Computational Materials Physics

Center for Molecular Modeling

Department of Materials Science and Engineering

what are elastic constants ?

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http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

Hooke's law

Hooke's law for the elongation of a spring subject to a given force:

$$F = k\,(\ell - \ell_0)$$
$$= kx$$

force applied to the spring (F); displacement (elongation of the spring) (x)

Hooke's law for the elongation of a rod subject to a given axial stress:

$$P = \frac{F}{S} = \frac{k}{\sqrt{S}}\,\frac{x}{\sqrt{S}} = C\,\epsilon$$

(axial) stress (P) — Dutch: "spanning"

strain (ϵ) — Dutch: "vervorming"

Hooke's law

Hooke's law for the elongation of a spring subject to a given force:

$$F = k\,(\ell - \ell_0)$$
$$= kx$$

[N] = [N/m] [m]

Hooke's law for the elongation of a rod subject to a given axial stress:

$$P = \frac{F}{S} = \frac{k}{\sqrt{S}}\,\frac{x}{\sqrt{S}} = C\,\epsilon$$

[Pa] = [Pa] [1]

Hooke's law

Elastic energy of the spring :

$$E = \frac{1}{2}kx^2$$

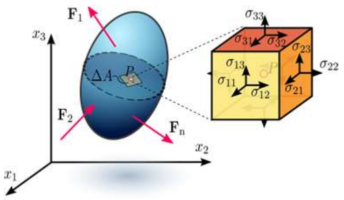
Elastic energy *density* of the rod :

$$\frac{E}{V} = \frac{1}{2}C\epsilon^2$$

Hooke's law
for three-dimensional anisotropic materials

$$P \longrightarrow \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{bmatrix}$$

Stress tensor
(your action on the material)
(symmetric, 3x3)



From: http://en.wikipedia.org/wiki/Stress_(mechanics)

σ_{ij} : if we cut the material along a plane perpendicular to the i-direction, then the j-component of the force per unit area exerted by one half of the material on the other half is given by σ_{ij}. These forces are the internal forces that hold the material together.

Hooke's law
for three-dimensional anisotropic materials

- Stress tensor is position dependent: in general different values at different points inside a macroscopic material
- Stress tensor is time dependent: in general different values at different moments in time during a process

Force per unit area in a plane perpendicular to the unit vector **n**=(n_x,n_y,n_z):

$$\begin{bmatrix} P_x^n \\ P_y^n \\ P_z^n \end{bmatrix} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{bmatrix} \cdot \begin{bmatrix} n_x \\ n_y \\ n_z \end{bmatrix}$$

Hooke's law
for three-dimensional anisotropic materials

$$\epsilon \longrightarrow \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{xy} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{xz} & \epsilon_{yz} & \epsilon_{zz} \end{bmatrix}$$

Strain tensor
(response of the material)
(symmetric, 3x3)

Notes:

- *Displacement vector* for any point of a material: from where to where did this point move under the effect of applied stress?
- This version is valid for *small deformations* only (infinitesimal strain theory)

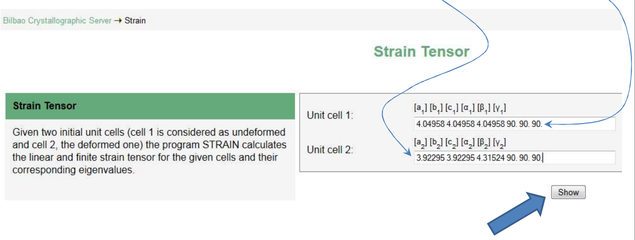
ε_{ij} = how does the j-component of the displacement vector change if you inspect the material along the i-direction?

More info: http://en.wikipedia.org/wiki/Strain_tensor

Use http://www.cryst.ehu.es/cryst/strain.html to determine the strain tensor corresponding to a given deformation.

Example: fcc Al

- take the experimental lattice parameters as the undeformed cell
- apply a volume-conserving elongation along the c-axis



Use http://www.cryst.ehu.es/cryst/strain.html to determine the strain tensor corresponding to a given deformation.

Example: fcc Al

Result:

Linear Lagrangian Strain Tensor (small deformation)

```
[ -0.031270  0.000000 -0.000000 ]
[  0.000000 -0.031270 -0.000000 ]
[ -0.000000 -0.000000  0.065602 ]
```

Eigenvalues

```
-0.03127 -0.03127 0.06560
```

$$\begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{xy} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{xz} & \epsilon_{yz} & \epsilon_{zz} \end{bmatrix}$$

Hooke's law

for three-dimensional anisotropic materials

$$P = C\,\epsilon$$

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ 2\epsilon_{yz} \\ 2\epsilon_{xz} \\ 2\epsilon_{xy} \end{bmatrix}$$

stress tensor (your action) | (36 → 21) elastic constants (material's property) | strain tensor (response of material)

Hooke's law

for three-dimensional anisotropic materials

$$\frac{E}{V} = \frac{1}{2} C \epsilon^2$$

$$\frac{E_{\text{elast}}}{V} = \frac{1}{2} \begin{bmatrix} \epsilon_{xx} & \epsilon_{yy} & \epsilon_{zz} & 2\epsilon_{yz} & 2\epsilon_{xz} & 2\epsilon_{xy} \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ 2\epsilon_{yz} \\ 2\epsilon_{xz} \\ 2\epsilon_{xy} \end{bmatrix}$$

Hooke's law

for materials with cubic symmetry

Depending on the crystal symmetry, these general expressions take on simpler forms. Example for cubic symmetry:

Hooke's law :

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ 2\epsilon_{yz} \\ 2\epsilon_{xz} \\ 2\epsilon_{xy} \end{bmatrix}$$

3 independent elastic constants only

Hooke's law

for materials with cubic symmetry

Depending on the crystal symmetry, these general expressions take on simpler forms. Example for cubic symmetry:

Elastic energy:

$$\frac{E_{\text{elast}}}{V} = \frac{1}{2}\begin{bmatrix} \epsilon_{xx} & \epsilon_{yy} & \epsilon_{zz} & 2\epsilon_{yz} & 2\epsilon_{xz} & 2\epsilon_{xy} \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ 2\epsilon_{yz} \\ 2\epsilon_{xz} \\ 2\epsilon_{xy} \end{bmatrix}$$

$$\frac{E_{\text{elast}}}{V} = \frac{1}{2}C_{11}\left(\epsilon_{xx}^2 + \epsilon_{yy}^2 + \epsilon_{zz}^2\right) + C_{12}\left(\epsilon_{xx}\epsilon_{yy} + \epsilon_{xx}\epsilon_{zz} + \epsilon_{yy}\epsilon_{zz}\right) + 2C_{44}\left(\epsilon_{xy}^2 + \epsilon_{xz}^2 + \epsilon_{yz}^2\right)$$

In a course on continuum mechanics:

- You get the C-tensor for a material, and determine the strain resulting from a given stress
- You get the C-tensor for a material, and determine the stress that explains a given strain
- You get an unknown material, and by applying a known stress and *measuring* the resulting strain, you determine the C-tensor.

In this course:

- You learn how to predict the C-tensor for a given crystalline material from quantum physics, without any experiment.