

Unit 1

Crystal Structure:

- (i) Crystalline Solids → atoms are arranged in regular manner.
- (ii) Amorphous Solids → atoms are arranged randomly.

⇒ Solids are divided into two categories:

- ① Crystalline Solids
- ② Amorphous Solids

Crystalline Solids: Those solids in which the particles arranged in a regular repeating 3-dimensional lattice is known as crystalline solid.

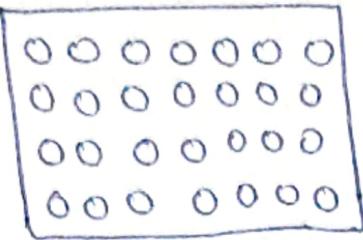
They have sharp melting point

for ex. % NaCl, diamond, Quartz etc

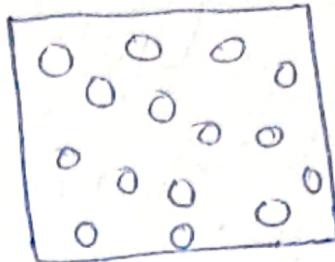
Amorphous Solids: Those solids in which particles are arranged randomly or in a irregular manner in 3-dimensional lattice is known as amorphous solid.

They melt over a range of temperature.

e.g. % Glass, Plastic etc.



[Crystalline Solid]

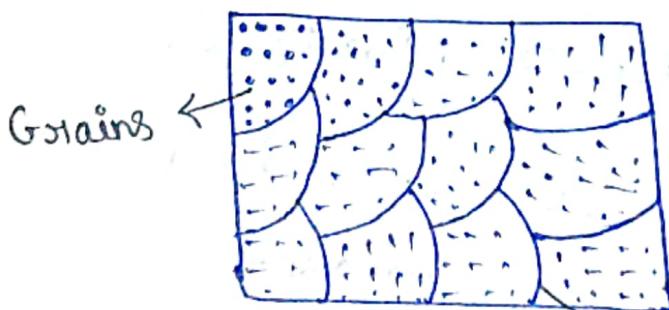


[Amorphous Solid]

Poly-crystalline Solids is a type of crystalline solid which made up of many crystals or grains known as polycrystalline solids.

Grains are separated by a boundary known as Grain boundary.

Grains are randomly oriented with respect to each other for ex. common metal, many ceramics, rocks etc are the example.

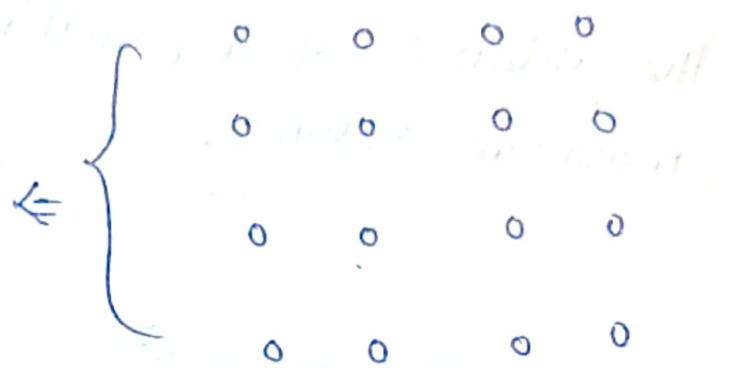


→ Poly-crystalline Solid
e.g. rock.

[Polycrystalline Solid] → Grain boundary

⇒ Orientation are same (of atom) in each crystal but when we compare to other here. Then it is different.

Space Lattice : Space lattice is a three dimensional ordered array of points describing the arrangement of particle has identical surrounding.



Basis or Motif : Basis may be atom or group of atom present in the crystal, when Basis is attached to every lattice point a crystal structure is formed.

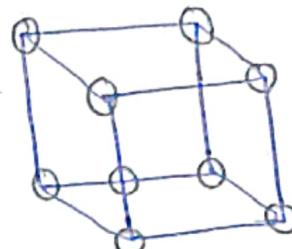
Couystal Structure : when lattice and Basis join together crystal structure is formed.



