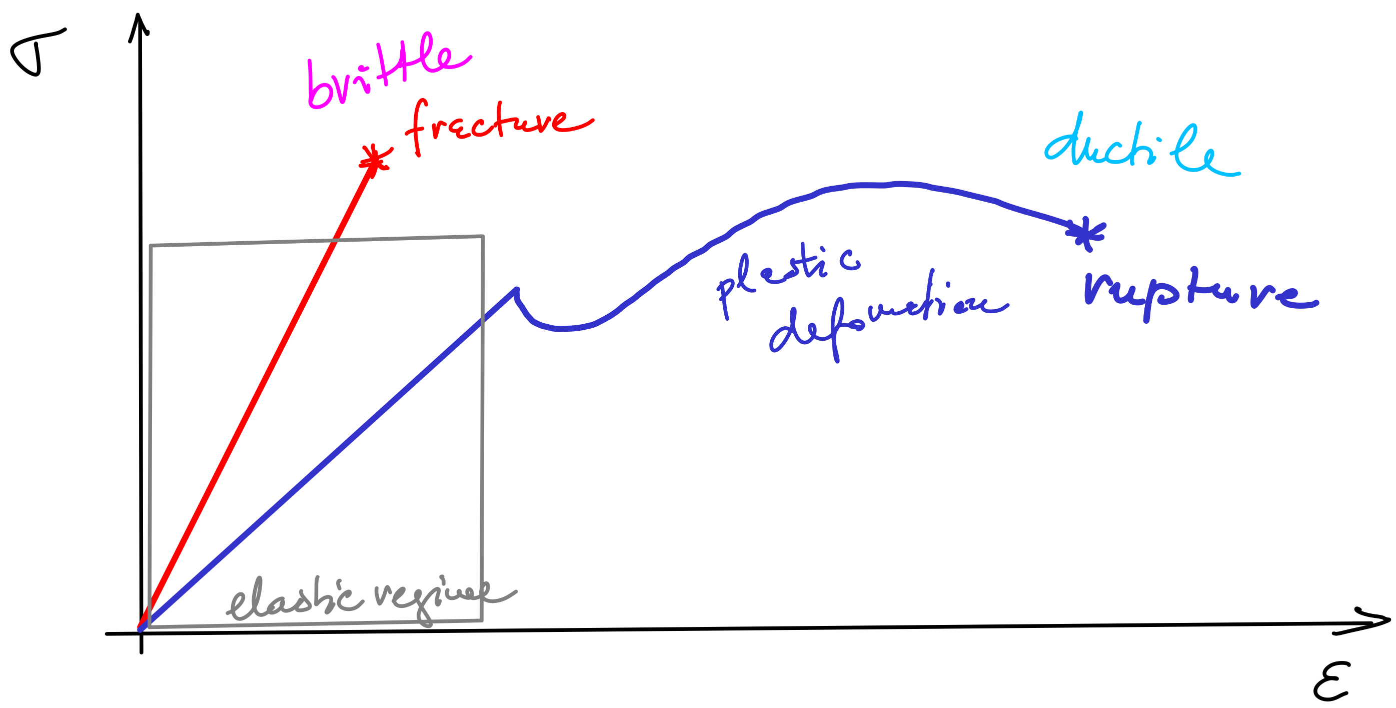
Elastic Properties of Material

1. Elastic deformation

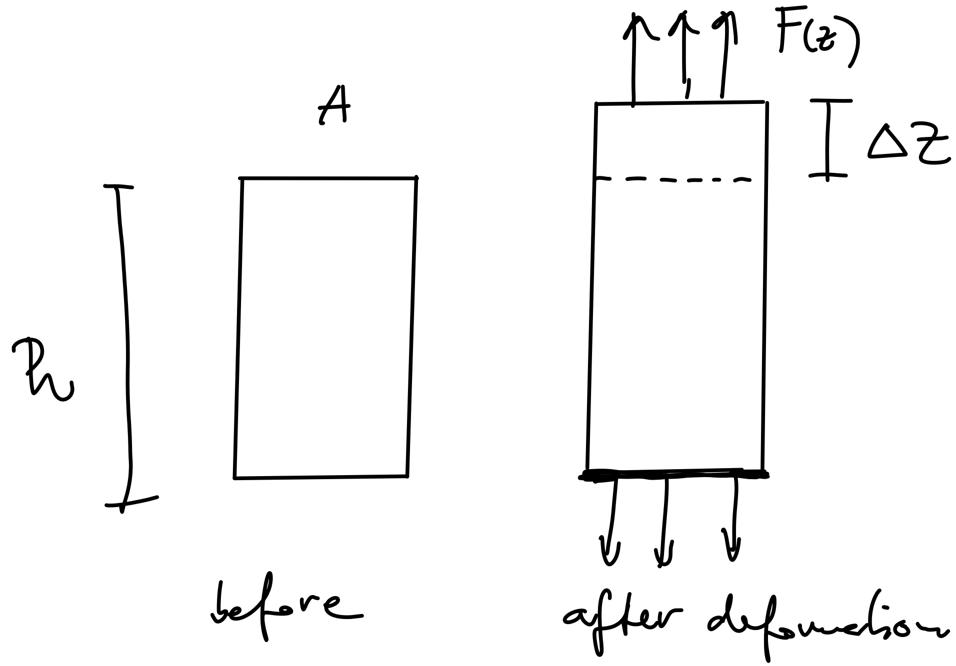
„stress–strain" curve of solid



$\sigma / \varepsilon = Y$

Young modulus

(2.) Calculation of strain and stress



$$\Delta U = \int_{h}^{h+\Delta z} F(z)\, dz$$

applied stress per unit area $\sigma = \frac{F}{A}$

strain due displacement of the top layer $\varepsilon = \frac{\Delta z}{h}$

$$\Delta U = A h \int_0^{\varepsilon} \sigma \, d\varepsilon \quad ; \quad \Omega = A h$$

→ volume of the calculated cell

$\sigma = C \varepsilon$; C – elastic constant

