Properties of Materials: Elasticity

1. Bonding between atoms.

Primary bonds:

Metallic bond – Nuclei are glued together by a sea of electrons. **Strong/weak** bond; **directional/non-directional**; strong thermal and electrical conductivities (electrons are very mobile); free electrons reflect photons so metals are shiny. Typical materials: Al, Mg, Ag ….

Ionic bond - Two different families of ions (one +ve and one -ve) attract each other and pack in a regular, stable way that allows balancing electrostatic actions. **Strong/weak** bond; **directional/non-directional**. Electrons are confined and ionic solids **do/don't** conduct electricity and are good insulator (in solid state only!). Typical materials: NaCl, SiC.

Covalent bond - Adjacent atoms share one or more electron in common orbitals. Bond is highly **directional/non-directional** and very strong; no conductivity and good isolator. Typical material: diamond.

Secondary bonds: electrons are not shared but bonding is by electrostatic attraction between 2 or more electrically neutral molecules.

Van der Waals – **Strong/weak** bond; **directional/non-directional**. Typical materials: graphite between layers, argon gas.

Hydrogen bonds – **Strong/weak** bond; **directional/non-directional**. Typical materials: water.

2. Different materials have different bonds.

Metals have mainly metallic but also covalent bond: stiff and strong, high melting point, **conductive/non-conductive** materials.

Ceramics have mainly covalent bond: very stiff and very strong, very high melting point, very good insulator.

Polymers (thermoplastic) have within long chains of the macromolecules covalent bonds but among the chains is e.g. Van der Waals bond: low stiffness and strength, very low melting point, **no/good** conductivity.

3. Potential energy and force between two atoms.

U is the interatomic potential energy ; r is the bond length between two atoms. Their relation is shown in the equation below.

Which part of the equation is attractive potential energy and which part is the repulsive potential energy between two atoms?

$$U(r) = -\frac{A}{r^m} + \frac{B}{r^n}, \quad n > m$$

attractive repulsive

Figure 1a is the curve of potential energy vs. bond length. U_0 is bond energy and r_0 is equilibrium bond length. In Figure 1b, mark r_0, F_{max}, attraction force and repulsive force, r_D (dissociation radius).

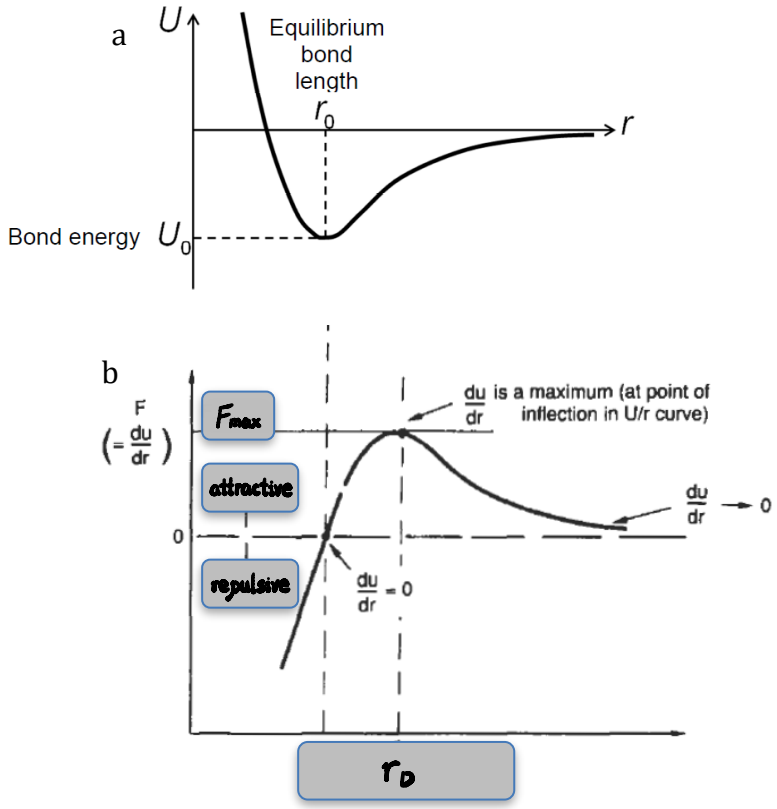


Figure 1 a. Potential energy vs. atom bond length; b. Force vs atom bond length.