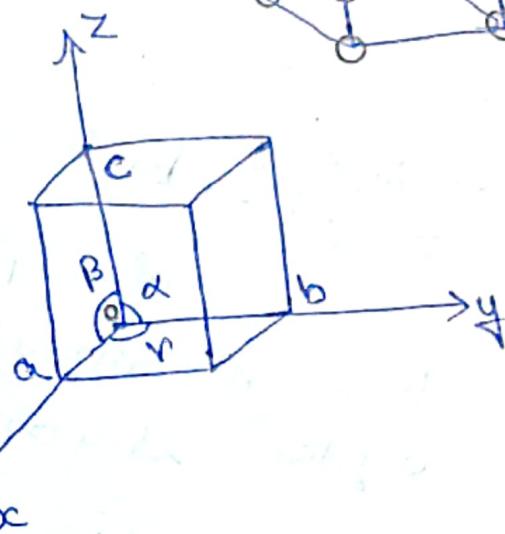
Unit Cell : Unit cell is the basic building of crystal which one repeated again and again in different directions in space, forms the entire crystal lattice or crystal structure.

Primitive Cell :- when the atoms on the lattice points are present only at the corners of unit cell, then the unit cell is called Primitive cell.

The volume of a primitive cell has a minimum volume.



Lattice Parameters



④ Crystallographic axis
($0x, 0y, 0z$)

- ⑤ Edges
(a, b, c)
- ⑥ Interfacial angles
(α, β, γ)

The shape of the unit cell depends on edges and angles between them.

Crystallographic axis :- The imaginary line parallel to the edges of the unit cell which are not lying in the same plane is called crystallographic axis.

In diagram $0x, 0y, 0z$ are crystallographic axis in the

Interfacial Angle: The angle between the edges of crystallographic axis is known as interfacial angles.

Here, α, β, γ are the interfacial angles and a, b, c are the intercept of edges.

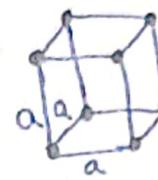
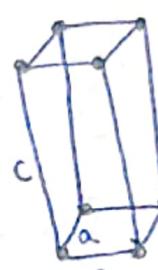
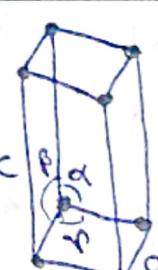
Crystal System & Bravais Lattice:

There are seven types of crystal depending upon their interfacial angle and edges ratio.

Bravais shows that they give rise to 14 type of space lattice due to simple cubic, body centered, face centered, base centered type.

The Seven Crystal System are:

- ① Cubic
- ② Tetrahedral
- ③ Ortho-rhombic
- ④ Trigonal (Rhombohedral)
- ⑤ Hexagonal
- ⑥ Monoclinic
- ⑦ Tri-clinic

	Crystal System	Axial Relationship	Interaxial Angle	Bravais Lattice	Unit Cell Geometry
①	Cubic	$a=b=c$	$\alpha=\beta=\gamma=90^\circ$	Simple cubic, body centered, face centered	
②	Tetrahedral	$a=b \neq c$	$\alpha=\beta=\gamma=90^\circ$	Simple cubic, body centered	
③	Orthorhombic	$a \neq b \neq c$	$\alpha=\beta=\gamma=90^\circ$	Simple cubic, body centered, base centered, face centered	
④	Monoclinic	$a \neq b \neq c$	$\alpha=\gamma=90^\circ \neq \beta$	Simple cubic, base centered	
⑤	Tetragonal	$a \neq b \neq c$	$\alpha=\beta=\gamma \neq 90^\circ$	Simple cubic	
⑥	Hexagonal	$a=b \neq c$	$\alpha=\beta=90^\circ, \gamma=120^\circ$	Simple cubic	
⑦	Rhombohedral (or Trigonal)	$a=b=c$	$\alpha=\beta=\gamma \neq 90^\circ$	Simple cubic	

Types of cubic crystals : (three types)

- ① Simple Cubic Crystal (SCC)
- ② Body centered Cubic Crystal (BCC)
- ③ Face centered cubic crystal (FCC)

Simple cubic cell (SCC) :

In simple cubic cell, the lattice points are situated at the corners of the unit cell.

