21_01_25

#2: Stiffness of a crystal: force displacement between neighboring atoms

Length Scales and other crystal geometric parameters.

•Assume a structure for the crystal. The simplest structure would be a cube with atoms placed at the corners.

•The important length scale for this crystal is the lattice parameter, we call is a.

•Now there are simple properties of this crystal that can be measured for calculating the value for a.

For example,

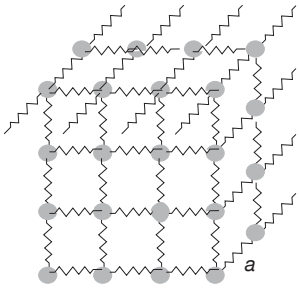
ρ is the density of the crystal in g cm^{-3}.

M_W is the molecular weight of the crystal in g mol^{-1}, where one mole is the Avogadro's number 6.02*10^{23} atoms/mol

Apply the above to the unit cell which is assumed to be a cube with atoms at the corners.

weight of the cube = #atoms per cube x weight per atom

volume of the cube = #atoms per cube x volume occupied per atom



Structure: how many atoms per unit cell: One

Weight of one unit cell= weight of one atom $= \frac{M_W}{N_A}$

$$density = \rho = \frac{\text{wt of a unit cell}}{\text{volume of a unit cell}} = \frac{M_W / N_A}{a^3} = \frac{M_W}{N_A \Omega}$$ (simple cubic structure)

More complex structures,

Body Centered Cubic Cell = atoms per unit cell = two (one from the corners and one from the center)

Face Centered Cubic Cell = atoms per unit cell = four (one-half from each face, and on from the corners)

number of atoms per unit cell n_{cell}

$$density = \rho = \frac{\text{wt of a unit cell}}{\text{volume of a unit cell}} = \frac{M_W n_{cell}}{N_A \Omega}$$ (simple cubic structure)

$$\Omega = \frac{M_W n_{cell}}{N_A \rho}$$

Copper face centered cubic structure
Problem Calculate the lattice parameter for copper.

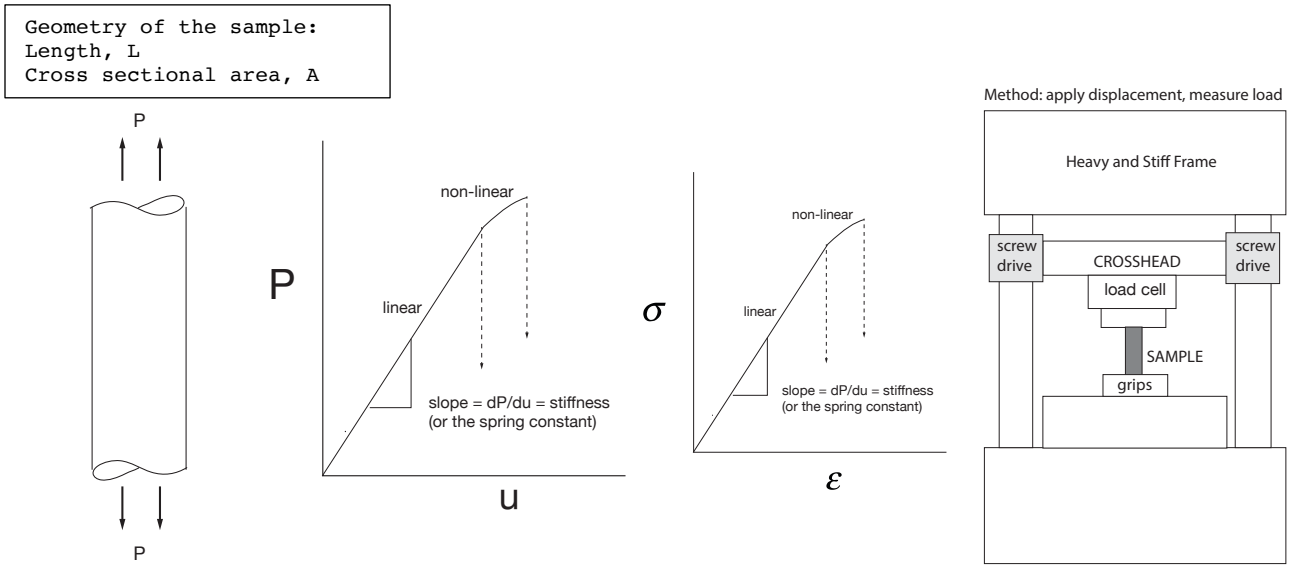
Structure

#atoms per unit cell	4
Density	8.96g/cm^3
At wt	63.55g/mole

N_A 6.02E+23atoms/mol

Omega 4.71E-23cm^3
4.71E-29nm^3

lattice par= 3.61E-10nm
3.61Angstrom



If the cross sectional area is doubled then the load required to achieve the same displacement will double..

$\text{stress} = \sigma = \frac{P}{A}$ units are Nm^{-2} or Pa

If the length of the sample is doubled then the displacement will also be twice as much.

$strain = \varepsilon = \frac{u}{L}$ dimensionless

The slope of the stress/strain curve is the elastic modulus

$E = \frac{d\sigma}{d\varepsilon}$ Young's Modulus units of the Youngs modulus are Pa or GPa

Copper $E = 117$ GPa (Diamond 1000 GPa)

As shown in the data map on the next page, the Young's modulus of polymers is only about 1-10 GPa. Also note that,

•Ceramics have a modulus in the 200 - 700 GPa range

•Metals are generally between 100 and 200 GPa

•Graphite fiber reinforced polymers have a modulus of about 100 GPa (scales with the volume fraction of the fibers - the volume fraction is equal to the area fraction seen in a cross section of the composite.

•In engineering design both E and the density are important; the higher the modulus to density ratio the better. The exact form of this ratio depends on different geometries of the design. For example consider the cylindrical sample above. Here the tensile stiffness to weight would be the figure of merit... this is given by

$$k = \frac{P}{u} = \frac{\sigma A}{\varepsilon L} = E\frac{AL}{L^2} = \frac{E}{\rho L^2}(AL\rho) = \frac{E}{\rho L^2}W$$

$$\frac{k}{W} = \frac{E}{\rho}\frac{1}{L^2}$$

Here W is the weight. Therefore for a given length the stiffness to weight ratio depends on $\frac{E}{\rho}$. Constant values of this parameter are shown by one of the dotted lines. The vertical displacement of these lines gives a higher figure of merit. The materials lying along one line have similar performance. A vertical shift of one order of magnitude will give a factor of ten improvement in performance.

Note the significance of using the logarithmic scale (various ratios of modulus and density can be drawn as straight lines).