Silicon as an anisotropic mechanical material

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This tutorial covers the calculation of silicon Young's modulus and Poisson's ratio from elastic constants in any crystal orientation. The algebra is the same for any elastic material with cubic symmetry but I am mostly interested in silicon as I have used it to make micromechanical components. The tutorial assumes knowledge of matrix algebra and some elementary mechanics concepts such as stress and strain. The material in this tutorial is mainly based on the paper by Wortman and Evans [1] with some concepts not familiar for a typical engineer briefly explained.

Figure 1 below shows how Young's modulus Y is defined: the bar is stretched in the x-direction while simultaneously it is allowed to move freely in y- and z-directions. The Young's modulus is then defined as the ratio of stress to strain in the direction of the stretching ($Y = T_{11}/\varepsilon_{11}$). The Poisson's ratio is defined as ratio of length extension to sideways contraction ($\nu = -\varepsilon_{22}/\varepsilon_{11}$). For reasons that should become obvious later, different directions are referred with numbers and letters interchangeable.

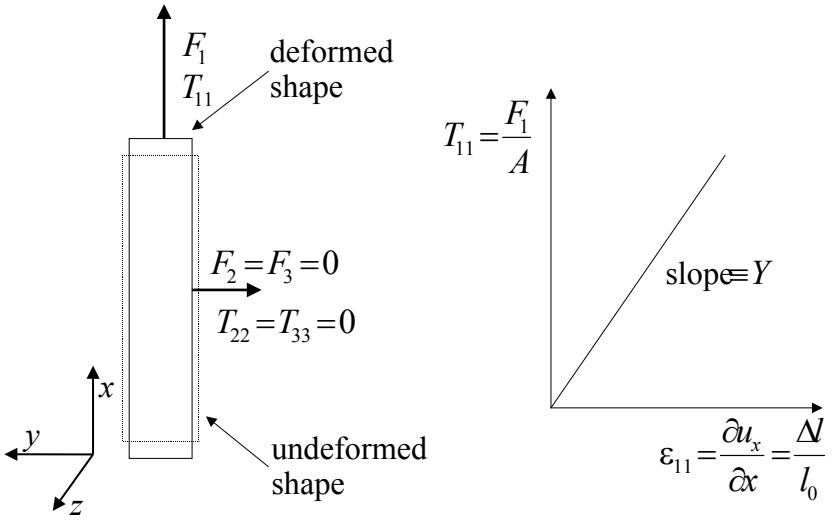


Figure 1. *Definition of Young's modulus Y. This tutorial uses numbers* 1, 2, *and* 3 *to indicate x, y, and z axes respectively.*

For an anisotropic material such as silicon the Young's modulus depends on which crystal direction the material is being stretched. Looking at Figure 2 this should be no surprise as the silicon crystal is highly structured. Figure 2 is also a quick introduction to the crystallographic notation: Different directions are indicated with respect to crystal basis using Miller indexes. In cubic crystal such as silicon the [100], [010] and [001]-directions can be chosen to coincide with x, y, and z-axes. However, this may not be true for crystal with different symmetry. The Miller indexes can be thought as vectors. For example [210] would mean two in [100]-direction and one in [010]-direction. Thus all other directions can be obtained with combination of indexes with [101]-direction shown as an example.

To account for anisotropy tensor formalism is required. The general relationship between stress and

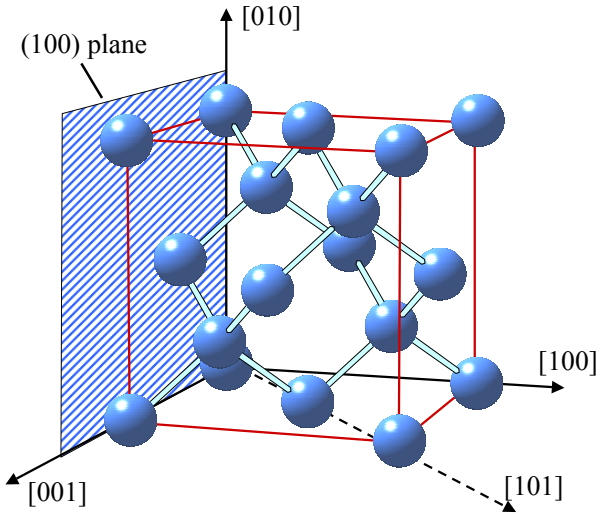


Figure 2. *Silicon crystal structure: Different crystal orientations are indicated with Miller indexes with [100] coinciding with x-axis. Also shown is (100)-plane (that is plane orthogonal to [100] direction) and crystal unit cell (red box).*

strain is

$$T_{ij} = \sum_{k=1}^{3}\sum_{l=1}^{3} C_{ijkl}\varepsilon_{kl}, \tag{1}$$

where C_{ijkl} is the second order stiffness tensor, ε_{kl} is strain and T_{ij} is stress. The subscripts ij refer to axes: For example T_{11} is stress in x-direction and T_{12} is shear stress between x-and y-axis.

