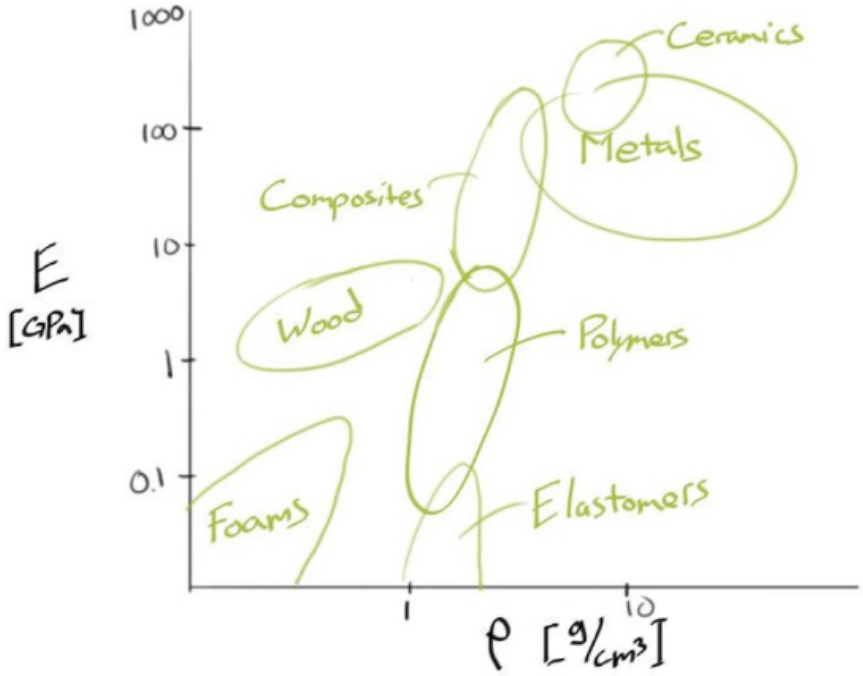
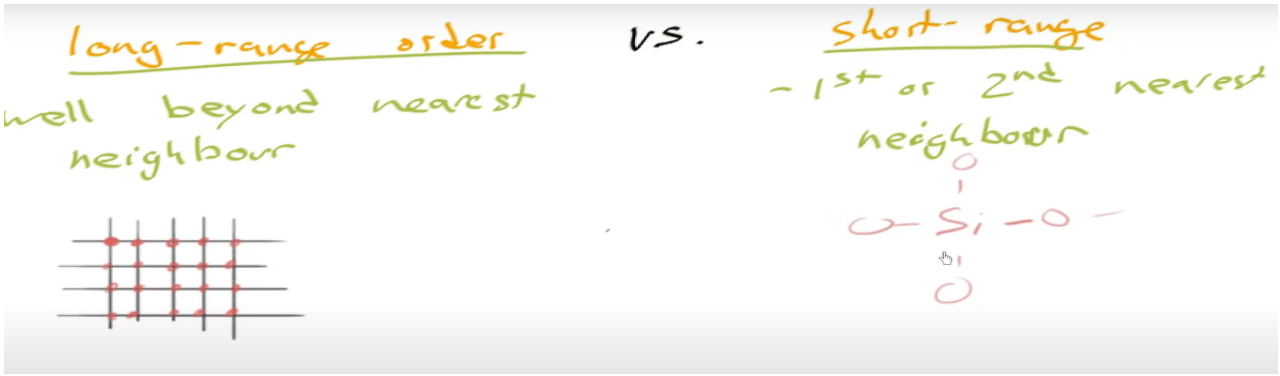
- **<u>Chapter 4: Structure-Property Relationship</u>**

❖ There is generally an increase in density as we move to higher Young's modulus.



❖ ORDERED SOLIDS:
- ➢ Metals are made of crystals (Polycrystalline)
- ➢ Each of these crystals is made of a massive number of atoms all positioned in regular repeating position
- ➢ Spaced roughly at the *atomic scale* = 10^-10 m
- ➢ These crystals that make up polycrystalline materials are called **<u>grains</u>**.
- ➢ Example- galvanized steel lamp posts, street signs, railings
- ➢ **Grain Boundaries-** etching away atoms that exist at the boundaries between grains
- ➢ *Long range order*- **highly ordered** repeating structure that extends <u>well beyond nearest neighbor atoms</u>
- ➢ *Short Range order*- nearest neighbor atoms



❖ SIMPLE CUBIC STRUCTURE:

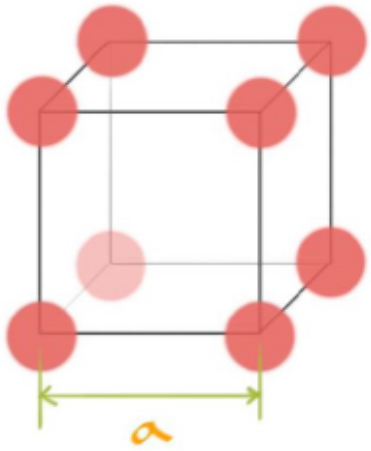


Figure 4: The simple cubic unit cell, showing an atom centred at each of the eight corners of a cube. The lighter red dots are the atoms located on the hidden parts of the cube. The cube edge length is known as the lattice parameter and is denoted with the letter a.