$$\frac{\Delta U}{\Omega} = \frac{1}{2} C \varepsilon^2 \longrightarrow \boxed{\sigma = \frac{1}{\Omega} \frac{\partial U}{\partial \varepsilon}}$$

3. General formulation

$$R'_{I\alpha} = \sum_{\beta} \left(\delta_{\alpha\beta} + e_{\alpha\beta}\right) R_{I\beta} \qquad \alpha,\beta = 1,2,3\,(x,y,z)$$

nuclear position of strained solid

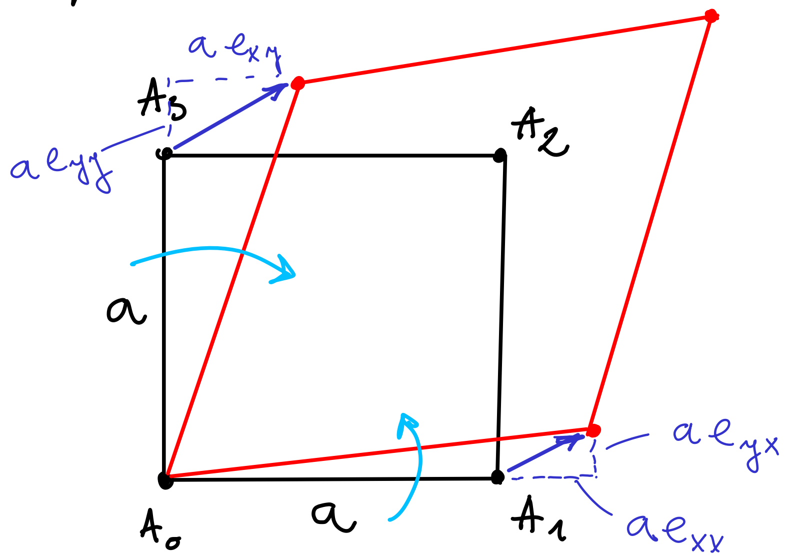
Kronecker's δ

3x3 matrix of small elements ($e_{\alpha\beta} \ll 1$)

nuclear position of unstrained solid

$$R'_{I\alpha} = \left(\delta_{\alpha\beta} + e_{\alpha\beta}\right) R_{I\beta} \qquad // \text{ Einstein notation}$$

