# UNIT – I CRYSTALLOGRAPHY AND ENGINEERING MATERIALS

## PART – A QUESTIONS

**1.What is a crystal? Give some examples.**

Regular arrangement of atoms in 3-dimensional space is called crystalline materials (or) crystal. Examples: Diamond, Gold, NaCl, Copper.

**2.What is amorphous solid? Give some examples.**

Irregular arrangement of atoms in 3-dimensional space is called amorphous solid. Examples: Plastics, Rubber, Glass.

**3.What are single and poly crystals?**

The entire solid material which has only one crystal is called single crystal.

A collection of many small crystals separated by well defined boundaries is called poly crystal.

**4.What is lattice?**

Lattice is defined as an array (group) of points to represent the position of atoms in the crystal. It is an imaginary concept.

**5.What is space lattice?**

A three dimensional collection of points in space is called space lattice. It is also called as crystal lattice.

**6.What are lattice planes?**

A set of parallel and equally spaced planes in a space lattice are called lattice planes. They are formed with respect to the lattice points.

**7.Define unit cell.**

Unit cell is defined as the smallest geometrical figure which is repeated to derive the actual crystal structure.

**8.Define packing factor (or) packing density (or) density of packing. Give its unit.**

It is defined as the ratio of the volume of atoms per unit cell to the total volume occupied by the unit cell.

$$APF = \frac{Number\ of\ atoms\ per\ unit\ cell \times Volume\ of\ one\ atom}{Volume\ of\ unit\ cell}$$

Since Atomic Packing factor is the ratio, it does not have any unit.

**9. Name the seven types of crystal systems (or) crystal structures.**

(i) Cubic
(ii) Tetragonal
(iii) Orthorhombic
(iv) Monoclinic
(v) Triclinic
(vi) Rhombohedral (Trigonal)
(vii) Hexagonal

**10. What are Bravais lattices?**

There are 14 possible ways of arranging points in space lattice from the seven crystal systems. All the lattice points have the same surroundings. These 14 space lattices are called the Bravais lattices.

**11. A unit cell has the dimensions a = b = c = 4.74 Å and $\alpha \neq \beta \neq \gamma \neq 60^0$, what is the crystal structure?**

For a = b = c = 4.74 Å and $\alpha \neq \beta \neq \gamma \neq 60^0$, the crystal structure is Trigonal (or) Rhombohedral.

**12. What is meant by primitive and Non-primitive Cell? Give an example.**

A primitive cell is the simplest type of unit cell which contains only one lattice point per unit cell. Example : Simple Cubic (SC).

If there are more than one lattice points in an unit cell, it is called Non-Primitive cell. Example: BCC & FCC.

**13. What is meant by loosely packed structure? Give an example.**

The loosely packed structure has the packing factor less than 0.74, i.e. in which more vacant site is available. Example: Simple cubic polonium & body centered sodium.

**14. What is meant by closely packed structure? Give an example.**

Closely packed structure has the highest packing factor of 0.74. Here the atoms are closely packed leaving a small space as vacant site in the crystal. Example: Face centered cubic copper & hexagonal closely packed magnesium.

**15. Write the parameters for Triclinic crystal.**

Axial lengths are $a \neq b \neq c$

Interfacial angles are $\alpha \neq \beta \neq \gamma \neq 90^0$.

**16. What are Miller Indices?**

Miller Indices are the reciprocal of the intercepts made by the plane on the three axes which are reduced to the smallest numbers. It is denoted as $(h\ \ k\ \ l)$.

**17. List out the procedure for finding Miller Indices.**

(i) Find the intercepts made by the plane along the three axes X, Y & Z.
(ii) Find the coefficients of the intercepts.
(iii) Find the reciprocal of the coefficients.
(iv) Convert these reciprocals into whole numbers by multiplying each with their LCM to get the smallest numbers.
(v) Enclose these numbers in a bracket like this (      ).

**18. A crystal plane cuts at 3*a*, 4*b* and 2*c* distances along the crystallographic axes. Find the Miller Indices of the plane.**

Given data : Intercepts = $3a : 4b : 2c$

Step (i) : Co-efficients of intercepts = 3: 4: 2

Step (ii) : Reciprocal of intercepts $= \frac{1}{3} : \frac{1}{4} : \frac{1}{2}$

Step (iii) : LCM = 12

Step (iv) : Multiplying by LCM with the reciprocals

$$12 \times \frac{1}{3} \quad : \quad 12 \times \frac{1}{4} \quad : \quad 12 \times \frac{1}{2}$$

We have 4 3 6

**Miller Indices = (4 3 6)**

**19. Calculate the value of d-spacing for (100) plane in a rock salt crystal of *a* = 2.814 Å.**

Given: $a = 2.814$ Å
$h = 1$
$k = 0$
$l = 0$

$$d - spacing\ (or)\ d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$d - spacing\ (or)\ d_{100} = \frac{2.814 \times 10^{-10}}{\sqrt{1^2 + 0^2 + 0^2}}$$

$$d = 2.814 \text{ Å}$$

## PART – B QUESTIONS

**1.Write the standard crystal systems corresponding to with their lattice parameters. What are Bravais lattices? How are they grouped into seven crystal systems?**

