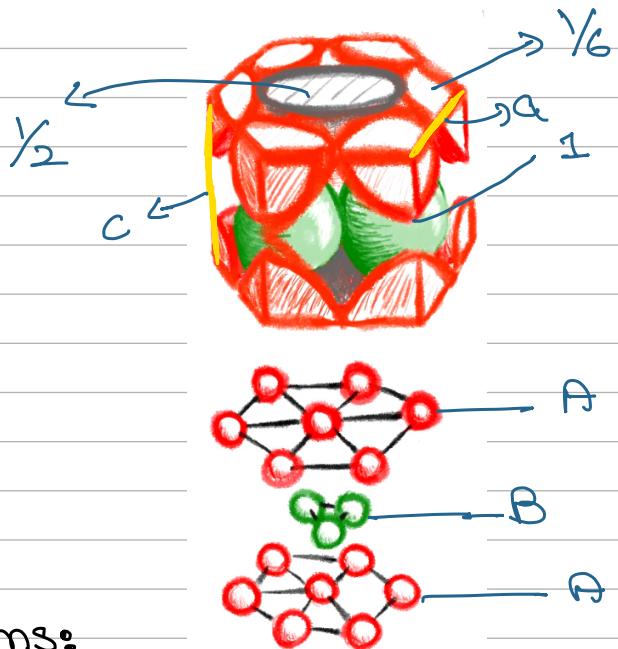


HCP:

12 corner atoms
2 middle atoms
3 centre atoms } contribution of each atom

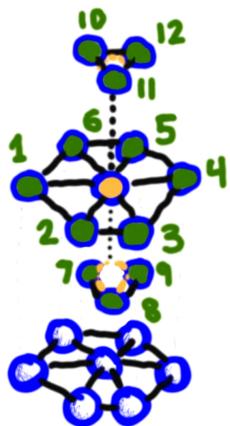


Equivalent atoms:

$$\frac{1}{6} \times 12 + \frac{1}{2} \times 2 + 3 = 6 \text{ atoms}$$

$$\frac{C}{a} = 1.633 \quad \text{— Determined experimentally}$$

Coordination number = 12



Atomic Packing factors:

Atomic packing factor = $\frac{\text{Volume of atom in unit cell} (V_s)}{\text{Total volume of unit cell} (V_c)}$

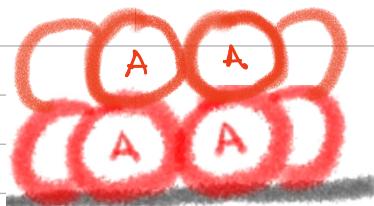
↓
Tells how packed / filled a structure is

$\uparrow \text{APF} \propto \text{Density} \uparrow$

Simple cubic:

$$V_s = \frac{4}{3}\pi R^3$$

$$\begin{aligned} V_c &= a^3 \\ &= (2R)^3 \\ &= 8R^3 \end{aligned}$$



$$\text{APF} = \frac{\frac{4}{3}\pi R^3}{8R^3}$$

Vacant space: 48%

= 0.52 → quite empty

Body centered cubic (BCC):

$$V_c = a^3$$

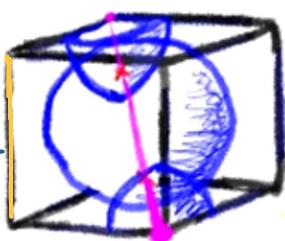
$$4R = \sqrt{3}a$$

$$a = \frac{4R}{\sqrt{3}}$$

$$V_c = \left(\frac{4R}{\sqrt{3}}\right)^3$$

a ←

$$\begin{aligned} V_s &= 2 \times \frac{4}{3}\pi R^3 \\ &= \frac{8}{3}\pi R^3 \end{aligned}$$



$$APF = \frac{\frac{8}{3}\pi R^3}{\left(\frac{4R}{\sqrt{3}}\right)^3}$$

Vacant space: 32%

$$= 0.68$$

Face centered cubic (FCC):