(total) No. of atoms in SCC : Number of atom

$$\text{in SCC} = 8 \times \frac{1}{8} = 1 \text{ atom per unit cell.}$$

Coordination Number

The coordination number is defined as the number of

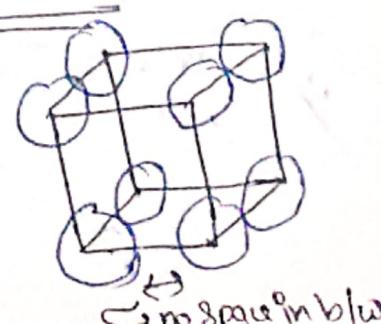
equidistant neighbours around an atom in the crystal.

In SCC unit cell, there are 6 equidistant neighbouring atom corresponding to each atom. Therefore, coordination number for SCC is 6.

⇒ The relation between atomic radius (r) and edge length (a) :

In 2-dimension of SCC from the diagram,

$$2r = a \Rightarrow r = \frac{a}{2}$$



Atomic Packing factor for FCC %

It is the ratio , volume occupied by atoms in unit cell to the total volume of unit cell.

then, APF = $\frac{\text{Total volume occupied by unit cell (of atom)}}{\text{Volume of unit cell.}}$

$$\text{APF} = \frac{\text{No. of atoms} \times \text{Volume of 1 atom}}{\text{Volume of unit cell.}}$$

↓
atomic
packing factor

$$\text{APF} = \frac{1 \times \frac{4}{3} \pi r^3}{a^3} = \frac{\frac{4}{3} \pi r^3}{(2r)^3} = \frac{\pi}{6}$$

$$\text{APF.} = 0.52$$

∴ 52% of the unit cell occupied by atom.

Body Centered Cubic cell (BCC) %

In Body centered cubic cell, 8 atoms are present at corners of unit cell and 1 atom is present at centre of the unit cell.

⇒ Then, Total number of atom per unit cell

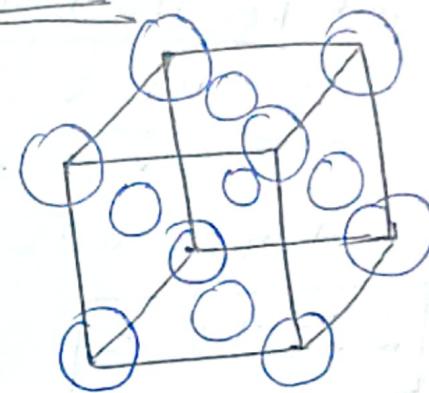
$$= \frac{1}{8} \times 8 + 1 = 2 \text{ atom / unit cell.}$$

⇒ The centre atom of BCC unit cell is equidistant from the corner atoms. So, its coordination number is 8.

Relation between π and a :

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

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



APF (atomic packing factor) of BCC:

$$\text{APF} = \frac{\text{No. of atom} \times \text{Volume of 1 atom}}{\text{Volume of unit cell.}}$$

$$\text{APF} = \frac{2 \times \frac{4}{3}\pi r^3}{a^3} = \frac{\frac{8}{3}\pi r^3}{2 \times 8 \times 4r^3} \times 8\sqrt{3} = 0.68$$

APF = 0.68 ∴ 68% of unit cell occupied by atom.

Face centered cubic crystal:

In face centered cubic cell, 6 atoms are present at the face centre and 8 atoms are present at the corners of unit cell.

