

IES / GATE

**Electronics &
Telecommunication
Engineering**

VOLUME-II

**Material Science
Electronic Measurement**

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Chemical Bond :-

- Binding forces b/w atoms or molecules in a material are known as chemical bonds
- There are two types of chemical bonds

(a) Primary bond :-

These bonds are having higher binding energy

eg:- Ionic bond, covalent bond & metallic bond

(b) Secondary bond :-

These bonds are having lesser binding energy as compared to primary bonds

eg:- Vanderwaal forces & hydrogen bond

Ionic Bond :-

- Ionic bond results from electrostatic interaction b/w oppositely charged ions by transfer of electrons fr one to another
- Ionic bond formed particularly b/w left hand side and right hand side of periodic table are strongly ionic
- eg:- Alkali halides

Covalent Bond :-

- It is formed due to sharing of electrons
- eg:- H_2O , CO_2 , Si , Ge
- Covalent bond formed b/w similar elements is very strong
- Covalent crystals are also known as valence cryst

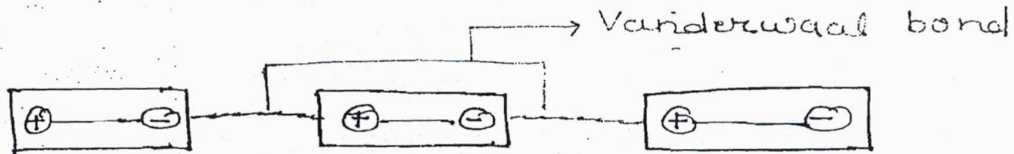
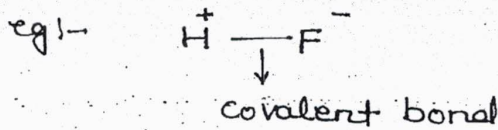
Metallic Bond :-

- Metallic bond is the characteristic of elements having small no. of valence electrons
- Metals are having large no. of free electrons in their conduction band even at room temperature because they require less amount of energy to be supplied to release their electrons from valence band to the conduction band

→ Metals can be considered as periodic structure of positive ions surrounded by large no. of electrons

Vanderwaal's Bond:-

→ Vanderwaal forces are weaker forces which are present in inert gases or materials having dipoles



→ Dipole interaction is due to the presence of vanderwaal forces

→ Hydrogen bond is a strong type of vanderwaal's bond

Atomic Arrangement in Solids:-

- Crystallinity
- Single crystal material
- Poly crystalline material
- Amorphous material.
- Epitaxial process

(i) Crystallinity :-

The property of solid in which atoms or molecules are arranged in a periodic and regular manner is called crystallinity

(ii) Single Crystal Material :-

If material is having only one type of periodic arrangement then material is called single crystal material

(iii) Poly Crystalline Material :-

A polycrystalline material is divided into no. of small regions. These regions are called grains. Each grain is having its own periodic arrangement but their periodic arrangement

varies from one grain to the other

eg:- polycrystalline silicon

Note:-

Anisotropic Material:-

If properties of material depends on the direction in which they are measured then material is called anisotropic material

eg:- single crystal materials

Isotropic Material:-

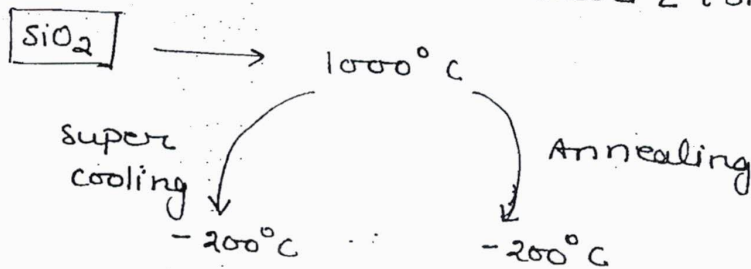
If properties of material are independent of the direction in which they are measured the material is called as isotropic material

Amorphous Material:-

→ In amorphous material, atoms upto first nearest neighbours are arranged periodically but the atoms which are away from the nearest atoms are found to be arranged randomly

→ When atoms or molecules are not given opportunity to arrange in regular and periodic manner, an amorphous material may be formed

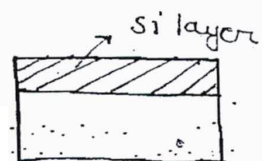
eg:- supercooled state of SiO_2 is known as Glass (Amorphous material), whereas on annealing SiO_2 may crystallise into Quartz (Single crystal material)



