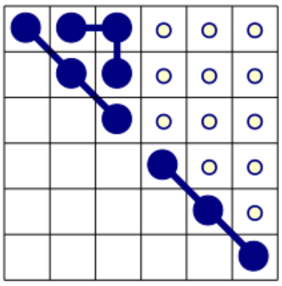
Exercise III
Crystal elasticity

Question 1

In a cubic system the stiffness matrix has the following shape

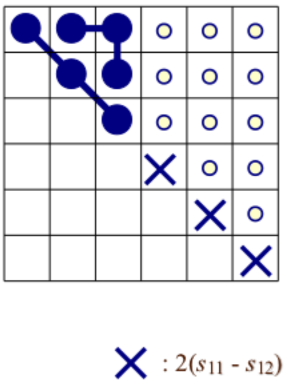


The anisotropy parameter is given and it's equal to 1:

$$A = \frac{2(s_{11} - s_{22})}{s_{44}} = 1$$

$$2(s_{11} - s_{22}) = s_{44}$$

But it's also $s_{44} = s_{55} = s_{66}$



and this matrix is the same of the isotropic continuum.

Question 2

Given the 3 elastic constants c_{11}, c_{12} and c_{44}, it is possible to find the compliance parameters from these equations:

$$\begin{cases} c_{11} = \frac{s_{11}+s_{12}}{(s_{11}-s_{12})(s_{11}+2s_{12})} \\ c_{12} = \frac{-s_{12}}{(s_{11}-s_{12})(s_{11}+2s_{12})} \\ c_{44} = \frac{1}{s_{44}} \end{cases} \tag{1}$$

$$\begin{cases} (s_{11}-s_{12})(s_{11}+2s_{12}) = \frac{s_{11}+s_{12}}{c_{11}} \\ (s_{11}-s_{12})(s_{11}+2s_{12}) = \frac{-s_{12}}{c_{12}} \\ s_{44} = \frac{1}{c_{44}} \end{cases} \quad \begin{cases} \frac{s_{11}+s_{12}}{c_{11}} = \frac{-s_{12}}{c_{12}} \\ (s_{11}-s_{12})(s_{11}+2s_{12}) = \frac{-s_{12}}{c_{12}} \\ s_{44} = \frac{1}{c_{44}} \end{cases}$$

$$\begin{cases} s_{11} = -\left(1+\frac{c_{11}}{c_{12}}\right) s_{12} \\ \left(-2-\frac{c_{11}}{c_{12}}\right) s_{12} \left(1-\frac{c_{11}}{c_{12}}\right) s_{12} = \frac{-s_{12}}{c_{12}} \\ s_{44} = \frac{1}{c_{44}} \end{cases} \quad \begin{cases} s_{11} = -\left(1+\frac{c_{11}}{c_{12}}\right) s_{12} \\ \left(-2-\frac{c_{11}}{c_{12}}\right) s_{12} \left(1-\frac{c_{11}}{c_{12}}\right) s_{12} = \frac{-s_{12}}{c_{12}} \\ s_{44} = \frac{1}{c_{44}} \end{cases}$$

$$\begin{cases} s_{11} = -\left(1+\frac{c_{11}}{c_{12}}\right) s_{12} \\ c_{12}\left(\frac{c_{11}+2c_{12}}{c_{12}}\right)\left(\frac{c_{12}-c_{11}}{c_{12}}\right) s_{12}^2 = s_{12} \\ s_{44} = \frac{1}{c_{44}} \end{cases}$$

$$\begin{cases} s_{11} = \frac{c_{11}+c_{12}}{(c_{11}-c_{12})(c_{11}+2c_{12})} \\ s_{12} = \frac{-c_{12}}{(c_{11}-c_{12})(c_{11}+2c_{12})} \\ s_{44} = \frac{1}{c_{44}} \end{cases} \tag{2}$$

Question 3

The expression of the bulk modulus is

$$\kappa = \frac{E}{3(1-2\nu)}$$

Using the following form

$$\frac{1}{3\kappa} = \frac{1-2\nu}{E} = \frac{1+\nu}{E} - 3\frac{\nu}{E}$$

it is easy to calculate for each of polycrystalline models the bulk modulus.

Reuss model

$$\begin{aligned} \frac{1}{3\kappa} &= \frac{2}{5}(s_{11}-s_{12}) + \frac{3}{10}s_{44} + 3\left(\frac{1}{5}s_{11} + \frac{4}{5}s_{12} - \frac{1}{10}s_{44}\right) = \\ &= s_{11} + \frac{10}{5}s_{12} = \\ &= s_{11} + 2s_{12} \end{aligned}$$