⇒ than total number of atom per unit

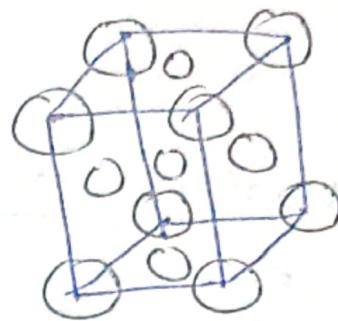
$$\text{cell} = \frac{1}{2} \times 6 + \frac{1}{8} \times 8 = 4 \text{ atom/unit cell.}$$

\Rightarrow There are 12 nearest neighbouring atom to face centered atom in fcc, hence its coordination number is 12

\Rightarrow and Relation b/w r_1 and a

$$4r_1 = a\sqrt{2}$$

$$2\sqrt{2}r_1 = a$$



\Rightarrow (APF) atomic packing factor in BCC

$$\text{APF} = \frac{\text{no. of atom} \times \text{volume of atom}}{\text{volume of 1 unit cell}}$$

$$\text{APF} = \frac{4 \times \frac{4}{3}\pi r_1^3}{a^3} = \frac{2 \times \frac{8}{3}\pi r_1^3}{8 \times 2\sqrt{2}r_1^3} = \frac{\pi}{3\sqrt{2}}$$

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

\Rightarrow \therefore 74% of the unit cell is occupied by the atom.

Relation between lattice constant (a) and density (ρ) ?

→ Volume of unit cell = a^3

→ If ρ is the density of unit cell, then its mass is equal to :

$$\text{mass} = \rho a^3 \quad \text{--- (1)}$$

of unit cell

→ Now, mass of each atom in unit cell = $\frac{M}{N_A}$

→ if there 'n' no. of atoms in unit cell,

$$\text{then mass of unit cell} = n \frac{M}{N_A} \quad \text{--- (2)}$$

→ equating (1) & (2),

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

Ans: Calculate the number of atoms per unit cell of a metal with lattice parameter 2.9 Å, given molecular weight is 55.85 and density is 7870 kg/m³. (2)

$$\text{Sol:} \quad \text{as } a^3 = \frac{n M}{\rho N_A} \Rightarrow n = \frac{a^3 \rho N_A}{M}$$

$$n = \frac{(2.9 \times 10^{-10})^3 \times 7870 \times 10^3 \times 6.023 \times 10^{23}}{55.85}$$

$$n = 2.069 \approx 2 \text{ atom/unit cell}$$

Ques: Germanium crystallizes in diamond structure with 8 atom per unit cell. If lattice constant is 5.6 \AA and molecular weight is 72.59, calculate its density. (5492)

Sol: $n = 8, a = 5.6 \text{ \AA}, M = 72.59 \text{ g/mol}$

$$\text{as } a^3 = \frac{nM}{\rho N_A} \Rightarrow \rho = \frac{nM}{a^3 N_A}$$

$$\rho = \frac{8 \times 72.59}{(5.6 \times 5.6 \times 5.6) \times 10^{-30} \times 6.023 \times 10^{23} \times 10^3} \approx 5492 \text{ kg/m}^3$$

for kg/m^3

Ques: A substance with face centered cubic lattice has density 6250 kg/m^3 and molecular weight 60.2, calculate the lattice constant (4 \AA)

Sol: $\rho = 6250 \text{ kg/m}^3, M = 60.2$

$$2 n = 4, a = ?$$

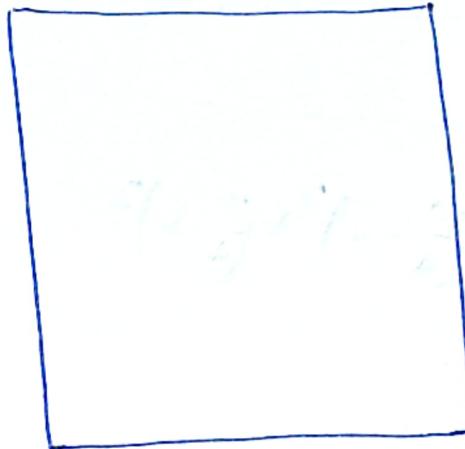
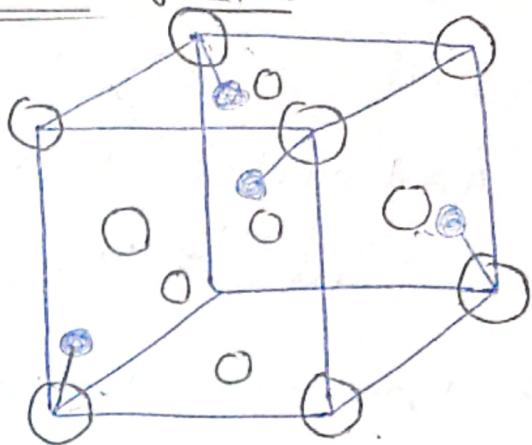
$$\text{as } a^3 = \frac{nM}{\rho N_A}$$

