Tutorial Class 1 – Week 2

Aims:

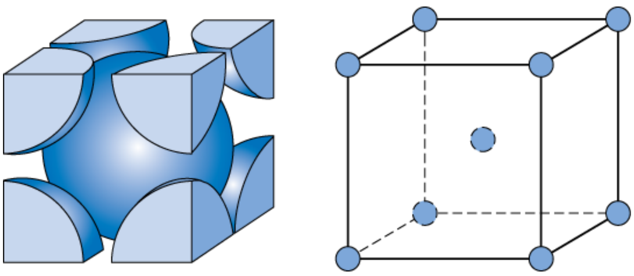
Upon successfully completing these tutorial exercises, students should be able to:

- Demonstrate and understanding of material structures
- Perform calculations to determine thermal properties of materials
- Solve problems related to imperfections in solids

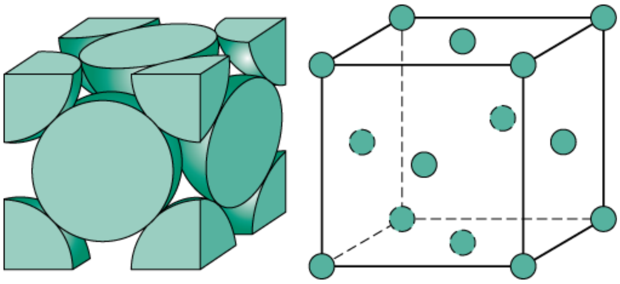
Exercise 1.1 Shown below are sketches of Body Centered Cubic (BCC) and Face-Centered Cubic (FCC) crystal structure.

i. How many atoms in a) BCC and b) FCC.

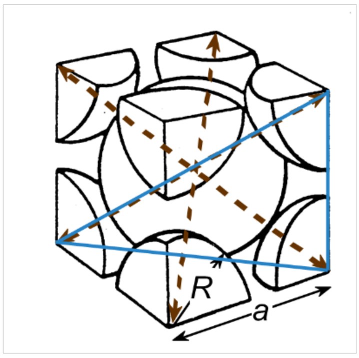
ii. Calculate the atomic Packing Factor (APF)

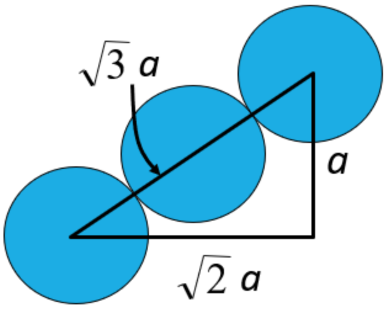


(a) **BCC structure**



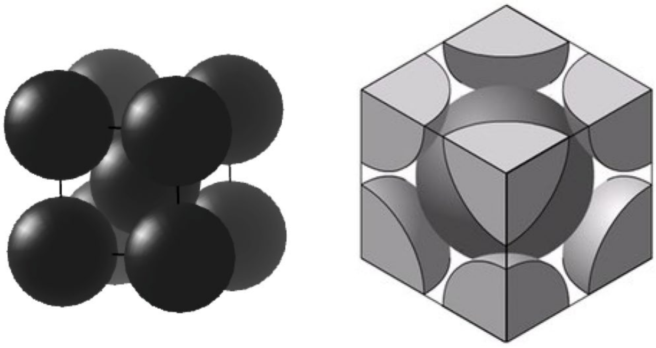
(b) **FCC structure**





Note: BCC was covered during lecture, but repeat calculation by yourself to test understanding.

Exercise 1.2 Iron has a BCC crystal structure, as shown in the figure below.



a) Given that the atomic radius of an iron atom is r (Fe) = 0.126 nm, calculate the lattice constant **a** for the iron unit cell.

b) Given the atomic mass of iron is ma (Fe) = 55.85 g/mol, calculate the theoretical density of iron. (Hint: Consider first the mass per atom and then the number of atoms in a unit cell).

c) Comment on why the calculated density may differ from the published value of 7850 kg/m^3 for plain carbon steel.

Note: Use your answer in Q1.1

Exercise 1.3 Imperfections in solids

Given:

$$N_v = N_s \exp\left(-Q_v / k_B T\right)$$ Refer to lecture notes

Boltzmann's constant k_B= 8.62x10^{-5} eV/K = 1.38x 10^{-23} J/atom-K

Calculate

a. The equilibrium number of vacancies per cubic meter in pure magnesium at 450 ^{o}C. Assume that the energy of formation of a vacancy in pure magnesium is 0.89eV/atom.
b. What is the vacancy fraction $\left(\frac{N_v}{N_s}\right)$ at 600 ^{o}C ?

Atomic weight of Mg = 24.31 g.mol^{-1}; Density of Magnesium = 1.74 g.cm^{-3}