

T.Y.B.Sc. SEM – VI

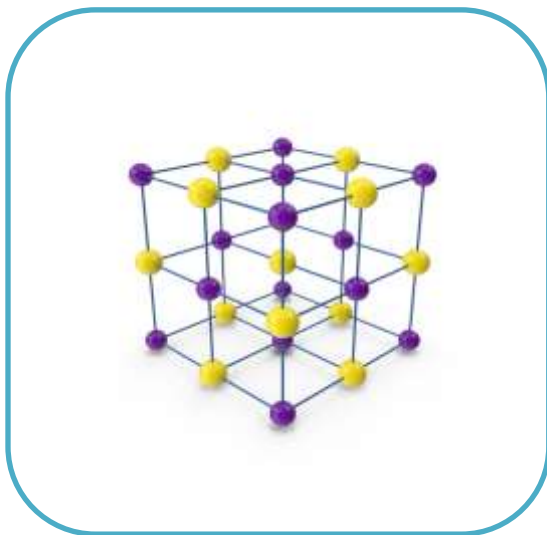
Subject: Physics

Paper- 602

Unit -2



CRYSTAL STRUCTURE



- Introduction
- Lattice
- Unit cell
- Bravais lattice
- Crystal planes
- Crystal structure
- Miller Indices
- Application

INTRODUCTION:

Part-A (SAQ-2Marks)

1) Define a) Space Lattice b) Basis c) Co-ordination number d) Packing factor e) Miller Indices.

a) **Space lattice:** is defined as an infinite array of points in three dimensions in which every point has surroundings identical to that of every other point in the array.

b) **Basis:** Group of atoms or molecules identical in composition.

Lattice + basis = crystal structure

c) **Co-ordination number:** The no of equidistant neighbors that an atom has in the given structure. Greater the co-ordination no, the atoms are said to be closely packed.

For Simple Cubic: 6, BCC: 8, FCC: 12

d) **Packing factor (PF):** It is the ratio of volume occupied by the atoms or molecule in unit cell to the total volume of the unit cell.

$$\text{Atomic Packing Factor (APF)} = \frac{\text{Volume of all the atoms in Unit cell}}{\text{Total Volume of the Unit cell}}$$

For Simple Cubic: 52%, BCC: 68%, FCC: 74%

e) **Miller Indices:** are the reciprocals of intercepts made by the planes on the crystallographic axis when reduced to smallest integers.

2) Describe seven crystal systems with lattice parameters and Bravais Lattice points.

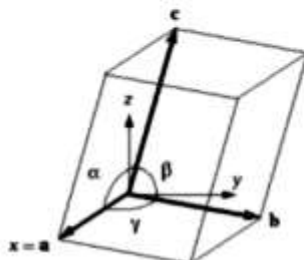
S:No	Name of the crystal systems	Primitives	Interfacial angles	Bravais Lattice points
1	Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	3(P,I,F)
2	Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	2(P,I)
3	Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	4(P,C,I,F)
4	Monoclinic	$a \neq b \neq c$	$\alpha = \beta = 90^\circ \neq \gamma$	2(P,C)
5	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	1(P)
6	Trigonal	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	1(P)
7	Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ$ and $\gamma = 120^\circ$	1(P)

3) Define a) Crystal Structure b) Lattice Parameters c) Unit Cell d) Atomic radius (r).

a) **Crystal structure:** periodic arrangement of atoms or molecules in 3D space.

b) **Lattice parameters:** the primitives (a,b,c) and interfacial angles (α, β, γ) are the basic lattice parameters which determine the actual size of unit cell.

c) **Unit cell:** is a minimum volume cell which on repetition gives actual crystal structure.



d) Atomic radius (r) – The atomic radius is defined as half the distance between neighboring atoms in a crystal of pure element.

4) What are properties of matter Waves.

De-Broglie proposed the concept of matter waves, according to which a material particle of mass 'm', moving with a velocity 'V' should have an associated wavelength ' λ ' called de-Broglie wavelength.

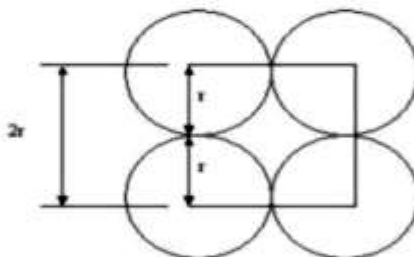
$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

Wavelength is associated with moving particle and independent of charge of the particles. Greater the mass, velocity of the particle, lesser will be the wavelength.

Part- B (Descriptive- 10marks)

1) Calculate the Packing factor of SC, BCC, FCC (or) Show that FCC is the closest packing of all the three cubic structures.