Seven crystal systems

1. Cubic
2. Tetragonal
3. Orthorhombic
4. Monoclinic
5. Triclinic
6. Rhombohedral (Trogonal)
7. Hexagonal

Bravais lattices

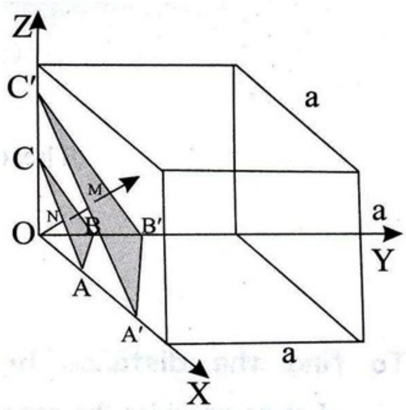
There are 14 possible ways of arranging points in space lattice from the 7 crystal system. All the lattice points have the same surroundings. These 14 space lattices are called as Bravais Lattices.

| S.No. | Crystal Systems | Intercepts (a, b, c) | Interfacial angles (α, β, γ) | Bravais Lattices | No. of lattices |
|---|---|---|---|---|---|
| 1. | Cubic | $a = b = c$ | $\alpha = \beta = \gamma = 90^o$ | Simple, Body centered & Face centered | 3 |
| 2. | Tetragonal | $a = b \neq c$ | $\alpha = \beta = \gamma = 90^o$ | Simple & Body centered | 2 |
| 3. | Orthorhombic | $a \neq b \neq c$ | $\alpha = \beta = \gamma = 90^o$ | Simple, Base centered, Body centered & Face centered | 4 |
| 4. | Monoclinic | $a \neq b \neq c$ | $\alpha = \beta = 90^o$, $\gamma \neq 90^o$ | Simple & Base centered | 2 |
| 5. | Triclinic | $a \neq b \neq c$ | $\alpha \neq \beta \neq \gamma \neq 90^o$ | Simple | 1 |
| 6. | Rhombohedral (Trigonal) | $a = b = c$ | $\alpha = \beta = \gamma \neq 90^o$ | Simple | 1 |
| 7. | Hexagoanal | $a = b \neq c$ | $\alpha = \beta = 90^o$, $\gamma \neq 120^o$ | Simple | 1 |
| Total | | | | | 14 |

**2.What is inter-planar spacing? Derive an expression for inter-planar spacing in terms of Miller Indices.**

**$d$-Spacing – Definition**

$d$-spacing or interplanar spacing is the distance between any two successive planes.



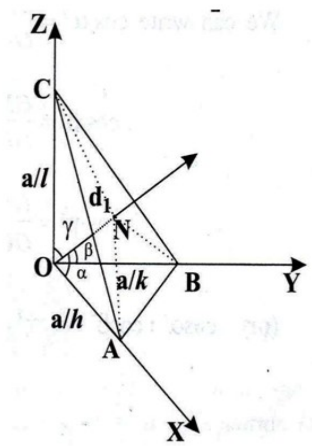

**Derivation**

- Consider a cubic lattice.
- $ABC$ & $A'B'C'$ are the two successive planes
- $O$ – Origin
- $(hkl)$ – Miller Indices of the planes
- Draw a perpendicular from $O$ to Plane $ABC$. It meets at $N$.

  $ON = d_1$
- Draw a perpendicular from $O$ to plane $A'B'C'$. It meets at $M$.

  $OM = d_2$
- Interplanar distance $d = d_2 - d_1$

**To calculate $d_1$**




$$OA = \frac{a}{h}$$

$$OB = \frac{a}{k}$$

$$OC = \frac{a}{l}$$

$$\angle ONA = \alpha, \qquad \angle ONB = \beta, \qquad \angle ONC = \gamma$$

$$\Delta ONA, \quad Cos\,\alpha = \frac{ON}{OA} = \frac{d_1}{a/h} \Rightarrow \frac{d_1 h}{a} \qquad ------(1)$$

$$\Delta ONB, \quad Cos\,\beta = \frac{ON}{OB} = \frac{d_1}{a/k} \Rightarrow \frac{d_1 k}{a} \qquad ------(2)$$

$$\Delta ONC, \quad Cos\,\gamma = \frac{ON}{OC} = \frac{d_1}{a/l} \Rightarrow \frac{d_1 l}{a} \qquad ------(3)$$

According to Cosine Rule,

$$Cos^2\alpha + Cos^2\beta + Cos^2\gamma = 1 \qquad ------(4)$$

Sub. (1), (2) & (3) in (4)

$$\left(\frac{d_1 h}{a}\right)^2 + \left(\frac{d_1 k}{a}\right)^2 + \left(\frac{d_1 l}{a}\right)^2 = 1$$

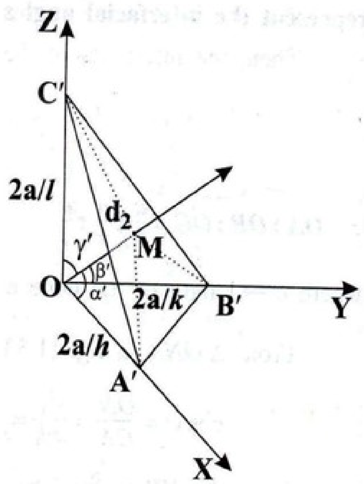
$$\left(\frac{d_1}{a}\right)^2 \left[h^2 + k^2 + l^2\right] = 1$$

$$\left(\frac{d_1}{a}\right)^2 = \frac{1}{h^2 + k^2 + l^2}$$

$$\frac{d_1}{a} = \frac{1}{\sqrt{h^2 + k^2 + l^2}}$$

$$\boxed{d_1 = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \qquad ------(5)}$$