→ In other cases molecules may be extremely long and irregular in shape so that periodic arrangement may not be obtained as in the case of polymers

v) Epitaxial Process:-

It refers growth of a layer of silicon on a substrate



Note :-

Annealing :-

It is a process of heating & slow cooling

Ques :- In a Si crystal, arrangement of atoms repeats periodically. This material can be classified as

- (a) Non-crystalline and amorphous
- (b) Epitaxial and non-crystalline
- (c) Single crystal and epitaxial
- (d) Single crystal and amorphous

Ans - (c)

Cubic Crystal Structure :-

Unit cell :-

It is defined as the minimum area cell in 2-dimension or the minimum volume cell in 3-dimension by repetition of which a crystal may be formed

Parameters of Unit cell :-

- (i) Unit cell dimension
- (ii) Angle b/w axis
- (iii) No. of atoms per unit cell
- (iv) Atomic packing factor (APF)

$$APF = \frac{\text{Sum of atomic volume}}{\text{Volume of unit cell}}$$

$$= \frac{\text{No. of atoms per unit cell} \times \text{Vol. of an atom}}{\text{Volume of unit cell}}$$

Coordination Number :-

The no. of atoms which are in physical contact with a particular atom in the crystal structure is known as coordination no

Type of cubic lattices :-

- (i) Simple cubic
- (ii) Body centred cubic (BCC)
- (iii) Face centred cubic (FCC)

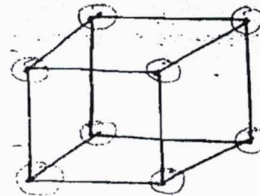
Simple Cubic :-

In simple cubic, there are 8 atoms at 8 corners of the cube

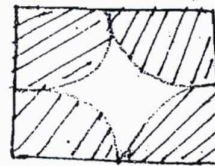
→ Atoms are in physical contact along edge of the cube

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

$$\rightarrow \text{No. of atoms per unit cell} = 8 \times \frac{1}{8} = 1$$



$$\rightarrow \text{APF} = \frac{1 \times \frac{4}{3} \pi r^3}{a^3} = 0.52$$



→ Coordination number : $3 \times 2 = 6$

eg:- Mn, Polonium, fluor spar etc

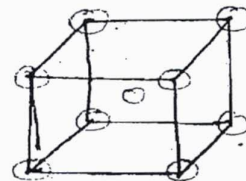
Body Centred Cubic :-

In BCC, there are 8 atoms at 8 corners of the cube and one atom is located at the center of the unit cell

→ Atoms are in physical contact along body diagonal

$$\rightarrow \sqrt{3}a = 4r \Rightarrow r = \frac{\sqrt{3}}{4}a$$

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



→ Coordination No : 8

eg:- Li, Na, K, Cr, Fe (α type), Fe (δ -type) etc

Face centred cubic :-

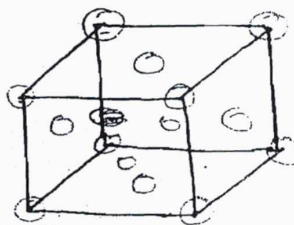
→ In FCC, there are 8 atoms at 8 corners of the cube and 6 atoms are located at the centre of six faces of the cube

→ Atoms are in physical contact along face diagonal

$$\rightarrow a\sqrt{2} = 4r \Rightarrow a = 2\sqrt{2}r$$

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

$$= 0.742$$



→ Coordination No : 12

→ eg:- Au, Ag, Cu, Pt, Pb, Ni, NaCl, Fe (V-type) etc

Note:-

→ FCC is an example of closed packed structure

→ It is also known as cubic closed packed

→ In FCC every third layer is identical

→ If an atom is surrounded by six other atoms in the same layer then structure is known as closed packed structure

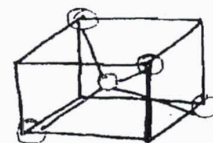
Diamond cubic :-

→ Diamond cubic unit cell is having contributions of 18 atoms (8 corner atoms, 6 face centred atoms & 4 atoms are completely inside)

→ No. of atoms per unit cell - $8 \times \frac{1}{8} + 6 \times \frac{1}{2} + 4 = 8$

→ In diamond cubic atoms are connected in tetrahedral form

smaller cell < Unit cell



→ Coordination No - 4

$$\rightarrow APF = \frac{8 \times \frac{4}{3} \pi r^3}{a^3} = \frac{32}{3} \times \frac{22}{7} \times \frac{a^3 \sqrt{3}}{64 \times 8 \times a^3}$$

$$= 0.34$$

→ Diamond cubic structure is also known as Zinc Blende (ZnS)