Simple cubic: There are 8 atoms at 8 corners of the cube. The corner atoms touch with each other. If we take a corner atom as a reference, this atom is surrounded by 6 equidistant nearest neighbors.



Co-ordination number: - (N) = 6:- is defined as number of equidistant nearest neighbors that an atom has in the given structure.

Total number of atoms :- (n) = 1:- each corner atom is shared by 8 unit cells, the share of each corner atom to a unit cell is $1/8^{\text{th}}$ of an atom ($8 \times 1/8 = 1$)

Nearest neighbor distance (2r):- the distance between centers of two nearest neighbor atoms will be $2r$ if ' r ' is the radius of the atom.

Atomic radius: - (r) = $2r$:- is defined as the distance between nearest neighbors in a crystal.

Lattice constant: - $a = 2r$

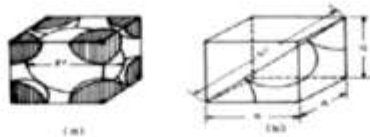
Atomic Packing Factor (APF) = $\frac{\text{Volume of all the atoms in Unit cell}}{\text{Total Volume of the Unit cell}}$

$$\frac{1 \times \frac{4}{3} \pi r^3}{a^3 = (2r)^3} = 52\%$$

Ex:-polonium at room temperature.

Body centered Cubic (BCC):

In a unit cell there are 8 atoms at 8 corners and another 1 atom at the body center. The 8 corner atoms are shared by 8 unit cells, and as the center atom is entirely within the unit cell, it is not shared by any surrounding unit cell.



Co-ordination number = 8

$$\text{Nearest neighbor distance} = \frac{a\sqrt{3}}{2}$$

$$\text{Lattice constant} = a = \frac{4r}{\sqrt{3}}$$

Number of atoms per unit cell = $v = 1$

$$\text{Volume of all atoms in unit cell} = v = 2 \times \frac{4}{3} \pi r^3$$

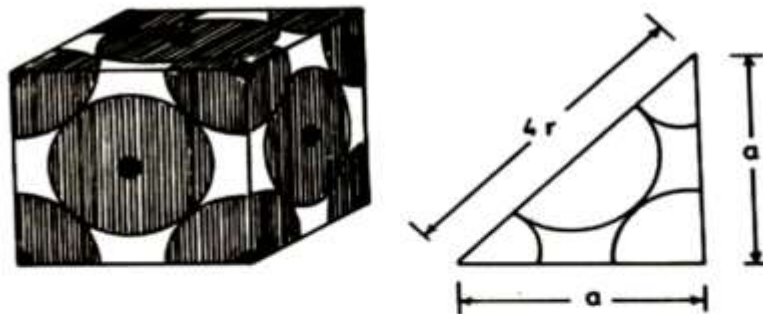
$$\text{Volume of unit cell} = V = a^3 = \left(\frac{4r}{\sqrt{3}}\right)^3$$

$$\text{Atomic Packing Factor is } \frac{2 \times \frac{4}{3} \pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3} = 0.68 = 68\%$$

Ex: - Li, Na, K, and Cr.

Face centered structure (FCC)

In FCC there are 8 atoms at 8 corners of the unit cell and 6 atoms at 6 faces. Considering the atoms at the face center as origin, it can be observed that this face is common to 2 unit cells and there are 12 points surrounding it situated at a distance equal to half the face diagonal of the unit cell.



Co-ordination number = $N = 12$

$$\text{Number of atoms in unit cell} = 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$$

$$\text{Lattice constant} = a = 2r = \frac{\sqrt{2}a}{2}$$

$$\text{Volume of the unit cell} = V = a^3 = \left(\frac{4r}{\sqrt{2}}\right)^3$$

$$\text{Volume of all atoms in unit cell} = v = 4 \times \frac{4}{3} \pi r^3$$

$$\text{Atomic Packing Factor} = \frac{v}{V} = \frac{4 \times \frac{4}{3} \pi r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3} = 0.74 = 74\%$$

Ex:- Cu, Al, Pb, and Ag.

By the above values of Atomic packing factors we can say that FCC is the closest packed structure of all the three cubic structures.

2) Explain the significance of Miller indices and derive an expression for interplaner distance in terms of Miller indices for a cubic Structure.

Miller indices: are the reciprocals of intercepts made by the crystal planes on the crystallographic axes when reduced to smallest integers.