$$a = \left[\frac{4 \times 60.2}{(6250 \times 10^3) (6.023 \times 10^{23})} \right]^{1/3}$$

$$a = 3.999 \times 10^{-10} \approx 4 \text{ \AA}$$

Structure of Diamond Crystal :

- ⊗ Structure \Rightarrow FCC
- ⊗ Total atoms involved = 18
- ⊗ Type of atom = 2
 - (i) at $(0,0,0)$, FCC
 - (ii) at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ \rightarrow (in Octahedral shape)
- ⊗ Coordination number = 4
- ⊗ no. of atoms per unit cell = 8
- ⊗



- \Rightarrow Diamond structure is face centered cubic lattice.
- \Rightarrow unit cell of diamonds contain 18 atom.
 - 8 atoms are placed at corners of the cube.
 - 6 atoms are placed at each face of the cube.
 - and 4 inside it.

⇒ Basis of carbon atom consist of 1 lattice point having 2 atoms placed at $(0,0,0)$ and at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$

⇒ Total number of atoms of diamond per unit cell

$$\text{cell} = \left(\frac{1}{8} \times 8\right) + \left(\frac{1}{2} \times 6\right) + 4 = 8 \text{ atoms / unit cell}$$

⇒ Diamond structure has tetrahedron shape of carbon atoms which means that each carbon atom is attached with four carbon atoms in tetrahedron shape.

⇒ The coordination number of diamond structure is 4.

Relation between lattice constant 'a' and 'r'

$$2r = \sqrt{\left(\frac{a}{4} - 0\right)^2 + \left(\frac{a}{4} - 0\right)^2 + \left(\frac{a}{4} - 0\right)^2}$$

$$2r = \frac{\sqrt{3}a}{4}$$

$$r = \frac{\sqrt{3}a}{8}$$

Atomic packing factor %

$$\text{APF} = \frac{\text{no. of atom} \times \text{volume of 1 atom}}{\text{Volume of unit cell}}$$

$$APF = \frac{8 \times \frac{4}{3}\pi r^3}{a^3} = \frac{8 \times \frac{4}{3}\pi r^3 \times 3\sqrt{3}}{64 \times 8} = \frac{r^3 \times 3\sqrt{3}}{16}$$

$$\therefore APF = \frac{\sqrt{3}\pi}{16} = 0.340$$

\therefore 34% of unit cell is covered by atom.

Ques: Lattice constant of BCC crystal is 0.36 nm. calculate its atomic radius.

$$\text{Sol: } \sqrt{3}a = 4r \Rightarrow r = \frac{\sqrt{3} \times 0.36}{4} \text{ nm}$$

$$r = 0.15 \text{ nm}$$

Ques: Copper is fcc whose atomic radius is 1.26×10^{-10} m. calculate its lattice constant.

$$\text{Sol: } a\sqrt{2} = 4r \Rightarrow a = \frac{4 \times 1.26 \times 10^{-10}}{\sqrt{2}} = 3.56 \times 10^{-10} \text{ m}$$

Ques: which of the following an amorphous material?

- (A) Mica ~~(B)~~ Lead ~~(C)~~ Rubber ~~(D)~~ Glass

Ques: The unit cell of certain type of crystal is defined by three vectors. a, b, c. these vectors are mutually perpendicular but $a \neq b \neq c$. The crystal structure is?

- (A) Triclinic ~~(B)~~ Tetragonal ~~(C)~~ Orthorhombic
(D) Monoclinic

Ques ③ Which of the following is correct sequence of the crystal structure with respect to percentage of voids (SCC - simple cubic, BCC - body centered, FCC - face centered).

(A) SCC < FCC < BCC

~~(B)~~ FCC < BCC < SCC

(C) SCC < BCC < FCC

(D) More than one of the above.