$$V_c = a^3$$

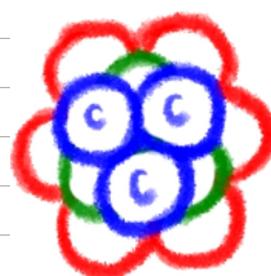
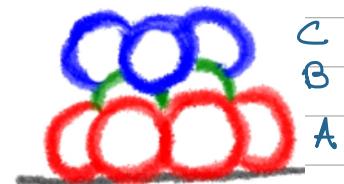
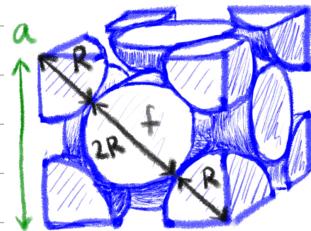
$$V_s = 4 \times \frac{4}{3}\pi R^3$$

$$4R = \sqrt{2} a$$

$$a = \frac{4R}{\sqrt{2}}$$

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

$$= \frac{16}{3}\pi R^3$$



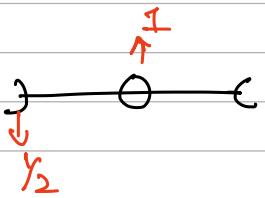
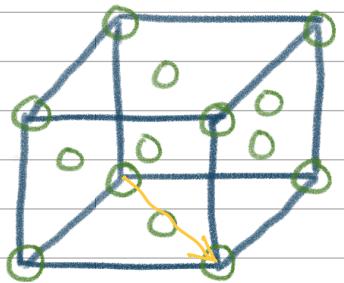
$$APF = \frac{\frac{16}{3}\pi R^3}{\left(\frac{4R}{\sqrt{2}}\right)^3}$$

$$= 0.74$$

Vacant space: 26%

Linear density: [110]

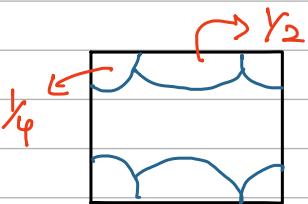
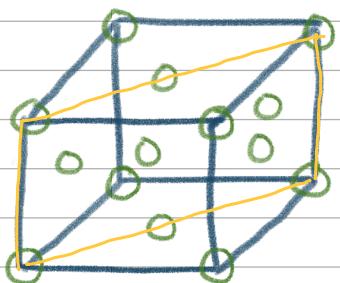
$$LD = \frac{\text{atom centered on direction vector}}{\text{Length of direction vector}}$$



$$LD = \frac{\frac{1}{2} + 1 + \frac{1}{2}}{4R} = \frac{2}{4R}$$

Planar density:

PD: Number of atoms in plane
Area of plane



$$PD = \frac{\frac{1}{4} + \frac{1}{4} + \frac{1}{4} + \frac{1}{4} + \frac{1}{2} + \frac{1}{2}}{8R^2\sqrt{2}}$$

$$= \frac{2}{8R^2\sqrt{2}} \rightarrow \left(\frac{4R}{\sqrt{2}}\right)^2 \times \sqrt{2}$$

$$\text{Area} = \sqrt{2} a^2$$

$$\frac{16R^2}{2} \times \sqrt{2}$$

$$8R^2\sqrt{2}$$

Theoretical density:

No of atoms/unit cell

$$\frac{A}{VcN_A} \rightarrow \text{Avagadro's No}$$

↑
A → Atomic No
Volume of unit cell

Impurities:

- When molten metals & alloys solidify, the resulting solid is imperfect in many ways.