For convenience short hand matrix notation can be used. The notation takes use of symmetry relationships $\varepsilon_{12} = \varepsilon_{21}$, $\varepsilon_{13} = \varepsilon_{31}$, and $\varepsilon_{23} = \varepsilon_{32}$ between shear stresses to write $11 \rightarrow 1$, $22 \rightarrow 2$, $33 \rightarrow 3$, $32 \rightarrow 4$, $31 \rightarrow 5$, and $21 \rightarrow 6$. For example C_{1132} then becomes C_{14} and ε_{32} is simply ε_4. With this notation Equation (1) can be rewritten as

$$\begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}. \tag{2}$$

The main advantage of short hand notation is that we have gotten rid of the nasty tensor double sum in Equation (1) and many calculations can be solved with matrix algebra. For silicon the stiffness matrix **C** in [100]-crystal axes is

$$\mathbf{C} = \begin{bmatrix} 1.66 & 0.64 & 0.64 & 0 & 0 & 0 \\ 0.64 & 1.66 & 0.64 & 0 & 0 & 0 \\ 0.64 & 0.64 & 1.66 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.80 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.80 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.80 \end{bmatrix}, \tag{3}$$

where all values are in units of 10^{11} Pa. Equation (2) allows direct calculation of the Young's modulus. To obtain Young's modulus in [100] direction (remember, that is also the x-direction), set all other stresses to

zero and solve for $Y_{[100]} = T_1/\varepsilon_1$. This gives

$$Y_{[100]} = C_{11} - 2\frac{C_{12}}{C_{11}+C_{12}}C_{12} = 130 \text{ Gpa}. \tag{4}$$

The Poisson's ratio can similarly be obtained as

$$\nu_{[100]} = \frac{C_{12}}{C_{11}+C_{12}} = 0.28. \tag{5}$$

The values for Young's modulus to [110]- and [111]-direction are $Y_{[110]} = 168$ GPa and $Y_{[111]} = 187$ GPa respectively.

Unfortunately calculations can become complicated very quickly and computerized method can be desirable. Since the stiffness matrix is known, the Young's modulus can be numerically computed by taking inverse of $\mathbf{C}$. This is called compliance matrix $\mathbf{S} = \mathbf{C}^{-1}$. The compliance matrix can be used to calculate strains due to applied stress in desired directions. If stress is applied x-direction, the stresses other than T_1 are zero. From $\varepsilon = \mathbf{S}T$ Young's modulus is then simply (Why?)

$$Y = \frac{T_1}{\varepsilon_1} = 1/S_{11}. \tag{6}$$

Similarly, Poisson's ratio is

$$\nu_{ij} = -\frac{\varepsilon_j}{\varepsilon_i} = -\frac{S_{ij}}{S_{ii}}. \tag{7}$$

Compliance matrix is useful in other situations too. Figure 3 shows 2D stretching of a plate. In this case $T_1 = T_2$ and the other stresses are zero. This gives $Y_{2D} = T_1/\varepsilon_1 = 181$ GPa. Interestingly this does not depend on axis orientation.

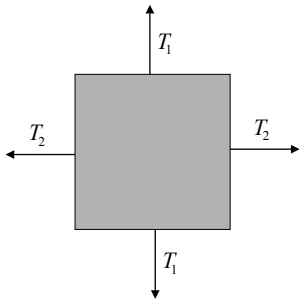


Figure 3. *2D stretching of a silicon plate.*

The Young's modulus in any direction can be obtained by calculating the stiffness matrix in rotated coordinates. For example, to obtain Young's modulus in $[110]$-direction, do a 45° rotation around the [001]-axis. Once stiffness matrix is known in the new coordinates, one can follow the calculation algorithm above. Example of axis rotation is shown in Figure 4. In calculating the rotated stiffness matrix, it has the be remembered that $\mathbf{C}$ is really based on a second-order tensor and that tensor rotation is slightly more complicated than for matrix rotation. The rotated $\mathbf{C}'$ can be found in literature [1] but due to complex algebra, I find it easier to calculate it numerically. The rotated $\mathbf{C}'$ is obtained from

$$C'_{ijkl} = \sum_{p=1}^{3}\sum_{q=1}^{3}\sum_{r=1}^{3}\sum_{s=1}^{3} Q_{pi}Q_{qj}Q_{rk}Q_{sl}C_{pqrs}, \tag{8}$$