(E) None than one of the above.

Ques ④ % Packing efficiency of the body centered crystal is

~~(A)~~ 0.68 (B) 0.74 (C) 0.50 (D) 1.00

Ques ⑤ If the atomic radius of aluminium is r_1 , what is the unit cell volume.

(A) $\left(\frac{2r_1}{\sqrt{2}}\right)^3$ ~~(B)~~ $\left(\frac{4r_1}{\sqrt{2}}\right)^3$ (C) $\left(\frac{2r_1}{\sqrt{3}}\right)^3$ (D) $\left(\frac{2r_1}{\sqrt{5}}\right)^3$

Ques ⑥ Coordination number for FCC crystal is

(A) 4

(B) 8

~~(C)~~ 12

(D) 16

Ques(7) :- If atom is assumed to be hard sphere, the maximum value of APP in metals will be

- (A) 0.65 (B) 0.74 (C) 0.85 (D) 0.98

Ques(8) :- The crystal structure of cementite (Fe_3C) is

- (A) FCC (B) BCC (C) Tetragonal (D) Orthorhombic

Ques(9) :- The effective number of lattice points in the unit cell of Scs, Bcc and fcc lattices respectively is

- (A) 1, 2, 3 (B) 1, 2, 4 (C) 4, 2, 1 (D) 3, 2, 1

Ques(10) :- The coordination number of fcc is

- (A) 4 (B) 8 (C) 12 (D) 16

Ques(11) :-

(A) Assertion :- Solids have definite mass, volume & shape.
Reason (R) :- Solids can be classified as crystalline and amorphous.

~~(A)~~ Both (A) & (R) are correct and (R) is correct explanation of the (A).

(B) Both (A) & (R) are correct statements, but (R) is not correct explanation of (A).

(C) (A) is correct but (R) is incorrect.

(D) (A) is incorrect, but (R) is correct.

Ques 12 & Assertion (A) :- Solids have definite mass, volume and shape.

✓
repeated
written

Reason (R) :- Solids can be classified as crystalline and amorphous.

~~(a)~~ Both Assertion (A) and Reason (R), are correct statement, and (R) is correct explanation of A.

(b) both (A) & (R) are correct but (R) is not correct explanation of (A).

(c) (A) is correct, but (R) is incorrect statement

(d) (A) is incorrect but (R) is correct statement

Ques 13 & (A) assertion :- Packing efficiency of body centered cubic structure is 68%.

(R) Reason :- 68% is the maximum packing efficiency any crystal can have.

(a) both (A) & (R) are true and (R) is correct explanation of (A).

(b) both (A) and (R) are true but (R) is not correct explanation of (A)

~~(c)~~ (A) is true but (R) is false

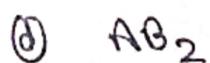
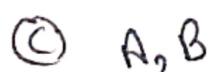
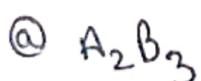
(d) (A) and (R) is false.

Ques 14 & (A) assertion :- Glass panes fixed to windows or doors of old building are slightly thicker at the bottom than at the top.

(a) Glass is a pseudo solid or supercold liquid.

- ~~(A)~~ both (A) and (R) are true and (R) is correct explanation of (A). ✓
- (B) both (A) and (R) are true but (R) is not correct explanation of (A)
- (C) (A) is true but (R) is false
- (D) both (A) & (R) are false.
- Ques(5) :- (A) Assertion :- CsCl has body-centered cubic arrangement
- (B) Reason :- CsCl has one and $\delta\text{-Cl}^-$ in unit cell.
- ~~(A)~~ both (A) and (R) are true and (R) is correct explanation of (A).
- (B) both (A) and (R) are true and (R) is not correct explanation of (A).
- (C) (A) is true but (R) is false.
- (D) both (A) and (R) are false.

Ques(16) :- In a face-centered cubic lattice, atom A occupies the corner positions and atom B occupies the face center positions. If one atom of B is missing from one of the face centered points, the formula of the compound is :-



$$\left. \begin{array}{l} \text{atom of A} = 1 \\ \text{atom of B} = 5/2 \\ \therefore \text{A B}_{5/2} \end{array} \right\}$$

Ques 17 In a monoclinic unit cell, the relation of sides and angles are respectively.