**To calculate $d_2$**




$$OA' = \frac{2a}{h}$$

$$OB' = \frac{2a}{k}$$

$$OC' = \frac{2a}{l}$$

$$\angle OMA' = \alpha', \qquad \angle OMB' = \beta', \qquad \angle OMC' = \gamma'$$

$$\Delta OMA', \quad Cos\,\alpha' = \frac{OM}{OA'} = \frac{d_2}{2a/h} \Rightarrow \frac{d_2 h}{2a} \qquad ------(6)$$

$$\Delta OMB', \quad Cos\,\beta' = \frac{OM}{OB'} = \frac{d_2}{2a/k} \Rightarrow \frac{d_2 k}{2a} \qquad ------(7)$$

$$\Delta OMC', \quad Cos\,\gamma' = \frac{OM}{OC'} = \frac{d_2}{2a/l} \Rightarrow \frac{d_2 l}{2a} \qquad ------(8)$$

$$Cos^2\alpha' + Cos^2\beta' + Cos^2\gamma' = 1 \qquad ------(9)$$

Sub. (6), (7) & (8) in (9)

$$\left(\frac{d_2 h}{2a}\right)^2 + \left(\frac{d_2 k}{2a}\right)^2 + \left(\frac{d_2 l}{2a}\right)^2 = 1$$

$$\left(\frac{d_2}{2a}\right)^2 \left[h^2 + k^2 + l^2\right] = 1$$

$$\left(\frac{d_2}{2a}\right)^2 = \frac{1}{h^2 + k^2 + l^2}$$

$$\frac{d_2}{2a} = \frac{1}{\sqrt{h^2 + k^2 + l^2}}$$

$$\boxed{d_2 = \frac{2a}{\sqrt{h^2 + k^2 + l^2}} \qquad ------(10)}$$

**Interplanar distance** $d = d_2 - d_1$

(10) – (5)
$$d = \frac{2a}{\sqrt{h^2 + k^2 + l^2}} - \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

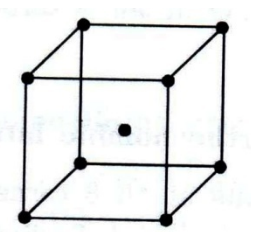
$$\boxed{d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \qquad ------(11)}$$

(11) is the expression for interplanar spacing.

3. **Describe the arrangement of atoms in BCC and FCC structures and also determine the atomic radius, coordination number and packing factor for the same structures.**

BODY CENTERED CUBIC (BCC) STRUCTURE

Arrangement of atoms

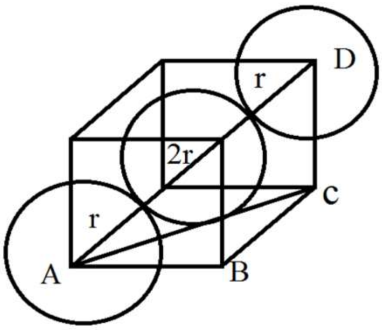


In BCC, each unit cell has the atoms in all the corners and one individual atom at the centre of the unit cell.

Atomic radius

The half of the distance between two nearest neighbouring atoms in a crystal is known as atomic radius.

Here the corner atoms do not touch each other.



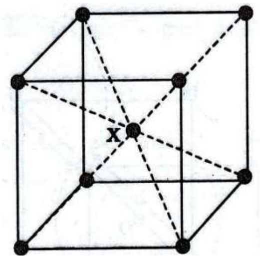

But each corner atom touches the body centered atom.

Consider the Δ ACD

$$(AD)^2 = (AC)^2 + (CD)^2$$
$$(AD)^2 = (AB)^2 + (BC)^2 + (CD)^2$$
$$(4r)^2 = a^2 + a^2 + a^2$$
$$(4r)^2 = 3a^2$$
$$4r = \sqrt{3}\ a$$
$$4r = \sqrt{3}\ a$$
$$\boxed{r = \frac{\sqrt{3}}{4}\ a}$$

Coordination number

It is defined as the number nearest neighbouring atoms to a particular atom.




Here body centered atom is the reference atom.

All the corner atoms are very near to the body centered atom.

$$\boxed{Co-ordination\ number = 8}$$

Packing factor for BCC

$$APF = \frac{No.of\ atoms\ per\ unit\ cell \times Volume\ of\ one\ atom}{Volume\ of\ the\ unit\ cell}$$

Number of atoms per unit cell = 2

$$APF = \frac{2 \times \frac{4}{3}\pi r^3}{a^3}$$

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

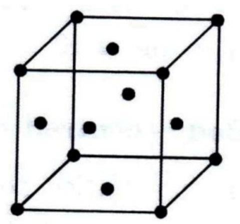
$$APF = \frac{\frac{\cancel{8}^{2}}{\cancel{3}}\pi \frac{\cancel{\sqrt{3}\times\sqrt{3}}\times\sqrt{3}}{\cancel{4}\times\cancel{4}_{2}\times 4}\cancel{a^3}}{\cancel{a^3}}$$

$$\boxed{APF = \frac{\sqrt{3}}{8}\pi = 0.68}$$

68 % is occupied by the atoms and 32 % is vacant (or) void space. So BCC is a tightly (or) closely packed structure compared with SC.

## FACE CENTRED CUBIC (FCC) STRUCTURE

### Arrangement of atoms



In FCC, each unit cell has the atoms at all the corners and all the faces.