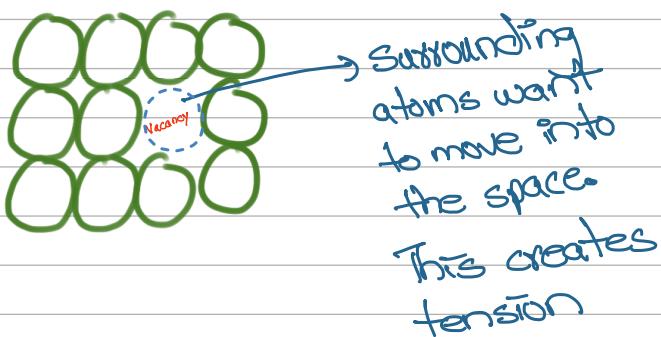
Types of defects in crystals:

- 1) Point defects 0D
- 2) Line defects 1D
- 3) Surface defect 2D
- 4) Volume defect 3D

Point Defects:

1) Vacancy:

When an atom is missing from its original lattice site

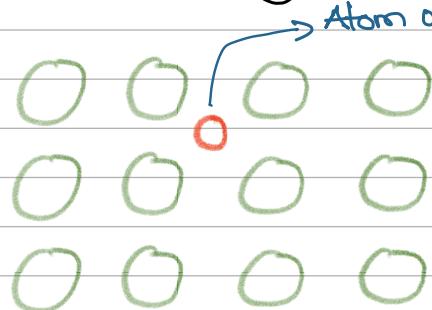


- Temp > Ok, then vacancy is possible

- Can occur in any crystalline solid
- Temp \propto number of vacancy Increases exponentially

2) Interstitial defect:

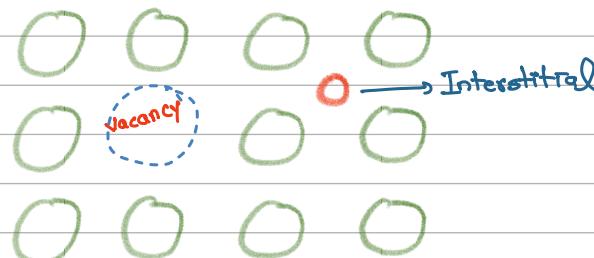
- Atom takes the interstitial position of lattice structure.
- This interstitial atom may be of same crystal or foreign



- If the atom is of the crystal, then it is called self-interstitial defect.
- Carbon occupies interstitial position from iron to steel.

3) Frenkel Defect:

- Combination of both vacancy & interstitial defect.



Criteria for formation of good substitution solution:

- 1) Atomic size close ($Cu/Ni: 128/125 \text{ pm}$)

- 2) Crystal structure same ($\text{Cu}/\text{Ni} : \text{FCC}/\text{FCC}$)
- 3) Electro-negativity close ($\text{Cu}/\text{Ni} : 1.9/1.8$)
- 4) Valency same ($\text{Cu}/\text{Ni} : +2/+1 \text{ or } +2$)

Interstitial solution:

- A type of solid where smaller atoms or molecules occupy the spaces in a crystal structure.

Eg: $\text{Fe}(0.124\text{nm}) + \text{C}(0.071\text{nm})$

- metals can be purified to 99.9999%.

Composition of solid solutions:

$$\text{wt\% } C_1 = \frac{m_1}{m_1 + m_2} \times 100$$

$$\text{At\% } \bar{C}_1 = \frac{n_m 1}{n_{m1} + n_{m2}} \times 100$$

$$C_1 = \frac{m_1}{M} \times 100$$

$$m_1 = \frac{C_1 M}{100}$$

$$\bar{C}_1 = \frac{m_1}{A_1}$$

$$\frac{m_1 + m_2}{A_1 + A_2}$$

$$= \frac{C_1 M}{100 A_1}$$

$$= \frac{\frac{C_1 M}{100} + \frac{C_2 M}{100}}{\frac{100 A_1}{100} + \frac{100 A_2}{100}}$$

$$= \frac{C_1 A_2}{C_1 A_2 + C_2 A_1}$$

$$\text{At\% } \leftarrow \bar{C} = \frac{C_x A_y}{C_x A_y + C_y A_x}$$

↑ atomic no
from wt%

$$C = \frac{\bar{C}_x A_x}{\bar{C}_x A_y + \bar{C}_y A_x}$$

↑ atomic no
↓ wt%
from At%

Point Defects:

