of the window.

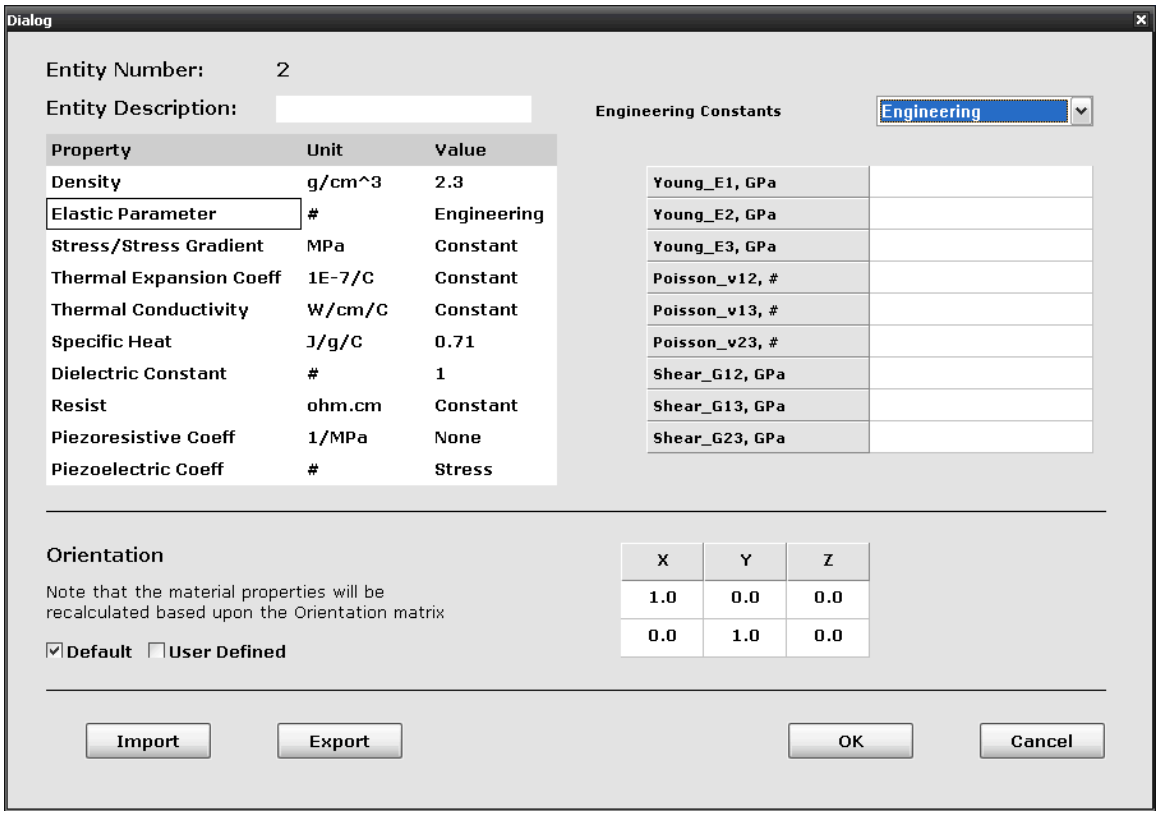


Figure 8: Orthotropic Material Settings

The other way to define the elasticity of an orthotropic material is to use the 9 elements of the stiffness matrix. The stress-strain relation of an orthotropic material is given as

$$\begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \gamma_{23} \\ \gamma_{13} \\ \gamma_{12} \end{Bmatrix} = \begin{bmatrix} C11 & C12 & C13 & 0 & 0 & 0 \\ & C22 & C23 & 0 & 0 & 0 \\ & & C33 & 0 & 0 & 0 \\ & & & C44 & 0 & 0 \\ & symm & & & C55 & 0 \\ & & & & & C66 \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix}$$

When the *Elastic Parameter* option is set to *Orthotropic,* the stiffness matrix values can be input in the fields on the right side of the window.