### Atomic radius

The half of the distance between two nearest neighbouring atoms in a crystal is known as atomic radius.

Here the corner atoms do not touch each other.

But each corner atom touches the face centered atom

Consider the Δ ABC

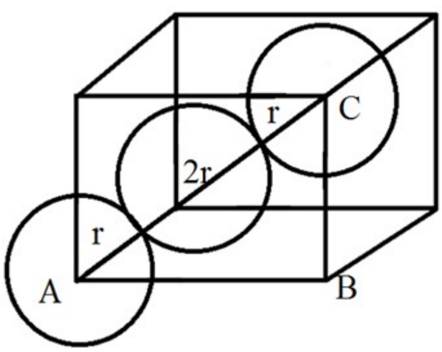
$(AC)^2 = (AB)^2 + (BC)^2$

$(4r)^2 = a^2 + a^2$

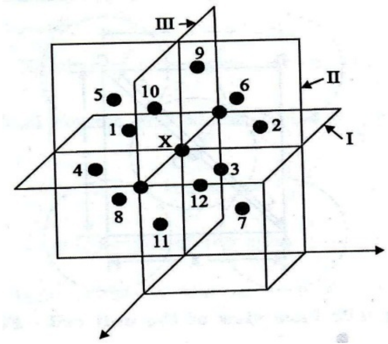
$(4r)^2 = 2a^2$

$4r = \sqrt{2}\,a$

$$\boxed{r = \frac{\sqrt{2}}{4}a}$$




### Coordination number




It is defined as the number nearest neighbouring atoms to a particular atom.
For any corner atom, the nearest atom is face centered atom.
There are 4 face centered atoms in its plane
4 atoms above its plane &
4 atoms below its plane.

$$\boxed{Co-ordination\ number = 4+4+4 = 12}$$

Atomic packing factor for FCC

$$APF = \frac{No.of\ atoms\ per\ unit\ cell \times Volume\ of\ one\ atom}{Volume\ of\ the\ unit\ cell}$$

Number of atoms per unit cell = 4

$$APF = \frac{4 \times \frac{4}{3}\pi r^3}{a^3}$$

$$APF = \frac{\frac{\cancel{16}}{3}\pi \frac{\cancel{\sqrt{2}\times\sqrt{2}}\times\cancel{\sqrt{2}}}{\cancel{4\times4}\times\cancel{4}\,\cancel{2}\sqrt{2}}\cancel{a^3}}{\cancel{a^3}}$$

$$\boxed{APF = \frac{\pi}{3\sqrt{2}} = 0.74}$$

74 % is occupied by the atoms and 26 % is vacant (or) void space. So BCC is a tightly (or) closely packed structure.

**4.What is packing factor? Obtain packing factor for SC, BCC and FCC structures.**

Packing factor – Definition

It is defined as the ratio between the volume occupied by the atoms per unit cell (v) to total volume of the unit cell (V).

$$APF = \frac{No.of\ atoms\ per\ unit\ cell \times Volume\ of\ one\ atom}{Volume\ of\ the\ unit\ cell}$$

Packing factor for SC

$$APF = \frac{No.of\ atoms\ per\ unit\ cell \times Volume\ of\ one\ atom}{Volume\ of\ the\ unit\ cell}$$

Number of atoms per unit cell = 1

$$APF = \frac{1 \times \frac{4}{3}\pi r^3}{a^3}$$

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

$$APF = \frac{\frac{\cancel{4}}{3}\pi \frac{\cancel{a^3}}{\cancel{2}\times\cancel{2}\times 2}}{\cancel{a^3}}$$

$$\boxed{APF = \frac{\pi}{6} = 0.52}$$

52 % is occupied by the atoms and 48 % is vacant (or) void space. So SC is a loosely packed structure.

Packing factor for BCC

$$APF = \frac{No.of\ atoms\ per\ unit\ cell \times Volume\ of\ one\ atom}{Volume\ of\ the\ unit\ cell}$$

Number of atoms per unit cell = 2

$$APF = \frac{2 \times \frac{4}{3}\pi r^3}{a^3}$$

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

$$APF = \frac{\frac{\cancel{8}^{2}}{3}\pi \frac{\cancel{\sqrt{3}\times\sqrt{3}}\times\sqrt{3}}{\cancel{4}\times\cancel{4}_{2}\times 4}\cancel{a^3}}{\cancel{a^3}}$$

$$\boxed{APF = \frac{\sqrt{3}}{8}\pi = 0.68}$$

68 % is occupied by the atoms and 32 % is vacant (or) void space. So BCC is a tightly (or) closely packed structure compared with SC.

Packing factor for FCC

$$APF = \frac{No.of\ atoms\ per\ unit\ cell \times Volume\ of\ one\ atom}{Volume\ of\ the\ unit\ cell}$$

Number of atoms per unit cell = 4

$$APF = \frac{4 \times \frac{4}{3}\pi r^3}{a^3}$$

$$APF = \frac{\frac{\cancel{16}}{3}\pi \frac{\cancel{\sqrt{2}\times\sqrt{2}}\times\cancel{\sqrt{2}}}{\cancel{4\times4}\times\cancel{4}\ 2\sqrt{2}}\cancel{a^3}}{\cancel{a^3}}$$

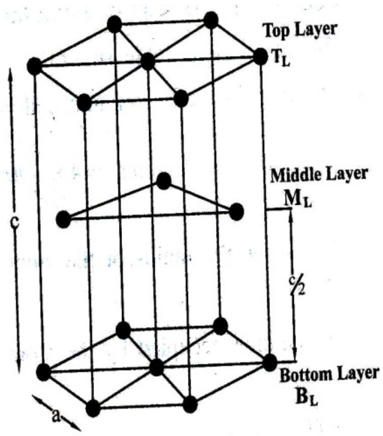
$$\boxed{APF = \frac{\pi}{3\sqrt{2}} = 0.74}$$

74 % is occupied by the atoms and 26 % is vacant (or) void space. So BCC is a tightly (or) closely packed structure.