→ Group - III - V compounds are having zinc blend structure

eg:- Diamond, C, Si, Ge. & Group III-V compounds [GaAs, GaP, AlP etc]

Hexagonal Close Packing (HCP):-

→ HCP unit cell is having

(i) 12 corner atoms

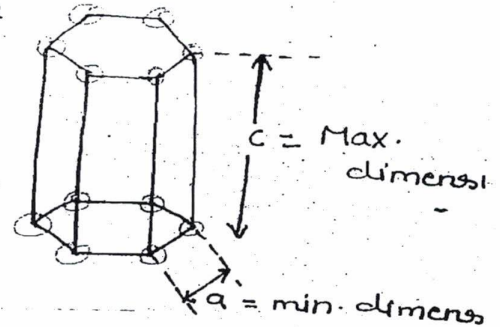
(ii) 2 face centred atoms, in top and bottom hexagon

(iii) 3 atoms are completely inside

→ No. of atoms = $8 \times \frac{1}{6} + 6 \times \frac{1}{6} + 2 \times \frac{1}{2} + 3$

$$= 1 + 1 + 1 + 3$$

$$= 6$$



$$\rightarrow \text{APF} = \frac{6 \times \frac{4}{3} \pi r^3}{a^3}$$

$$= 0.74$$

→ Coordination No: 12

$$\rightarrow \frac{c}{a} = \frac{\text{Max. dimension}}{\text{Min. dimension}} = 1.63$$

→ It is an example of closed pack structure

→ In HCP, every alternate layer is identical

eg:- Be, Cd, Co, Zn, Mg etc

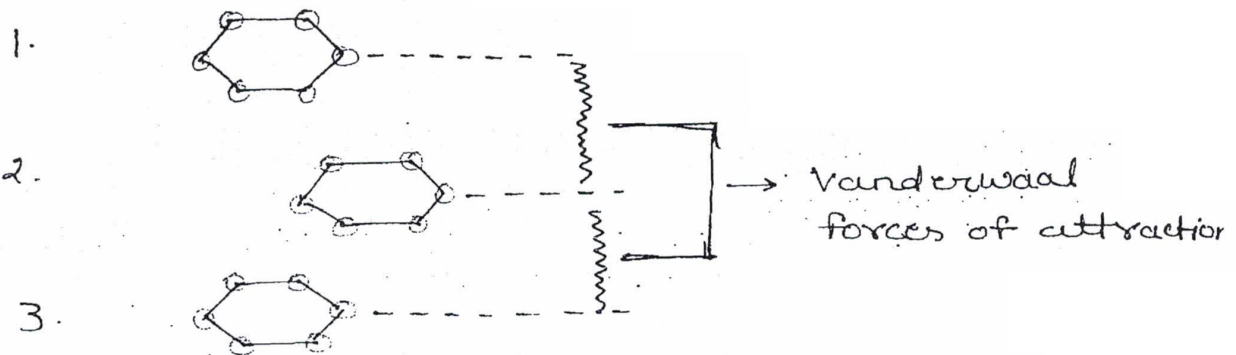
Graphite:-

→ Structure of graphite is hexagonal but it is not HCP as there is no centre atom in the hexagon

→ Each carbon atom has 4 valence electrons, 3 of these valence electrons are used in forming covalent

bond with adjacent atoms in the same layer. The 4th electron is free to move over the surface of the layer making graphite an electrical conductor.

→ Between layers force of attraction is van der Waals because these forces are weak, layers of graphite can slide on each other. Due to sliding property of layers, graphite is used as a lubricant.



Comparison b/w Diamond and Graphite :-

| <u>Property</u> | <u>Diamond</u> | <u>Graphite</u> |
|-------------------------|----------------|--------------------|
| Hardness | Extremely hard | Soft |
| Transparency | Transparent | opaque |
| Electrical conductivity | Insulator | conductor |
| Structure | Tetrahedral | Hexagonal ≠ HCP |

Ques:- Consider the statements related to FCC structure

- (i) Coordination No. is 12
- (ii) APF is 0.74
- (iii) There is an atom at the body centre of the unit cell.

Which of these statements are correct?