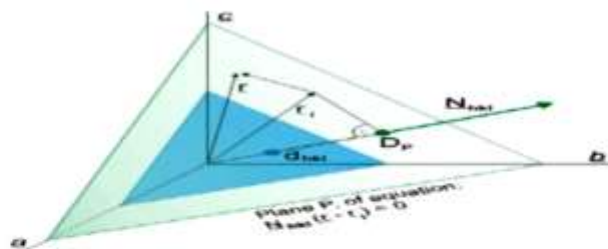
Important features of Miller indices:

- Miller indices represent a set of parallel equidistant planes.
- All the parallel equidistant planes have the same Miller indices.
- If a plane is parallel to any axis, then the plane intersects that axis at infinity and Miller indices along that direction is zero.
- If the miller indices of the two planes have the same ratio (844,422,211), then the planes are parallel to each other.
- If a plane cuts an axis on the -ve side of the origin, then the corresponding index is -ve, and is indicated by placing a minus sign above the index.

Ex: if a plane cuts -ve y-axis, then the miller index of the plane is $(h \bar{k} l)$

Derivation:

- Consider a crystal in which the three axes are orthogonal and the intercepts are same. Take 'o' as origin, and the reference plane passes through the origin i.e entirely lies on the axis.
- The next plane ABC is to be compared with the reference plane which makes the intercepts $\frac{a}{h}, \frac{b}{k}, \frac{c}{l}$ on x,y,z axes respectively.
- Let $(h k l)$ be the miller indices.
- Let $ON=d$ be a normal drawn to the plane ABC from origin 'o' which gives the distance of separation between adjacent planes.
- Let the normal ON makes an angles α, β, γ with x,y,z axes respectively. Angle $\alpha = NOA$, angle $\beta = NOB$, angle $\gamma = NOC$.



- Then form Δ i.e NOA

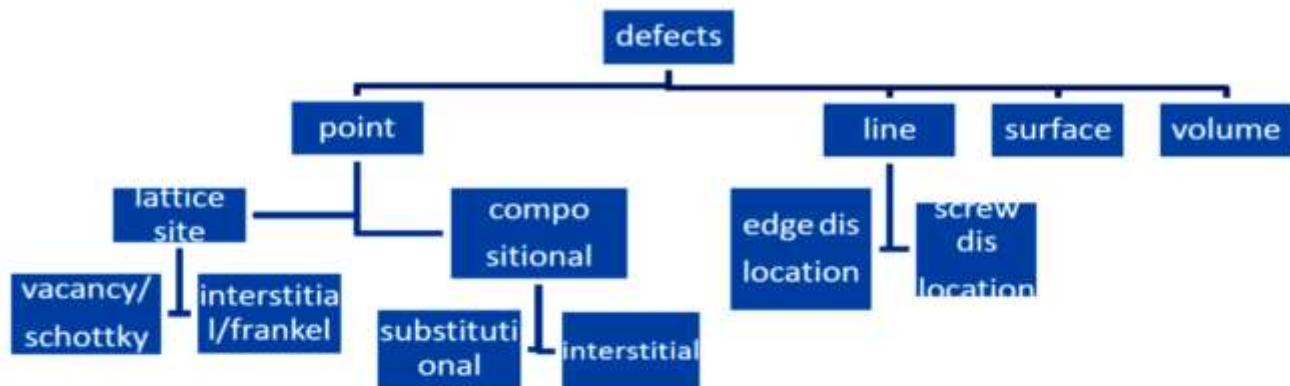
$$\cos \alpha = \frac{ON}{OA} = \frac{d}{a/h} = \frac{dh}{a}$$
- Similarly $\cos \beta = \frac{ON}{OB} = \frac{d}{b/k} = \frac{dk}{b}$
- $\cos \gamma = \frac{ON}{OC} = \frac{d}{c/l} = \frac{dl}{c}$
- According to cosine law of directions, $\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = 1$
- Therefore $\left(\frac{dh}{a}\right)^2 + \left(\frac{dk}{b}\right)^2 + \left(\frac{dl}{c}\right)^2 = 1$
- $d^2 \left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right] = 1$
- In a cubic crystal $a = b = c$,
- Therefore

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

- Therefore $d^2 = \frac{a^2}{h^2+k^2+l^2}$
i.e $d = \frac{a}{\sqrt{h^2+k^2+l^2}}$

3) Classify the defects and write a short note on Point defects.

- Defects are broadly classified into



Point defects: (zero dimensional defects) arises when an atom is absent from the regular position, presence of impurity atom or atom in the wrong place during crystallization. These are small defects which extends its influence in all directions but limited to a specific region of small order (two or three atomic orders).

Vacancy: missing of an atom from its original lattice site. Generally arises due to thermal vibrations during crystallization and influenced by external parameters. Vacancies may be single, two or more depending on crystal type. For most of the crystals, in order to create one vacancy thermal energy of 1.1 eV is required.