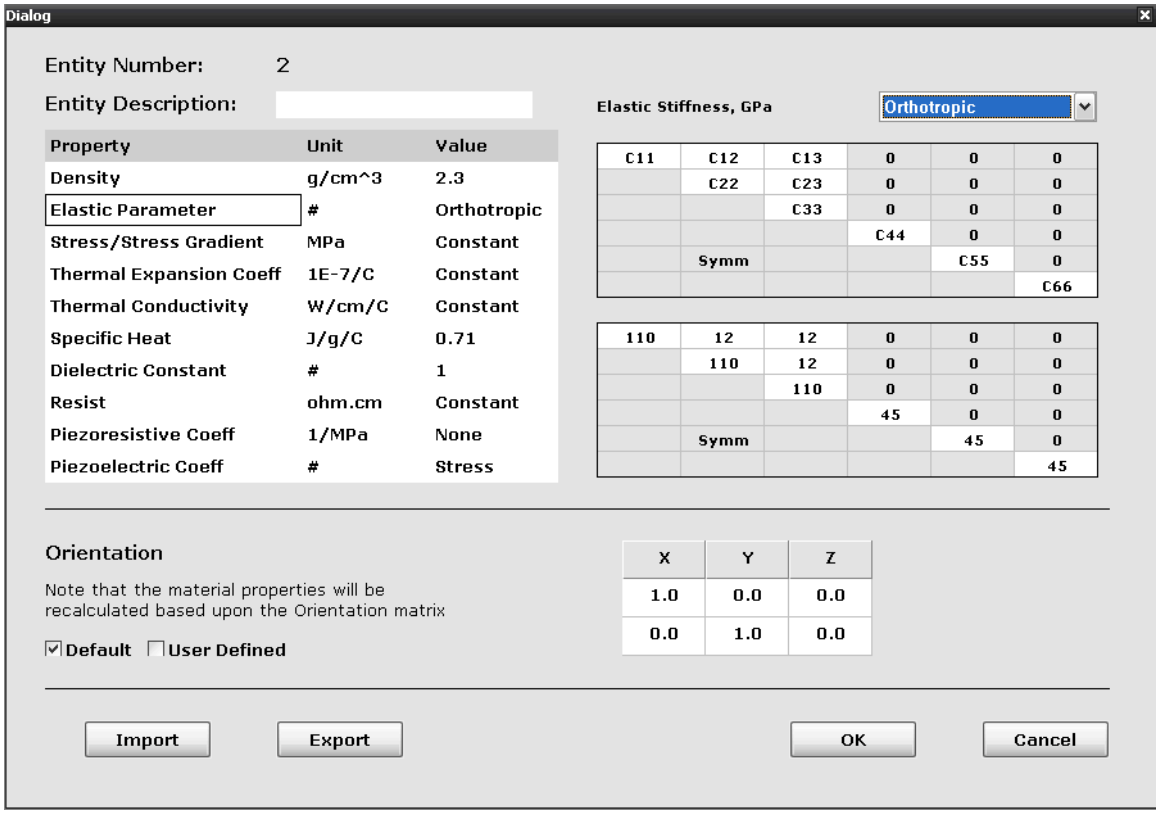


Figure 9: Orthotropic material settings

2.3 Fully Anisotropic Materials

For fully anisotropic elastic materials, 21 independent elastic stiffness elements are needed. The stress-strain relation is as follows.

$$\begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \gamma_{23} \\ \gamma_{13} \\ \gamma_{12} \end{Bmatrix} = \begin{bmatrix} C11 & C12 & C13 & C14 & C15 & C16 \\ & C22 & C23 & C24 & C25 & C26 \\ & & C33 & C34 & C35 & C36 \\ & & & C44 & C45 & C46 \\ & symm & & & C55 & C56 \\ & & & & & C66 \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix}$$

The elasticity can be set as shown in the figure below.