4. Understand the physical origin of Young's modulus

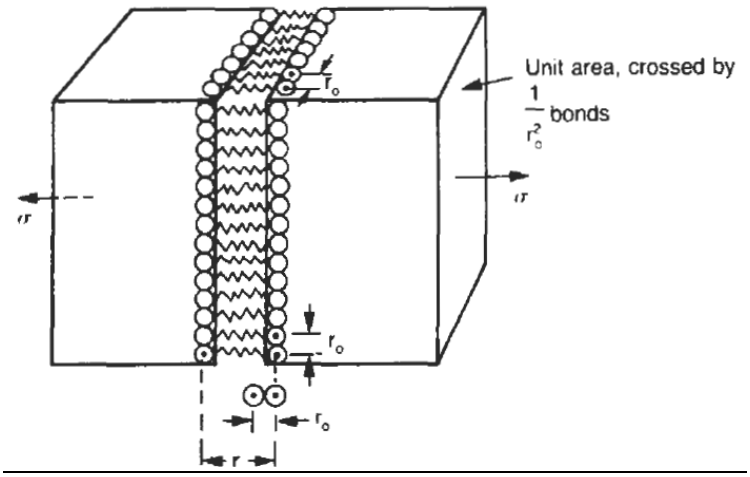


Figure 2 Physical origin of Young's modulus regarding atom bond stiffness

To understand where Young's modulus is physically coming from, the atom bonds come into place. If the atom bonds are stretched, one can image the bonds acting like springs between atoms in the elastic region. Stretch of the bonds gives the elastic strain. Basically the Young's modulus can be calculated by counting the number of bonds (N) per unit area and using the strength (stiffness, S) of the atom bonds as follows:

Hook's law: $\sigma = E\varepsilon$

And looking at Figure 2: $\sigma = NS(r - r_0)$

Bond number per unit area: $N = \frac{1}{r_0^2}$

$$\sigma = \frac{1}{r_0^2} S(r - r_0)$$

$$= \frac{S}{r_0} \frac{r - r_0}{r_0}$$

$$= \frac{S}{r_0} \frac{\Delta r}{r_0}$$

$$= \frac{S}{r_0} \varepsilon = E\varepsilon \qquad \therefore E = \frac{S}{r_0}$$

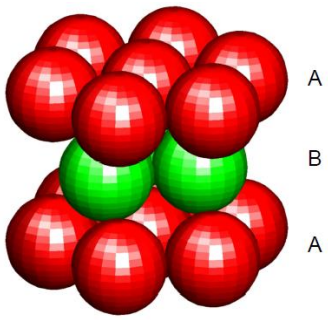
5. Metal atom packing

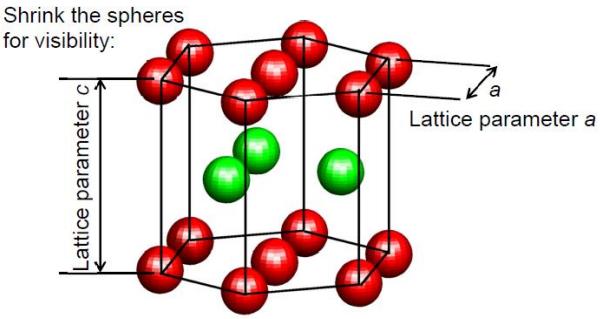
(i)

Closed packed structure (densely packed):

HCP (hexagonal packing): A large HCP crystal can be thought of as numerous repetitions of the hexagonal "unit cell" represented below.

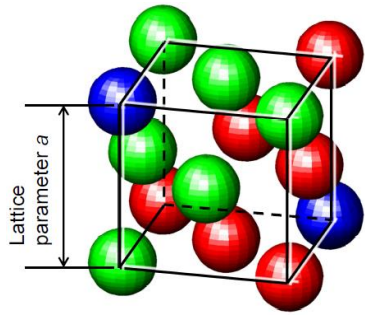
Coordination number 12. Typical material: Mg.

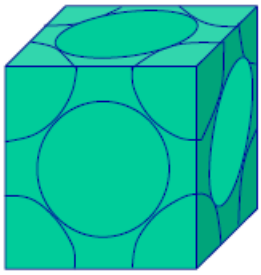




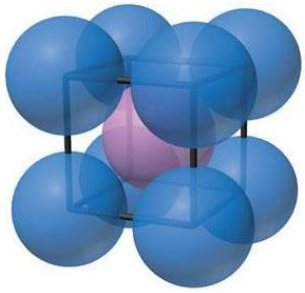
FCC (Face Centered Cubic): Unit cell is a cube of side length *a*, which is also called lattice parameter, with 8 atoms centred in the corners and 6 atoms centred on the 'face-centres'.

Coordination number 12. Typical material: Al, Cu.

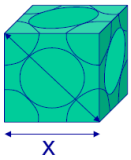




BCC (Body Centered Cubic): Unit cell is a cube of side length *a* (also lattice parameter), with 8 atoms centred in the corners and 1 atoms centred on the 'body-centre'. Coordination number 8.



(ii) Calculate the packing density of FCC.



$V_{cube} = x^3$

$N = \frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$

$r \times (1 + 2 + 1) = 4r = \sqrt{x^2 + x^2} = \sqrt{2}x$

$\therefore r = \frac{\sqrt{2}}{4}x$

$\therefore V = 4 \cdot \frac{4}{3}\pi(\frac{\sqrt{2}}{4}x)^3$

$= \frac{\sqrt{2}}{6}\pi x^3$

$\therefore$ packing density

$= \frac{V}{V_{cube}}$

$= 0.740$