Interstitial: this defect arises when an atom of same kind or different kind occupies the void space between the regular atomic sites.

Impurity atom: an atom that does not belong to the parent lattice (original crystal).

Substitution defects: this defect arises when an impurity atom replaces or substitutes parent atom. Ex: in brass, zinc is a substitution atom in a copper lattice

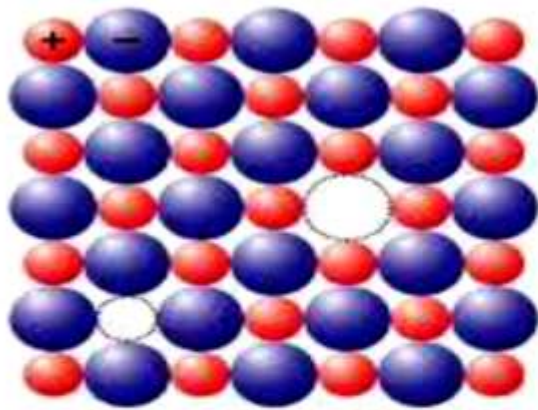
Interstitial impurity: this defect arises when an impurity atom which is small in size is placed between the regular atomic sites.

Ex: when pentavalent and trivalent impurities are added to pure Si or Ge, we get n- type and P-type semiconductors.

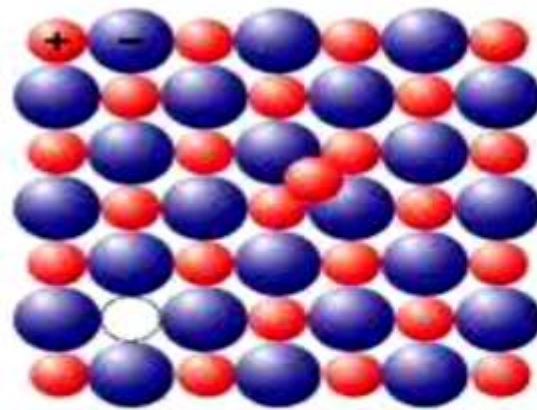


In case of ionic crystals imperfections appear in crystals while maintaining the electrical neutrality. Two types of defects (point defects) occur in ionic crystals.

1. Frenkel defect 2. Schottky defect.



(a) Schottky defect



(b) Frenkel defect

Frenkel defect: When an ion is displaced from a regular lattice site to an interstitial site is called Frenkel defect. Generally cations which are small in size are displaced to an interstitial site as the interstitial space is small. A Frenkel imperfection does not change the overall electrical neutrality of the crystal.

Schottky defect: A pair of one cation and one anion missing from the original lattice site on to the surface of the crystal so that charge neutrality is maintained in the crystal is called Schottky defect.

4) Write a short note on line defects. (or) What are edge and screw dislocations?

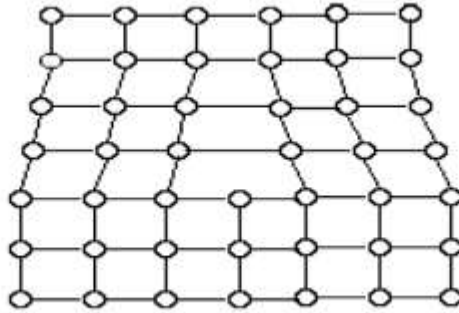
Line defects (or) dislocations (one dimensional defect) are defined as the disturbed region between the two perfect parts of the crystal and these defects are formed in the process of deformation.

Edge dislocation:

- A perfect crystal is composed of several parallel vertical planes which are extended from top to bottom completely and parallel to side faces. The atoms are in equilibrium positions and the bond lengths are in equilibrium value.
- If one of the vertical planes does not extend from top to bottom face of the crystal, but ends in midway within the crystal, then crystal suffers with a dislocation called edge dislocation.
- In imperfect crystal all the atoms above the dislocation plane are squeezed together and compressed there by the bond length decreases. And all the atoms below the dislocation plane are elongated by subjecting to the tension and thereby the bond length increases.
- There are two types of edge dislocation. They are 1. Positive edge dislocation 2. Negative edge dislocation.

Positive edge dislocation: if the vertical plane starts from top of the crystal and never reaches to the bottom.

Negative edge dislocation: if the vertical plane starts from bottom of the crystal and never reaches top.



Screw dislocation:

- Atoms are displaced in two separate planes perpendicular to each other or defects forming a spiral around the dislocation line.
- A screw dislocation marks the boundary between slipped and unslipped parts of the crystal that can be produced by cutting the crystal partway and then sheering down one part relative to the other by atomic spacing horizontally.