**5.Describe HCP structure. Show that a HCP structure demands an axial ratio of 1.6333. Hence prove that HCP and FCC structures have the same atomic packing factor.**

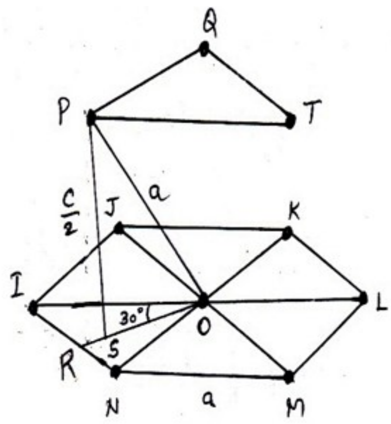
<u>HCP structure – Description</u>

- HCP structure has 3 layers.
  - (i) Top layer
  - (ii) Middle layer
  - (iii) Bottom layer




- Top layer has one atom at each corner and one atom at the centre of the face. Totally top layer has 6 corner atoms and 1 face centered atom.
- Middle layer has 3 individual atoms.
- Bottom layer has one atom at each corner and one atom at the centre of the face. Totally bottom layer has 6 corner atoms and 1 face centered atom.
- The height of the unit cell is '*c*'.
- The side of the unit cell is '*a*'.

Axial ratio (*c/a* ratio) – Proof




- I, J, K, L, M & N – Corner atoms of the bottom layer.
- P, Q & T – Middle layer atoms.
- *c* – Height of the unit cell.
- *a* – Distance between two atoms.
- *O* – Face centered atom.
- Draw a line from '*O*' to *IN*. It meets at '*R*'.
- Draw a line from '*P*' to '*OR*'. It meets at '*S*'.
- '*S*' – Orthocentre.

Consider Δ IRO

$$\cos 30^{\circ} = \frac{OR}{OI}$$

$$\frac{\sqrt{3}}{2} = \frac{OR}{a}$$

$$\boxed{OR = \frac{\sqrt{3}}{2} a \qquad ---------(1)}$$

According to Orthocentre theorem

$$OS = \frac{2}{3} OR \qquad --------(2)$$

Sub.(2) in (1)

$$OS = \frac{\cancel{2}}{\cancel{3}} \frac{\cancel{\sqrt{3}}}{\cancel{2}} a$$

$$\sqrt{3}$$

$$\boxed{OS = \frac{a}{\sqrt{3}}}$$

Consider $\Delta$ SOP

$(OP)^2 = (OS)^2 + (SP)^2$ ---------- (3)

$$\left.\begin{aligned} OP &= a \\ OS &= \frac{a}{\sqrt{3}} \\ SP &= \frac{c}{2} \end{aligned}\right\} \quad \text{----------- (4)}$$

Sub. (4) in (3)

$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2$$

$$a^2 = \frac{a^2}{3} + \frac{c^2}{4}$$

$$a^2 - \frac{a^2}{3} = \frac{c^2}{4}$$

$$a^2\left(1 - \frac{1}{3}\right) = \frac{c^2}{4}$$

$$a^2\left(\frac{3-1}{3}\right) = \frac{c^2}{4}$$

$$a^2\left(\frac{2}{3}\right) = \frac{c^2}{4}$$

$$\frac{2 \times 4}{3} = \frac{c^2}{a^2}$$

$$\frac{8}{3} = \frac{c^2}{a^2}$$

$$\frac{c^2}{a^2} = \frac{8}{3}$$

$$\boxed{\frac{c}{a} = \sqrt{\frac{8}{3}} = 1.6333}$$

<u>Atomic packing factor for HCP</u>

$$APF = \frac{No.of\ atoms\ present\ in\ a\ unit\ cell \times Volume\ of\ one\ atom}{Volume\ of\ the\ unit\ cell} \quad \text{--------(1)}$$

Number of atoms per unit cell = 6 -------------- (2)

$$Volume\ of\ one\ atom = \frac{4}{3}\pi r^3$$

$$= \frac{4}{3}\pi\left(\frac{a}{2}\right)^3 \qquad \left[\because r = \frac{a}{2}\right]$$

$$= \frac{\cancel{4}}{3}\pi \frac{a^3}{\cancel{8}_2}$$

$$\boxed{Volume\ of\ one\ atom = \frac{\pi a^3}{6}} \quad \text{--------------- (3)}$$

$$Volume\ of\ unit\ cell = Area\ of\ base \times Height$$
$$= 6 \times Area\ of\ one\ \Delta(INO) \times c$$
$$= 6 \times \frac{1}{2} \times IN \times RO \times c$$
$$= \cancel{6}^{3} \times \frac{1}{\cancel{2}} \times a \times \frac{\sqrt{3}}{2} a \times c$$

$$\boxed{Volume\ of\ unit\ cell = \frac{3\sqrt{3}\ a^2 c}{2}} \qquad \text{------------ (4)}$$