$$\kappa = \frac{1}{3(s_{11}+2s_{12})}$$

Voigt model

$$\begin{aligned}
\frac{1}{3\kappa} &= \frac{5(s_{11}-s_{12})s_{44}}{6(s_{11}-s_{12})+2s_{44}} + 3\frac{(2s_{11}-2s_{12}-s_{44})(s_{11}+2s_{12})+5s_{12}s_{44}}{6(s_{11}-s_{12})+2s_{44}} = \\
&= \frac{5s_{11}s_{44}-5s_{12}s_{44}+3(2s_{11}^2-2s_{11}s_{12}-s_{11}s_{44}+4s_{11}s_{12}-4s_{12}^2-2s_{12}s_{44}+5s_{12}s_{44})}{6(s_{11}-s_{12})+2s_{44}} = \\
&= \frac{2s_{11}s_{44}+4s_{12}s_{44}+6s_{11}^2+6s_{11}s_{12}-12s_{12}^2}{6(s_{11}-s_{12})+2s_{44}} = \\
&= \frac{2(s_{11}+2s_{12})s_{44}+6(s_{11}^2+s_{11}s_{12}-2s_{12}^2)}{6(s_{11}-s_{12})+2s_{44}} = \\
&= \frac{2(s_{11}+2s_{12})s_{44}+6(s_{11}+2s_{12})(s_{11}-s_{12})}{6(s_{11}-s_{12})+2s_{44}} = \\
&= s_{11}+2s_{12}
\end{aligned}$$

$$\kappa = \frac{1}{3(s_{11}+2s_{12})}$$

Kröner model

$$\kappa = \frac{1}{3(s_{11}+2s_{12})}$$

Question 4

Choosing the Kröner model, it's one way to determine Young's modulus, Poisson's ratio and shear modulus of polycrystalline bulk silicon with the following constant: $c_{11} = 165.78\,GPa$, $c_{12} = 63.94\,GPa$, $c_{44} = 79.62\,GPa$.
The bulk modulus value is

$$\kappa = \frac{1}{3}(c_{11} + 2c_{12}) = 97.89\,GPa$$

To calculate the shear modulus we need these two constants:

$$\mu_1 = \frac{1}{2}(c_{11} - c_{12}) = 50.92\,GPa$$

$$\mu_2 = c_{44} = 79.62\,GPa$$

Solving the following expression, it is possible to find the value of G:

$$G^3 + \gamma_1 G^2 + \gamma_2 G + \gamma_3 = 0$$

where the three constants are

$$\gamma_1 = \frac{9\kappa + 4\mu_1}{8} = 135.59$$

$$\gamma_1 = -\mu_2 \frac{3\kappa + 12\mu_1}{8} = -9004.13$$

$$\gamma_3 = -\frac{3\kappa\mu_1\mu_2}{4} = -2.97e5$$

The only real solution of the previous equation is

$$G = 66.59\,GPa$$

Finally we cand find the Young's modulus and Poisson's ratio

$$E = -\frac{9\kappa G}{(3\kappa + G)} = 162.8\,GPa$$

$$\nu = \frac{3\kappa - 2G}{2(3\kappa + G)} = 0.223$$

Question 5

With the Reuss model, it's possible to calculate the Young's modulus on the directions of a silicon crystal. Using the equations found at Question 2 and the numerical value of the constant (Question 4):

$$\begin{cases} s_{11} = \frac{c_{11}+c_{12}}{(c_{11}-c_{12})(c_{11}+2c_{12})} & = 7.68e-3 \\ s_{12} = \frac{-c_{12}}{(c_{11}-c_{12})(c_{11}+2c_{12})} & = -2.138e-3 \\ s_{44} = \frac{1}{c_{44}} & = 1.26e-2 \end{cases}$$

$$s_0 = s_{11} - s_{12} - \frac{s_{44}}{2} = 3.52e-3$$

From these two equations, it is possible to calculate E:

$$\begin{cases} \frac{1+\nu}{E} = s_{11} - s_{12} - 3s_0\Gamma \\ -\frac{\nu}{E} = s_{12} + s_0\Gamma \end{cases}$$

$$\begin{cases} \nu = E\left(s_{11} - s_{12} - 3s_0\Gamma\right) - 1 \\ \nu = -E\left(s_{12} + s_0\Gamma\right) \end{cases}$$

$$E\left(s_{11} - s_{12} - 3s_0\Gamma\right) - 1 = -E\left(s_{12} + s_0\Gamma\right)$$

$$E = \frac{1}{s_{11} - 2s_0\Gamma}$$

The general expression for the orientation function is

$$\Gamma = \frac{h^2k^2 + k^2l^2 + l^2h^2}{(h^2 + k^2 + l^2)^2}$$

Direction <100>

$$\Gamma = \frac{h^2k^2 + k^2l^2 + l^2h^2}{(h^2 + k^2 + l^2)^2} = 0$$

$$E = \frac{1}{s_{11} - 2s_0\Gamma} = 130.21\, GPa$$

Direction <110>

$$\Gamma = \frac{h^2k^2 + k^2l^2 + l^2h^2}{(h^2 + k^2 + l^2)^2} = \frac{1}{4}$$

$$E = \frac{1}{s_{11} - 2s_0\Gamma} = 168.89\, GPa$$

Direction <111>

$$\Gamma = \frac{h^2k^2 + k^2l^2 + l^2h^2}{(h^2 + k^2 + l^2)^2} = \frac{1}{3}$$

$$E = \frac{1}{s_{11} - 2s_0\Gamma} = 187.45\, GPa$$