Ans:- (i) and (ii)

Ques :- Which of the following statements are true diamond structure

- i) Coordination No. is 4
- ii) Packing fraction is 0.34
- iii) Cu crystallises into diamond structure

Ans :- (i) and (ii)

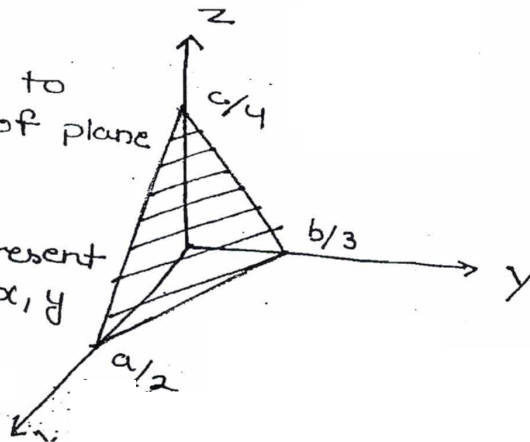
Comparison :-

| Structure | APF | No. of atoms per unit cell | Coordination No. | Atomic Radius (r) | Example |
|---------------------|------|----------------------------|------------------|-------------------------|---|
| Diamond Cubic | 0.34 | 8 | 4 | $\frac{a\sqrt{3}}{8}$ | Grp III-Compounds Si, Ge, C Diamond |
| Simple Cubic | 0.52 | 1 | 6 | $\frac{a}{2}$ | Mn, Polonium fluorspar |
| BCC | 0.68 | 2 | 8 | $\frac{a\sqrt{3}}{4}$ | Li, Na, K Cr, Fe α -type Fe (δ -type) |
| FCC (ABC ABC...) | 0.74 | 4 | 12 | $\frac{a\sqrt{2}}{4}$ | Au, Ag, Cu Pt, Al, Pb Ni, NaCl |
| HCP (ABAB AB) | 0.74 | 6 | 12 | $\frac{c}{a}$ = 1.63 | Fe (γ -type) Be, Cd, Co, Zn, Mg |

Miller Indices :-

> Miller indices are used to determine the direction of plane in a crystal structure

Where a, b and c represent unit cell dimension along x, y and z axis respectively



Steps to determine Miller Indices:-

(i) Determine intercept made by plane along x, y and z axis respectively

$$\frac{a}{2}, \frac{b}{3}, \frac{c}{4}$$

(ii) Express intercepts as multiples of unit cell dimensions

$$\frac{1}{2}, \frac{1}{3}, \frac{1}{4}$$

(iii) Get reciprocal of multiples

$$2, 3, 4$$

(iv) Reduce reciprocals to the smaller set of integers [2, 3, 4]

Ques:- Miller indices

| | |
|------------|---|
| Intercepts | 2a, 3b, 4c |
| Multiples | 2, 3, 4 |
| Reciprocal | $\frac{1}{2}, \frac{1}{3}, \frac{1}{4}$ |
| Integers | [6, 4, 3] |

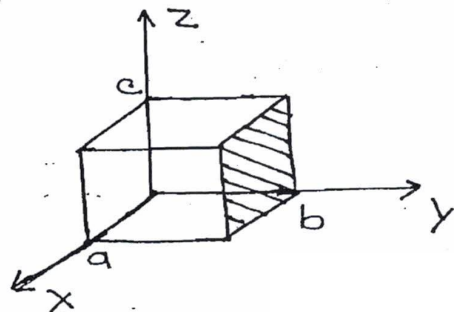
Ques:- Determine miller indices for black shaded position

Solⁿ:- Intercept :- ∞, b, ∞

Multiple :- $\infty, 1, \infty$

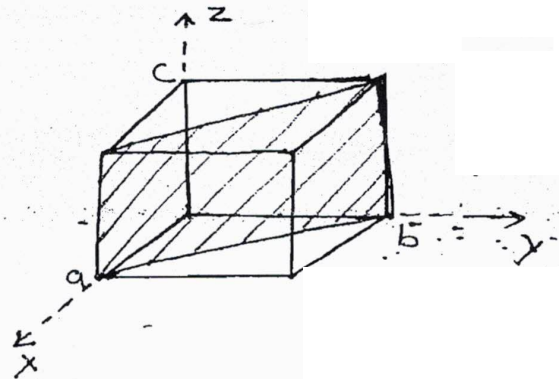
Reciprocal :- 0, 1, 0

Integers :- [0, 1, 0]