Example: 2d square lattice



e_{xx}, e_{yy} — normal components of strain (dilatation of solid)

e_{xy}, e_{yx} — „shear" strain (sliding)

Note: $a e_{\alpha\beta}$ are very small in reality $\approx 0.01\,a$

atom A_1 transforms: $\vec{R}_1' = \vec{R}_1 + a(e_{xx}\vec{u}_x + e_{yx}\vec{u}_y)$

atom A_3 transforms: $\vec{R}_3' = \vec{R}_3 + a(e_{xy}\vec{u}_x + e_{yy}\vec{u}_y)$

$A_0 - A_1$ bond:

$$e_{yx}\, a = tg\,\gamma \cdot (a + e_{xx}) \simeq a\, tg\,\gamma \;; \quad tg\,\gamma \simeq \gamma$$

$e_{xx} \ll a$

rotation is precisely e_{yx}

$A_0 - A_3$ bond: rotating e_{xy}

Averaged rotation (counterclockwise): $(e_{yx} - e_{xy})/2$

$$\vec{R}_1'' = \vec{R}_1' - \frac{a}{2}(e_{yx} - e_{xy})\vec{u}_y = \vec{R}_1 + a\left[e_{xx}\vec{u}_x + \frac{1}{2}(e_{xy} + e_{yx})\vec{u}_y\right]$$

$\vec{R}_3'' = \dots$

Pure elastic deformation of a solid $\rightarrow$ strain tensor

$$\varepsilon_{\alpha\beta} = \frac{1}{2}\left(e_{\alpha\beta} + e_{\beta\alpha} \right)$$

symmetric part ⊛

?

antisymmetric part (rotation)

$$\frac{\Delta U}{\Omega} = \frac{1}{2} C_{\alpha\beta\gamma\delta}\, \varepsilon_{\alpha\beta}\, \varepsilon_{\gamma\delta}$$

tensor
$3^4 = 81$
elastic constant

} Elastic moduli

Note: 2d system --- 16 components

$$\sigma_{\alpha\beta} = \frac{1}{\Omega} \frac{\partial U}{\partial \varepsilon_{\alpha\beta}}$$ ⊛

Note: Holds the following

$$\frac{\partial \varepsilon_{\alpha\beta}}{\partial \varepsilon_{\gamma\delta}} = \delta_{\alpha\gamma}\, \delta_{\beta\delta}$$

$$C_{\alpha\beta\gamma\delta} = C_{\gamma\delta\alpha\beta}$$ ⊛

$$\boxed{\sigma_{\alpha\beta} = C_{\alpha\beta\gamma\delta}\, \varepsilon_{\gamma\delta}}$$

Hooke's Law

$\circledast \quad \sigma_{\alpha\beta} = \sigma_{\beta\alpha} \Rightarrow e_{\alpha\beta} = e_{\beta\alpha}$

if not equal
$\Rightarrow$ global rotation

$\Rightarrow$ symmetry $\rightarrow$ 6 independent components

$$\varepsilon_{\alpha\beta} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ & \varepsilon_{yy} & \varepsilon_{yz} \\ & & \varepsilon_{zz} \end{pmatrix} \xrightarrow[\text{notation}]{\text{Voigh}} \varepsilon_i = \begin{pmatrix} \varepsilon_1 & \varepsilon_6 & \varepsilon_5 \\ & \varepsilon_2 & \varepsilon_4 \\ & & \varepsilon_3 \end{pmatrix}$$

$\Rightarrow$ $6 \times 6 = 36$ coefficients = independent components of elastic tensor (81 → 36)

$\Rightarrow$ ⊛ Due symmetry $\rightarrow$ 21 independent components (H.W.)

$$\boxed{\sigma_i = C_{ij}\,\varepsilon_j}$$

Hooke's law (Voigh notation)