Sub. (2), (3) & (4) in (1)

$$APF = \frac{\cancel{6} \times \frac{\pi a^{\cancel{3}}}{\cancel{6}}}{\frac{3\sqrt{3}}{2} a^{\cancel{2}} c}$$

$$= \frac{2\pi a}{3\sqrt{3}\,c} \Rightarrow \frac{2\pi}{3\cancel{\sqrt{3}}} \frac{\cancel{\sqrt{3}}}{\sqrt{8}}$$

$$= \frac{2\pi}{3\sqrt{8}} \Rightarrow \frac{2\pi}{3\sqrt{\cancel{2 \times 2} \times 2}}$$

$$\boxed{APF = \frac{\pi}{3\sqrt{2}} = 0.74}$$

So 74 % is occupied by the atoms and 26 % is vacant (or) void space. Hence HCP structure is a closely packed structure.

Atomic packing factor for FCC

$$APF = \frac{No.of\ atoms\ per\ unit\ cell \times Volume\ of\ one\ atom}{Volume\ of\ the\ unit\ cell}$$

Number of atoms per unit cell = 4

$$APF = \frac{4 \times \frac{4}{3} \pi r^3}{a^3}$$

$$APF = \frac{\frac{\cancel{16}}{3} \pi \frac{\cancel{\sqrt{2} \times \sqrt{2}} \times \cancel{\sqrt{2}}}{\cancel{4 \times 4 \times 4}\ \cancel{2}\sqrt{2}} \cancel{a^3}}{\cancel{a^3}}$$

$$\boxed{APF = \frac{\pi}{3\sqrt{2}} = 0.74}$$

Hence HCP and FCC have same atomic packing factor.

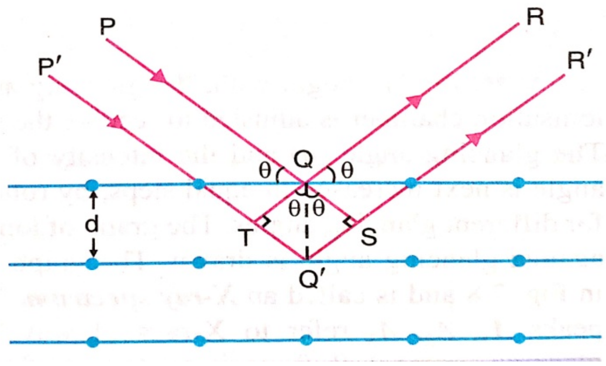
**6.What is Bragg's law? Derive the expression for Bragg's law.**

Bragg's law

When a beam of X-ray is incident on a crystal at an angle θ, the reflected beam of X-ray also has the same angle of scattering θ. The interference pattern will occur when the path difference 'd' between two reflected waves from two different planes is an integral multiple of λ.

$$2d \sin\theta = n\lambda \qquad n = 1, 2, 3 \ldots..$$

Diagram




Derivation

- Consider a set of parallel planes of atom.
- d – spacing between two successive planes.
- Let monochromatic X-rays are incident on the planes at an angle θ.
- PQ and P′Q′ – Two incident rays.
- These two rays are incident on first and second plane respectively and reflected.
- After reflection, PQ and P′Q′ travel along QR and Q′R′ respectively.
- Draw a normal from Q to P′Q′. It meets at T.
- Draw a normal from Q to Q′R′. It meets at S.
- Therefore, the path difference between the two waves PQR and P′Q′R′ is equal to TQ′ + Q′S.

In the Δ TQQ′

$$Sin\theta = \frac{TQ'}{Q'Q}$$

$$TQ' = Q'Q\, Sin\theta$$

$$TQ' = d\, Sin\theta$$

In the Δ QQ′S

$$Sin\theta = \frac{Q'S}{Q'Q}$$

$$Q'S = Q'Q\,Sin\,\theta$$

$$Q'S = d\,Sin\,\theta$$

Path difference = TQ′ + Q′S

Path difference = d Sin θ + d Sin θ = 2d Sin θ.

- If this path difference 2d Sin θ is equal to integral multiple of wavelength of X-ray i.e. nλ.

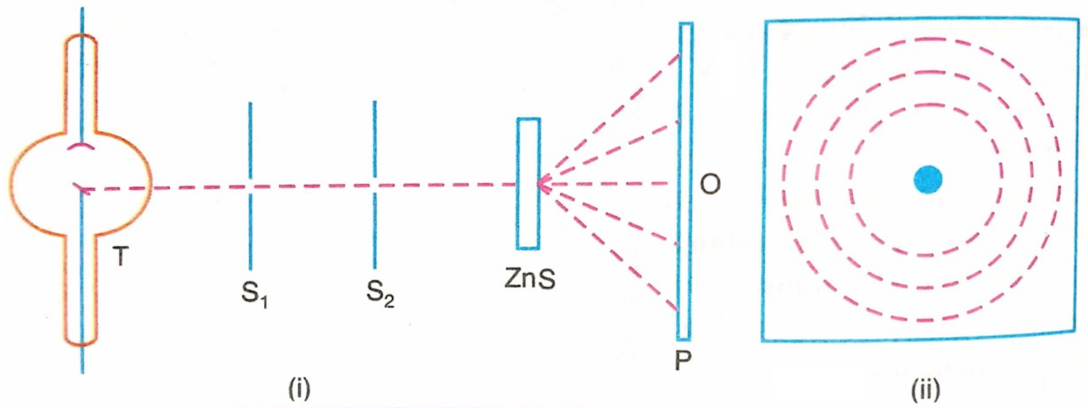
$$2d\,Sin\,\theta = n\lambda \qquad n = 1, 2, 3 \ldots..$$

where n – order of the scattered beam
λ – wavelength of incident X-ray
d – spacing of the crystal planes
θ – angle between incident ray and scattered plane

This is known as Bragg's law.