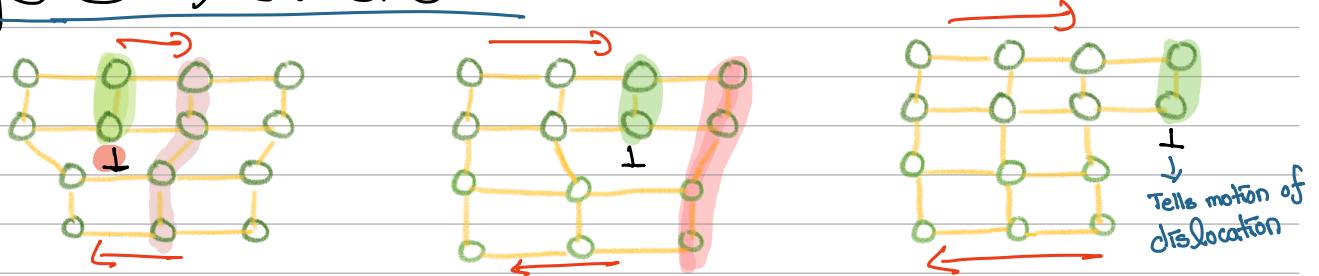
$$\frac{N_v}{N} = e^{\left(-\frac{Q_v}{kT} \right)}$$

$$N_v = N \times e^{\left(-\frac{Q_v}{kT} \right)}$$

$$P = \frac{NA}{N_A}$$

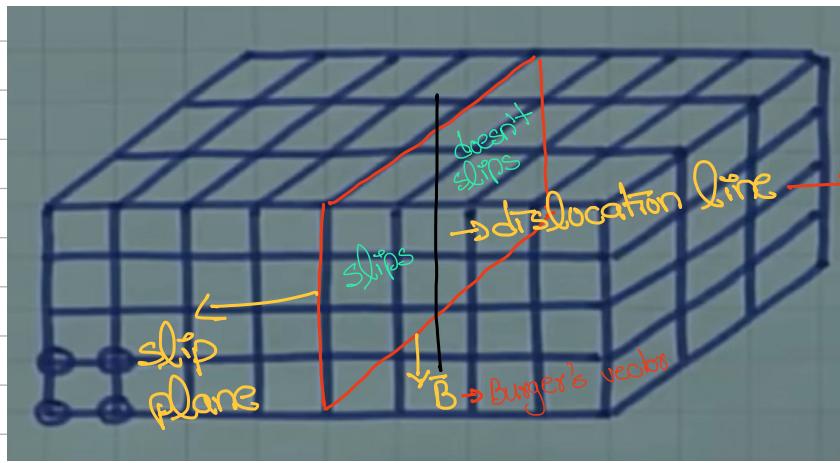
$$N = \frac{PN_A}{A}$$

Edge dislocations:



- Burgers vector is \perp to dislocation line

Screw dislocation:



Left half slips w.r.t Right half

- Burgers vector is \parallel to dislocation

\hookrightarrow Tells magnitude & direction of slip



Screw dislocation connected the planes in a spiral ram/helicooidal surface.

Mixed dislocation:

- Combination of edge & screw dislocation.

Facts of dislocations:

- A highly deformed metal will have miles of dislocation line.
- Ease of motion of dislocation line shows ductile material.
- Cold working creates dislocations & this strengthens metal because dislocation line blocks other dislocation motion.
- Second phase precipitate also block dislocation & strengthens crystal.
- Foreign atoms also block dislocation

Interfacial dislocations:

1) Twinning:

- Slipping happens such that both halves become mirror images.

2) Grain boundary

3) Stacking fault: A B A A B B

B is missing

4) External surface of the crystal

5) Phase boundary