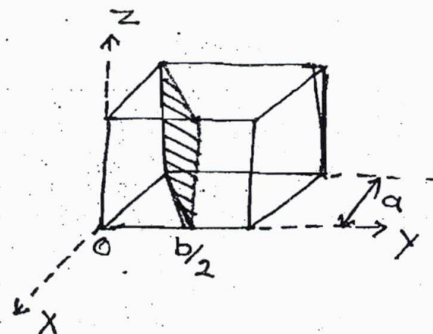
Ques:- Unit cell dimensions are a, b, c . Determine Miller indices for shaded portion

Soln:-
 Intercept:- a, b, ∞
 Multiplier:- $1, 1, \infty$
 Reciprocal:- $1, 1, 0$
 Integers:- $[1, 1, 0]$



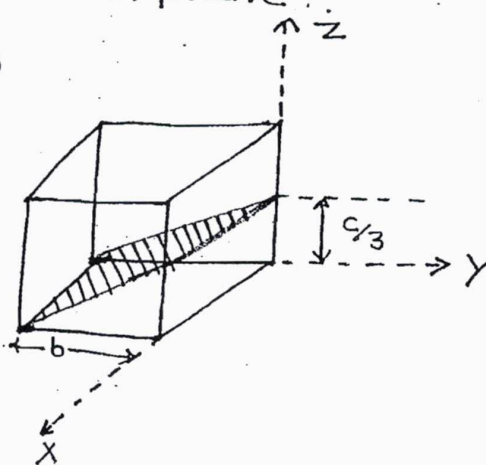
Ques:- Unit cell dimensions are a, b & c . Determine Miller indices for black shaded plane

Soln:-
 Intercepts:- $-a, b/2, \infty$
 Multiplier:- $-1, 1/2, \infty$
 Reciprocal:- $[-1, 2, 0]$
 Integers:- $[\bar{1}, 2, 0]$



Ques:- Unit cell dimensions are a, b & c . Determine the Miller indices for black shaded plane.

Soln:-
 Intercepts:- $\infty, -b, c/3$
 Multiplier:- $\infty, -1, 1/3$
 Reciprocal:- $0, -1, 3$
 Integers:- $[0, \bar{1}, 3]$



Interplanar Separation: -

Distance b/w two parallel adjacent p in a crystal structure is known as interplanar separation

For cubic crystal system, interplanar separation

$$d = \frac{a}{\sqrt{l^2 + m^2 + n^2}}$$

where a = edge length of cube

[l, m, n] = Miller indices for given plane

ques:- A material has a FCC structure with atom radius 1.06 \AA . Calculate the interplanar separation for [1, 1, 0] planes

Soln:- $\rightarrow r = 1.06 \text{ \AA}$

$\rightarrow [l, m, n] = [1, 1, 0]$

\rightarrow FCC:

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

$$\rightarrow d = \frac{a}{\sqrt{l^2 + m^2 + n^2}}$$

$$= \frac{2\sqrt{2}r}{\sqrt{2}} = 2r = 2 \times 1.06 \text{ \AA} = 2.12 \text{ \AA}$$

Equivalent Planes: -

\rightarrow Plane : [1, 0, 0]

[1, 0, 0] [0, 1, 0] [0, 0, 1]

[$\bar{1}$, 0, 0] [0, $\bar{1}$, 0] [0, 0, $\bar{1}$]

→ 13 Plane : $[1, 1, 0]$

$[1, 1, 0]$ $[1, 0, 1]$ $[0, 1, 1]$

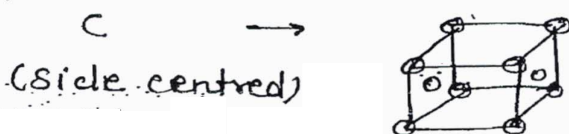
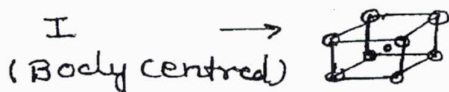
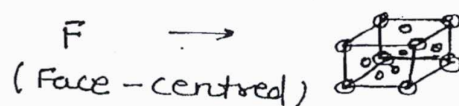
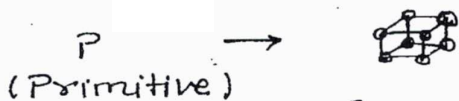
$[\bar{1}, 1, 0]$ $[\bar{1}, 0, 1]$ $[0, \bar{1}, 1]$