**7.**Describe the Laue method for studying crystal structures.

- This method was suggested by Von Laue in 1913.
- According to him, a crystal can act as a three-dimensional grating for an X-ray beam.
- If X-rays are allowed to pass through a crystal, the X-rays are diffracted.

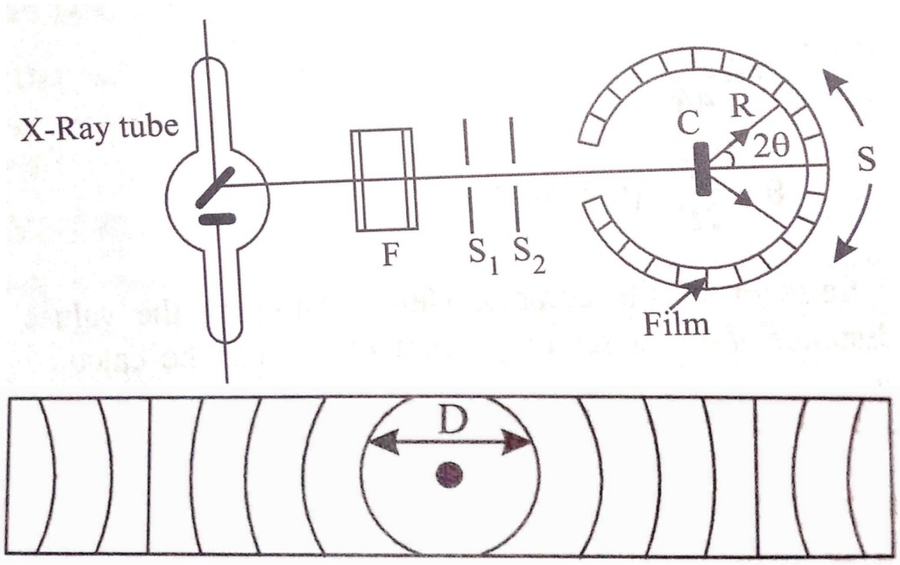



- This experimental arrangement consists of X-ray tube (T), slits (S1 & S2), crystal (ZnS) & photographic plate (P).
- The X-ray tube is used to produce a beam of X-rays.
- This beam of X-rays is collimated by two slits $S_1$ and $S_2$.
- The beam is now allowed to pass through a zinc sulphate (ZnS) crystal.
- The crystal transmits the X-ray beam.
- The transmitted beam is received on a photographic plate P.
- After exposure of many hours, the plate is developed.
- The Laue photograph is obtained on the plate.
- The plate consists of 2 kinds of spots.
  - (i) One central spot due to direct beam.
  - (ii) Many fainter parts due to diffracted beam
- These spots are known as Laue spots.

- From the experiment, the following facts are established.
  - (i) Regular arrangement of atoms three-dimensional space.
  - (ii) Shape of the unit cell.

**8.**Describe the Powder crystal method (or) Debye and Sherrer method for studying crystal structures.

- This method is suggested by Debye and Sherrer.
- This arrangement consists of X-ray tube, Filter (F), Slits ($S_1$ & $S_2$), Powder specimen (C) and Cylindrical camera (S).
- The specimen S is taken in the form of powder.
- An X-ray tube is used to produce a beam of X-rays.
- The X-rays are converted to monochromatic beam by the filter F.
- The monochromatic X-rays are collimated by two slits $S_1$ and $S_2$.
- Then they are allowed to fall on the powdered specimen S.
- The specimen is suspended vertically on the axis of a cylindrical camera (S).
- The photographic film is mounted round the inner surface of the camera S.




- The film covers diffracted beam in the whole circumference.
- Now the X-rays are allowed to fall on the powdered specimen S.
- The X-rays are diffracted by the powdered specimen S.
- The diffracted rays will be on the surface of a cone, vertex at the specimen, base on the photographic film.
- The traces are obtained in the photographic film.
- From the experiment, the following facts are established.
  - (i) Size of the unit cell.
  - (ii) Type of the lattice.
  - (iii) Calculation of d-spacing

**9.What is crystal growth? State the principle and describe the diagram with detailed working of Bridgmann method of crystal growth. Also state the advantages.**

