Crystal Structure

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Unit Cell

The smallest unit of crystal structure which completely defined the behaviour of a crystal.

Number of atoms per unit cell

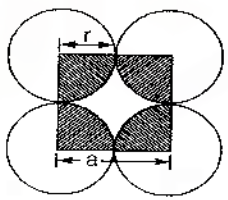
$$n = \frac{\rho a^3 N_A}{M}$$

where, a = Edge of unit cell
M = Atomic weight of element
ρ = Density of metal
N_A = Avogadro's number = 6.023×10^{23}

Note:

- Unit cell is cubic in shape.
- Unit cell is repeated to form a crystal. So most important characteristic of crystal is periodicity of unit cell inside the crystal.

Simple Cubic (SC)



- Distance between adjacent atom

$$d_{sc} = 2r = a$$

where, r = Radius of an atom
a = Edge length of cube

- Effective number of atom in a unit cell

$$Z_{sc} = 8 \times \frac{1}{8} = 1$$

- Atomic packing fraction

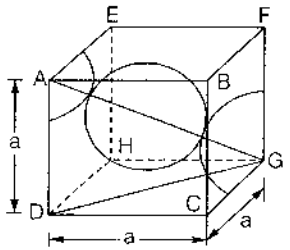
$$APF = \frac{\text{Volume occupied atoms}}{\text{Volume of the cell}}$$

$$APF_{SC} = \frac{\pi}{6} = 0.523$$

Example: Polonium

- Coordination number of simple cubic is 6.

Body Centered Cubic (BCC)



- The distance between adjacent atom

$$d_{BCC} = 2r = \frac{\sqrt{3}}{2}a$$

- Effective number of atom in unit cell

$$Z_{BCC} = 8 \times \frac{1}{8} + 1 = 2$$

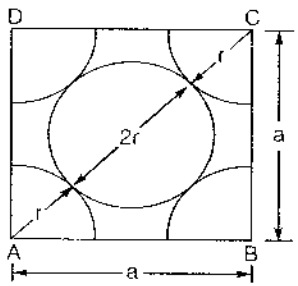
- Atomic packing fraction

$$APF_{BCC} = \frac{\sqrt{3}}{8}\pi = 0.68$$

Example: Cr, Li, Na, K, Fe

- The coordination number of body centered cubic is 8.

Face Centered Cubic (FCC)



- The distance between adjacent atom

$$d_{FCC} = 2r = \frac{a}{\sqrt{2}}$$

- Effective number of atom in a unit cell

$$Z_{FCC} = 4$$

- Atomic packing fraction

$$APF_{FCC} = \frac{\pi}{3\sqrt{2}} = 0.7404$$

Example: Fe, Al, Cu, Au, Ca, Pb

- The coordination number of face centered cubic is 12.

Miller Index

$$MI = \frac{\text{Cell edge length}}{\text{Intercept by plane}}$$

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