$[1, \bar{1}, 0]$ $[1, 0, \bar{1}]$ $[0, 1, \bar{1}]$

$[\bar{1}, \bar{1}, 0]$ $[\bar{1}, 0, \bar{1}]$ $[0, \bar{1}, \bar{1}]$

Bravais Crystal System : — } $\begin{cases} 7 \text{ Crystal System} \\ 14 \text{ Bravais lattices} \end{cases}$

| Crystal System | Unit cell Dimension | Angle b/w Axis | Bravais lattices |
|-------------------------|---------------------|---|------------------|
| Orthorhombic | $a \neq b \neq c$ | $\alpha = \beta = \gamma = 90^\circ$ | P, I, C, F |
| Monoclinic | $a \neq b \neq c$ | $\alpha = \beta = 90^\circ \neq \gamma$ | P, C |
| Triclinic | $a \neq b \neq c$ | $\alpha \neq \beta \neq \gamma \neq 90^\circ$ | P |
| Hexagonal | $a = b \neq c$ | $\alpha = \beta = 90^\circ, \gamma = 120^\circ$ | P |
| Tetragonal | $a = b \neq c$ | $\alpha = \beta = \gamma = 90^\circ$ | P, I |
| Trigonal / Rhombohedral | $a = b = c$ | $\alpha = \beta = \gamma \neq 90^\circ$ | P |
| Cubic | $a = b = c$ | $\alpha = \beta = \gamma = 90^\circ$ | P, I, F |



Ques:- Match List I & List -II

List - I

List - II

1. Hexagonal

A $a=b=c$, $\alpha = \beta = \gamma \neq 90^\circ$

2. Rhombohedral

B $a=b \neq c$, $\alpha = \beta = \gamma = 90^\circ$ $\neq \gamma$

3. Triclinic

C $a \neq b \neq c$, $\alpha = \beta = \gamma \neq 90^\circ$

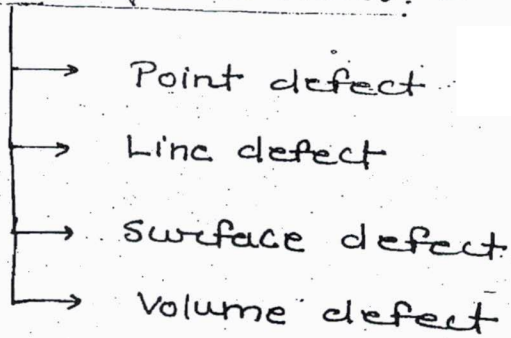
4. Monoclinic

D $a \neq b \neq c$, $\alpha \neq \beta \neq \gamma \neq 90^\circ$

Soln

1 2 3 4
 → B A B C

Structural Imperfections:-



Point defect:-

Point defect is a localised imperfection which does not spread more than 1 or 2 unit cells

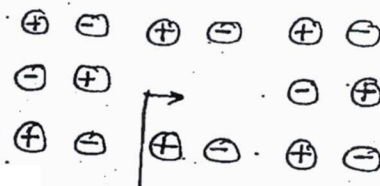
→ There are two types of point defect

- (i) Vacancy defect (ii) Impurity defect

1) Vacancy defect:-

It arises due to absence of atom or molecule in the crystal structure

eg:- Schottky defect



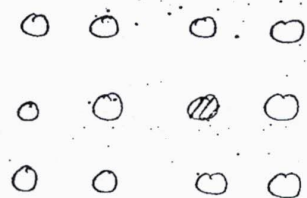
Missing pair of ions

2. Impurity Defect :-

It arises when an impurity atom is introduced in the crystal structure either as an interstitial or substitutional

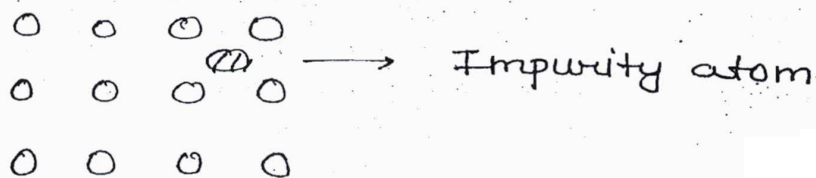
(a) Substitutional type Impurity defect :-

It arises when impurity atom replaces a parent atom of crystal.



(b) Interstitial type Impurity defect :-

It arises when an impurity atom occupy free space or void available in the crystal structure



Dielectric Properties of Material :-

→ Dielectrics are non-conducting material which can be polarised with an application of electric field

→ Non-conducting materials are divided into two categories

- (i) Insulator (ii) Dielectric

(i) Insulator :-

If the main function of non-conducting material is to provide electric insulation then material is called insulator