$\alpha\beta \longrightarrow i$
$\gamma\delta \longrightarrow j$

$$\boxed{\frac{\Delta U}{\Omega} = \frac{1}{2} C_{ij}\, u_i u_j} \circledast$$

with $u_i = \begin{cases} \varepsilon_i & ; \; i = 1,2,3 \\ 2\varepsilon_i & ; \; i = 4,5,6 \end{cases}$

$$
\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix}
=
\begin{bmatrix}
C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\
 & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\
 & & C_{33} & C_{34} & C_{35} & C_{36} \\
 & & & C_{44} & C_{45} & C_{46} \\
 & & & & C_{55} & C_{56} \\
 & & & & & C_{66}
\end{bmatrix}
\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}
$$

$$
\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix}
=
\begin{bmatrix}
C_{1111} & C_{1122} & C_{1133} & C_{1123} & C_{1113} & C_{1112} \\
 & C_{2222} & C_{2233} & C_{2223} & C_{2213} & C_{2212} \\
 & & \ddots & & & \\
 & & & & & \\
 & & & & & \\
 & & & & &
\end{bmatrix}
\begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix}
$$

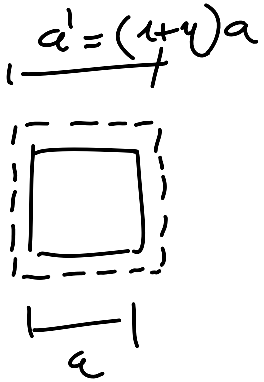
5. Calculation of the elastic constants by DFT using (*)

Example: Cubic lattice

$$c_{ij} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & & & \\ c_{12} & c_{11} & c_{12} & & & \\ c_{12} & c_{12} & c_{11} & & & \\ & & & c_{44} & & \\ & & & & c_{44} & \\ & & & & & c_{44} \end{bmatrix}$$

$$\frac{\Delta U}{\Omega} = \frac{1}{2} C_{11}\left(u_1^2 + u_2^2 + u_3^2\right) + C_{12}\left(u_1 u_2 + u_1 u_3 + u_2 u_3\right) + \frac{1}{2} C_{44}\left(u_4^2 + u_5^2 + u_6^2\right)$$

- isotropic deformation

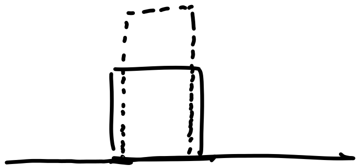


normal strain as η ; shear strain $= 0$

$u_1 = u_2 = u_3 = \eta$; $u_4 = u_5 = u_6 = 0$

$$\frac{\Delta U}{\Omega} = \frac{3}{2}\left(C_{11} + 2C_{12}\right)\eta^2$$

- tetragonal deformation



$a' = (1-\eta)a$

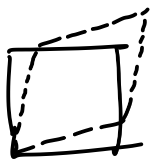
$c' = (1+2\eta)a$

no shear : $u_4 = u_5 = u_6 = 0$

$u_3 = 2\eta \quad ; \quad u_1 = u_2 = -\eta$

$$\frac{\Delta U}{\Omega} = 3\left(C_{11} - C_{12}\right)\eta^2$$

- trigonal deformation



$u_1 = u_2 = u_3 = 0$

$u_4 = u_5 = 0$

$u_6 = \eta$

$$\frac{\Delta U}{\Omega} = \frac{1}{2} C_{44} \eta^2$$

$a'_{1x} = a_{1x} + \eta\, a_{1y}/2$

$a'_{1y} = a_{1y} + \eta\, a_{1x}/2$

$a'_{1z} = a_{1z}$

6. Bulk modulus B_0

$$\bar{\bar{\varepsilon}} = \begin{pmatrix} 1+\eta & & \\ & 1+\eta & \\ & & 1+\eta \end{pmatrix}$$

Birch–Murnaghan state equation:

$$U(V) = U_0 + \frac{9V_0B_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{2/3}-1\right]^3 B_0' + \left[\left(\frac{V_0}{V}\right)^{2/3}-1\right]^2\left[6-4\left(\frac{V_0}{V}\right)^{2/3}\right]\right\}$$

B_0 – bulk modulus

B_0' – 1st derivative of B_0

V_0 – equilibrium volume

U_0 – equilibrium total energy