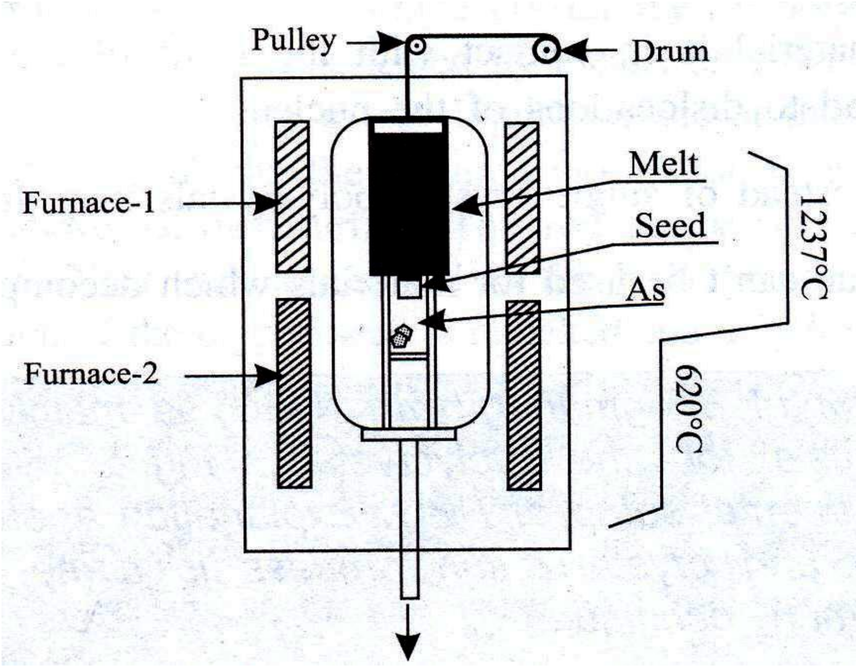
Crystal Growth

The process of making a crystal by continuing to remove a component from a solution is called crystal growth.

Principle

The material is heated to a very high temperature until the molten stage is reached. The molt is moved across a temperature gradient so as to solidify and form a seed. Such movements will lead to the crystal growth.

Diagram




Description (or) Construction

- The material is taken in a crucible inside the vertical cylindrical container.
- A seed crystal is placed at the bottom of the crucible.
- The container is surrounded by two furnaces namely, Furnace 1 & Furnace 2.
- Furnace 1 is kept at hot zone (1237$^{o}$ C) and Furnace 2 is kept at cold zone (620$^{o}$ C).
- A pully and drum is used to move the container up and down during the crystallization process.
- This movement is used to heat and cool the crystal to be grown (melt).
- This movement is very slow in the range of 1 to 30 mm/hour.

Working

- Furnace 1 is switched ON and the material is heated to a very high temperature.
- Now the material is changed into molten state.
- The container is moved slowly towards the furnace 2 with the help of the pully and the drum.
- When the container enters into the furnace 2, the crystallization starts in the tip of the seed crystal.
- When the container is moved down continuously, the entire molten material will grow into a large crystal.

Advantages

- Cheaper than other techniques.
- Easiest method.
- Composition can be controlled during the growth.
- Good crystals can be formed.

**10. What is crystal growth? Explain the principle and describe the diagram with detailed working of Czochralski method of crystal growth. Also state the advantages.**

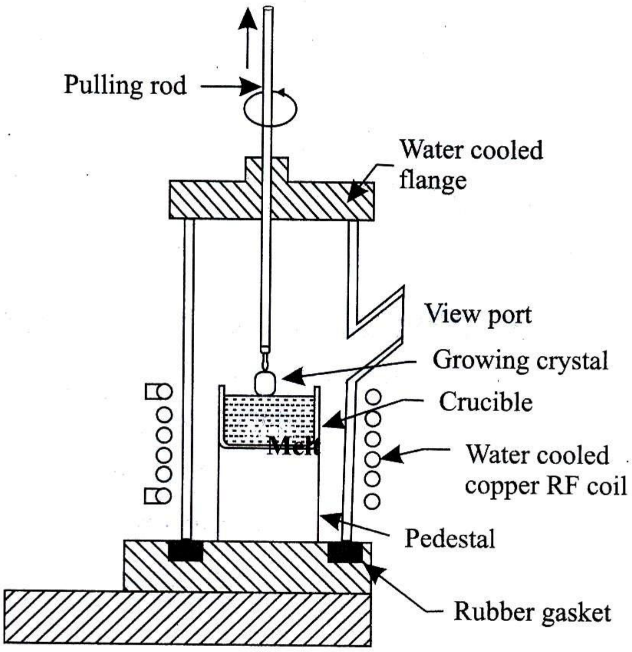
Crystal Growth

The process of making a crystal by continuing to remove a component from a solution is called crystal growth.

Principle

"Crystal pulling from the melt" is the principle used in Czochralski method. Here the material is melted over the monocrystalline seed and is rotated. Further, with the help of pull rod it is slowly drawn upwards and hence the melt freezes on the crystal and thus the crystal grows.

Diagram




Description (or) Construction

- The material is taken in a crucible.
- The material is heated by a radiofrequency heater to obtain melt.
- The seed crystal is attached to a pulling rod.
- The seed crystal is just touch on the melt surface.
- Water cooled flange is provided for cooling effect.
- The entire system is covered in a vessel with argon gas.
- Argon gas avoids combustion.
- The growing crystal can be seen through the view point.
- Pedestal and Rubber gasket give strong support to the system.

Working

- The seed crystal is attached to a pulling rod with a specific orientation.
- The heater is switched ON.
- The material in the crucible is melted and free liquid surface will be formed on the top.
- The pulling rod is allowed to rotate and pulled out gradually from the melt.
- The melt freezes on the seed crystal.
- Now a single crystal is grown as the seed crystal orientation.
- The shape of the crystal is initially in the form of a thin neck and then increased. It is known as necking procedure.
- By pulling mechanism and necking procedure, bulk crystal can be grown.
- The pulling rate, rotation rate and the power to the heater decide the diameter of the grown crystal.

Advantages

- This technique provides growth of crystal free from crystal defect.
- It can produce large single crystal.
- It allows convenient chemical composition of crystal.
- It enables easy control of atmosphere during growth.