(a)

$$a \neq b \neq c \text{ and } \alpha \neq \beta \neq \gamma \neq 90^\circ$$



(b)

$$a \neq b \neq c \text{ and } \beta = \gamma = 90^\circ \neq \alpha$$

(c)

$$a = b \neq c \text{ and } \alpha = \beta = \gamma = 90^\circ$$

(d)

$$a \neq b \neq c \text{ and } \alpha = \beta = \gamma = 90^\circ$$

Ques 18 All of the following share the same crystal structure except

(a) RbCl

(b) CsCl

~~(c) LiCl~~

(d) NaCl

Ques 19 Ammonium chloride crystallizes in a body centered cubic lattice with edge length of unit cell of 390 pm. If the size of chloride ion is 180 pm, the size of ammonium ion would be:-

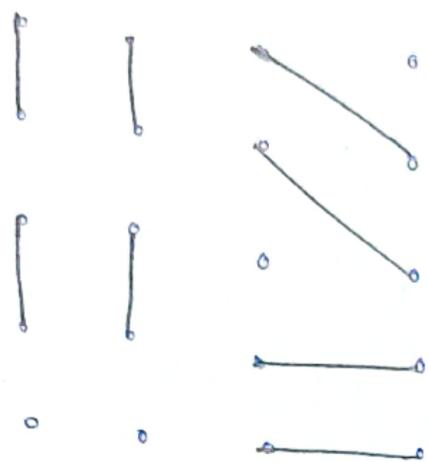
(a) 158 pm

(b) 74 pm

(c) 142 pm

(d) 126 pm

Crystal Planes :- when lattice point joined together in crystal lattice in different directions, these are known as crystal planes.



Miller Indices: The crystal lattice consists of many parallel planes, it is difficult to write their geometric equations.

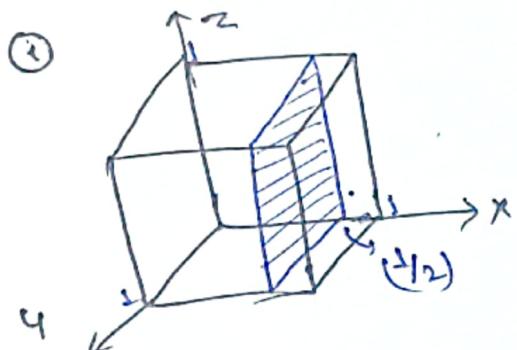
Miller evolved a method to designate a plane in a crystal by three numbers (hkl).

⇒ Miller indices of a plane is defined as the reciprocal of intercept which the plane make with the axis when reduced to the smallest number.

⇒ He used the following steps to find Miller indices of a plane :-

- ① Determine the intercept of plane along three coordinate axis.
- ② Secondly, take the reciprocal of slope intercepts.
- ③ Taking whole number of the reciprocal by multiplying with their LCM.
- ④ Write the integer in a bracket to get Miller indices.

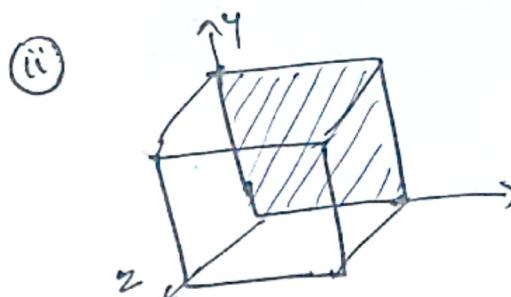
Ans: Get the miller indices of plane.