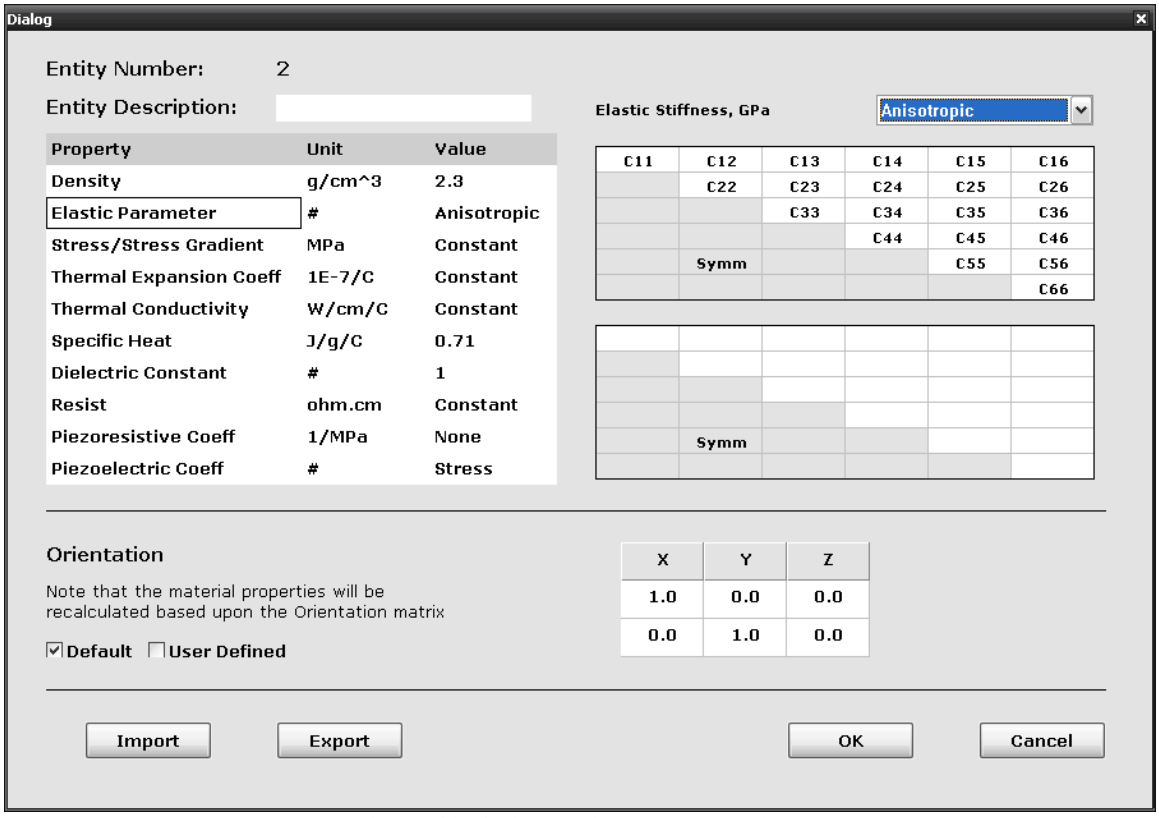


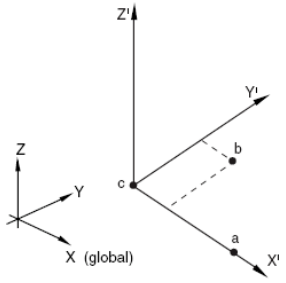
Figure 10: Anisotropic material settings

2.4 Orientation definition

This definition shows the orientation relation between the designed mechanical structure (global coordinate system) and the material crystals (local coordinate system). Note that the definition (or coordinate system transformation specification method) here is different from the coordinate axis transformation specification method in section 1. We used 2 vectors for coordinate axis transformation before. Here, we are going to use 3 points for coordinate transformation definition.

For example, the values in the table below define a rectangular Cartesian system by the 3 points a, b, and c as shown in figure (coordinates of point c not shown). Point c is the origin of the coordinate system. Point a must lie on the X'-axis, and point b must lie on the $X'Y'$- plane. Although not necessary, it is intuitive to select point b such that it is on or near the local Y'-axis.

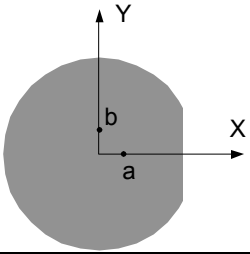
	X	Y	Z
a	1.0	0.0	0.0
b	0.33	0.67	0.0

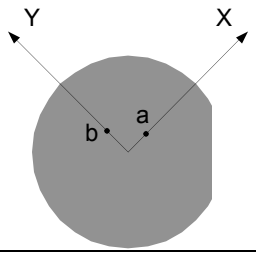
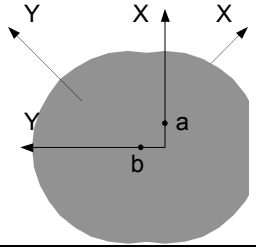
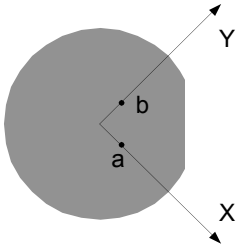
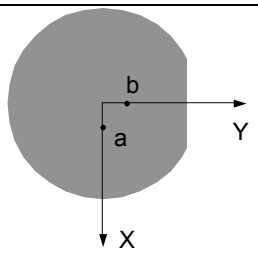


2.4.1 Typical orientations

Below is a table listing typical orientation relations between the designed mechanical structure (global coordinate system) and material crystals (local coordinate system). This table is the same as the table in Section 1 if points (1, 0, 0) and (0, 1, 0) in the global coordinate system are selected as points a and b, respectively.

On the wafer drawings, only the primary flat is shown for wafers, and the secondary flat is omitted. The X and Y axes are the global axes designers use to draw the mechanical structures. The Z axis can be obtained by cross multiplying the X and Y axes. Designers only need to specify the orientation relation between the flat of a wafer and the coordinate system of the designed mechanical structure by entering the corresponding coordinates of points a and b.

Orientation relation	Point	Point coordinates					
		{100}			{111}		
	a	1	-1	0	-1	1	0
	b	1	1	0	-1	-1	2
	a	1	0	0	-2	0	2

	a	1	0	0	-2	0	2
	a	1	1	0	-1	-1	1
	b	-1	1	0	1	-1	1
	a	0	-1	0	0	1	1
	b	1	0	0	-1	0	1
	a	-1	-1	0	1	1	1
	b	1	-1	0	-1	1	1