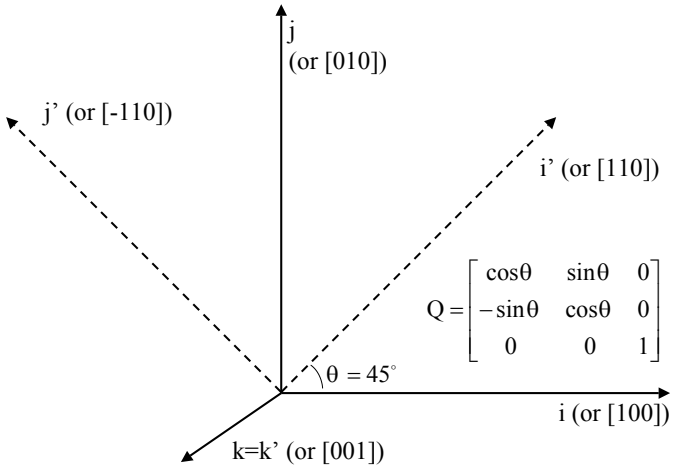
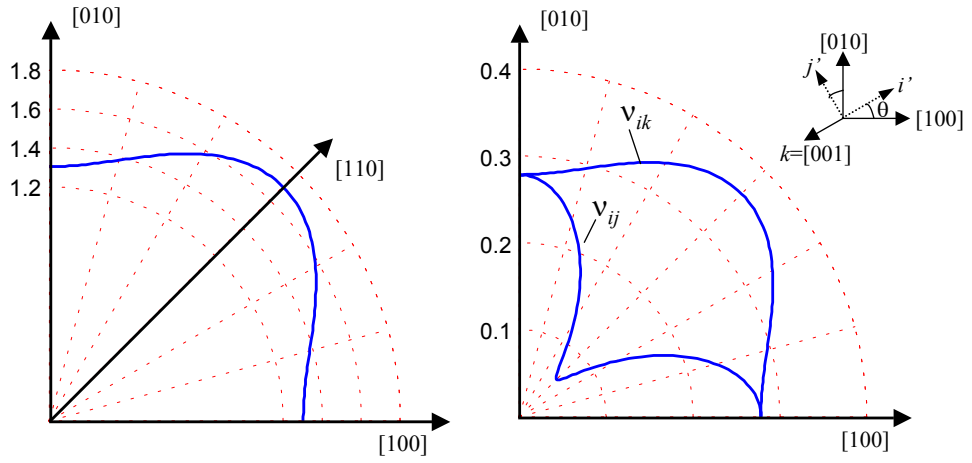


Figure 4. *Axis rotation using rotation matrix* **Q**. *The new axes is obtained with* $\mathbf{x}' = \mathbf{Q}\mathbf{x}$



(a) Young's modulus (units: 10^{11} Pa)

(b) Poisson's ratio

Figure 5. *Calculated silicon Young's modulus and Poisson's ratio in (100)-plane*

where **Q** is the rotation matrix. Tedious for hand calculation but a breeze for a computer.

This is all that is needed to calculate silicon Young's modulus and Poisson's ratio. As an example, they are shown in (100)-plane in Figure 5. You may obtain the Matlab-script used in calculating the images from http://www.kaajakari.net/~ville/research/tutorials/Yangle.m. With the script you should be able to calculate the Young's modulus in other planes. (111)-plane gives an interesting result of constant Young's modulus and Poisson's ratio. This makes (111) wafers an interesting material for micromachining.

I hope you enjoyed this little tutorial. I plan to improve it in the future so if you have any comments or feedback, please send me an e-mail to ville@kaajakari.net!

References

[1] J. J. Wortman and R. A. Evans, "Young's modulus, shear modulus, and Poisson's ratio in silicon and germanium", *J. Applied Physics*, vol. 36(1), pp. 153–156, Jan. 1965.