$$\text{intercept} = \left(\frac{1}{2}, 1, 1\right)$$

$$\therefore \text{reciprocal} = (2, 0, 0)$$

$$\therefore \text{Miller indices} = (2, 0, 0)$$



$$\text{intercept} = (\infty, 1, 1)$$

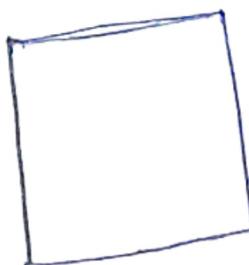
$$\therefore \text{reciprocal} = (0, 0, 1)$$

$$\therefore \text{m.i.} = (0, 0, 1)$$

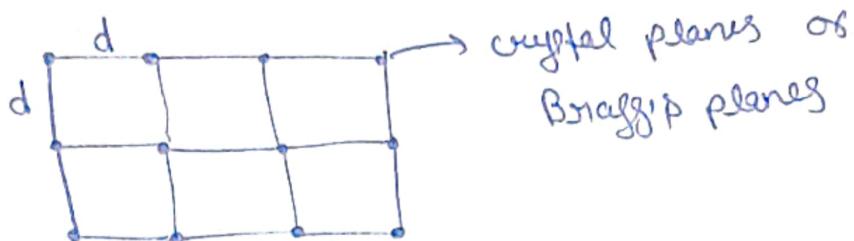
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Ans: Draw plane for miller indices (1, 0, 0). don't use comma
(negative axis lieg) use bar.

i (100)



Interplanar Distance (d): The separation b/w two successive planes is known as interplanar distance 'd'.



Relation b/w 'd' - edge length and interplanar distance 'd':

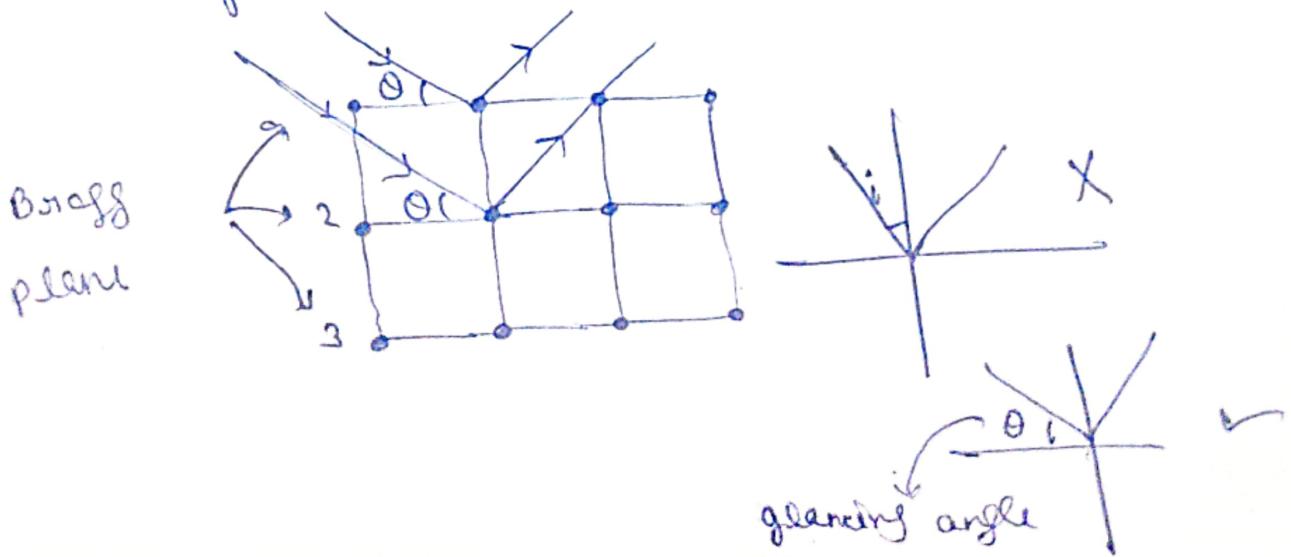
$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

where hkl are Miller indices.

In general

$$d = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$$

Glancing angle: The angle of incidence ' θ ' is measured by Bragg's plane in a crystal is known as glancing angle ' θ '



Bragg's law : (Crystal Study - X-ray)

To understand the Bragg's law consider a parallel beam of x-ray is incident on the crystal lattice at atom A and B then the light is reflected from atoms A and B. both reflected rays are coherent, interfere with each other, as a result we get constructive interference depending on their path difference.