- The cube edge length is known as the *lattice parameter a. Coordination number=8*

❖ FACE-CENTERED CUBIC (FCC):

- Highly Organized Material
- The atoms are centered on each of the six faces of the cube

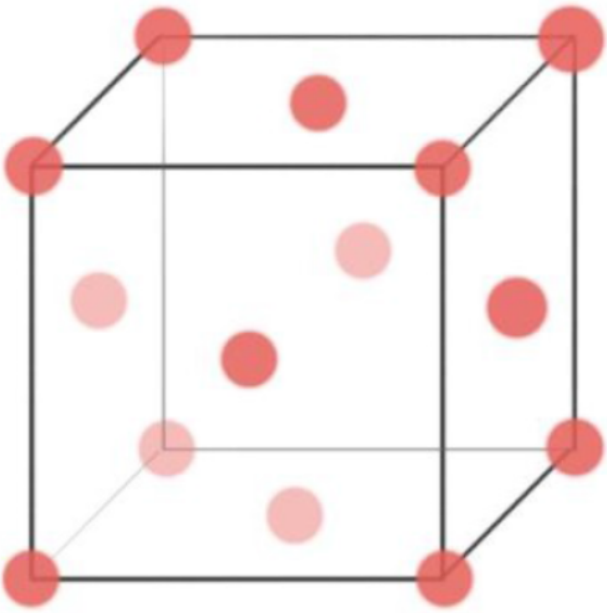
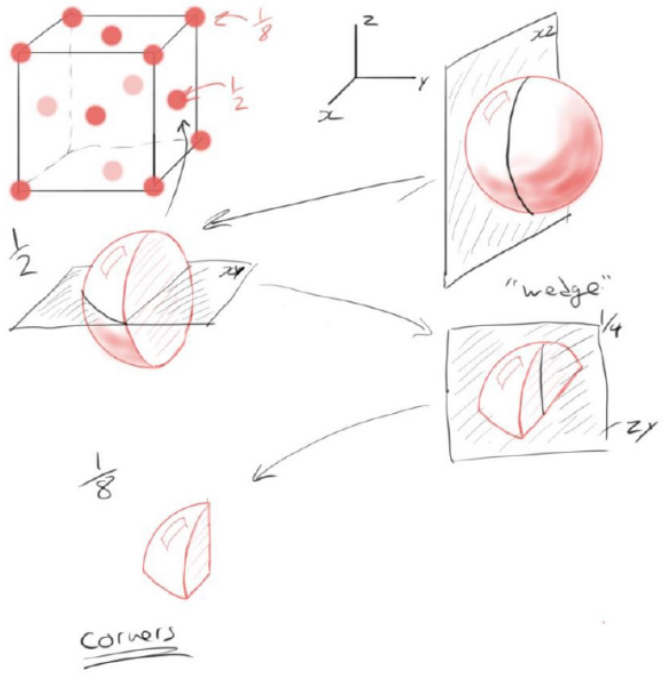


Figure 5: The FCC unit cell, showing an atom centred at each of the eight corners of a cube as well as one atom centred at the very centre of each of the six cube faces. The lighter red dots are the atoms located on the hidden parts of the cube.

FRACTIONAL ATOMS IN FCC:



- The **eight atoms** that result from a sphere being sliced in three orthogonal planes are found in the **eight corners**, while the **half atoms** are located at the face **centered** positions.
  - **Coordination Number= 12**
  - So, 8*⅛ = 1 atom from the corners + 6*½= 3 atoms from the faces
  - **4 atoms in the FCC unit cell**

    nFCC = 4
  - **a = 2√2 R**
  - **Volume =a^3**

PROOF:

$$a^2 + a^2 = (4R)^2$$
$$2a^2 = 16R^2$$

$$a_{FCC} = 2\sqrt{2}R$$

- ❖ DENSITY OF CRYSTALLINE SOLID:

- Density = Mass/ Volume
- MASS:

$$\text{Mass}_{\text{AtomsinUnitCell}} = \text{Number}_{\text{Atoms in Unit Cell}} \cdot \frac{\text{Molar Mass of Atom}}{\text{Avagadro's Number}}$$

or

$$m = n \cdot \frac{A}{N_A}$$

- So, Density (Divide by volume of unit cell):

$$\rho = \frac{nA}{V_C N_A}$$

- N_A= 6.02*10^23
- Vc for FCC is calculated as (**2**√**2 R)**^{3}

❖ **ATOMIC PACKING FACTOR FCC:**

This is a measure of the fraction of a volume that is occupied by atoms arranged in a particular crystal structure

$$\text{APF} = \frac{\text{Volume}_{\text{Spheres}}}{\text{Volume}_{\text{Unit Cell}}} \quad (5)$$

or, since the unit cell is a cube whose volume is a^3

$$\text{APF} = \frac{n\frac{4}{3}\pi R^3}{a^3} \quad (6)$$

and, specifically for FCC

$$\text{APF} = \frac{4\frac{4}{3}\pi R^3}{a^3} \quad (7)$$

$$APF = \frac{4\frac{4}{3}\pi R^3}{\left(2\sqrt{2}R\right)^3}$$

$$\text{APF}_{\text{FCC}} = 0.74$$