

THEORY & OBJECTIVE

MATERIAL SCIENCE

*By
Team of
Engineers Academy*



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BASICS OF ENGINEERING MATERIAL

THEORY

1.1 | CHEMICAL BONDS

The binding force between two or more atoms or molecules are known as chemical bonds.

There are two types of chemical bonds.

- Primary
- Secondary

1.1.1 Primary Bond

These bond are inter atomic bond.

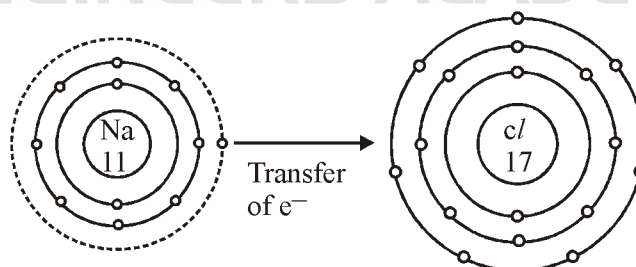
These bond are having higher bond energy.

Ex. Ionic, covalent and metallic bond.

Ionic Bond : Ionic bond is a bond resulting from the electrostatic interaction of opposite ions by transfer of e^- from one to another.

Ionic solid are formed particularly elements on the left and right hand side of the periodic table.

Ex. Alkali halide (Group I and Group VII elements) $NaCl$, KCl et.)

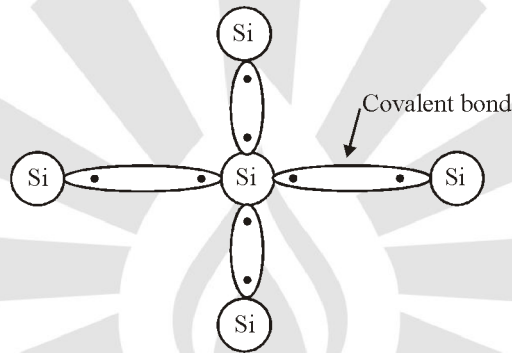


General Characteristic of Ionic Bond

- Moderate to high strength
- Higher hardness
- Brittle (can be break)
- Malleable (can be mould)
- Electrically neutral
- High melting point

Covalent Bond : Covalent bond is formed by sharing of e^- between neighboring atoms.

Ex. Si, Ge, CO_2 .



General Characteristic of Covalent Bond

- High strength
- High melting point
- Brittle
- Electrical conductivity depends upon Bond strength
- Tin : Conductor (weak covalent bond)
- Si, Ge : Semi conductor (moderate)
- Diamond : Insulator (High)

Metallic Bond : This type of bond is in the element having small number of valence electron, which are loosely held, so that they can be easily released to the common pool.

The Metallic bonding results when each of the atoms of the metal contributes its valence e^- to the formation of an e^- cloud that pervades the solid metal.

General Characteristic of Metallic Bond

- High electrical and thermal conductivity
- Metals are opaque

- They are having surface luster
- Metallic bond are non directional (it means bond strength is equal in all direction)

Ex. Alkali metals (highest metallic bonding)

1.1.2 Secondary Bond

These bonds are inter molecular bond.

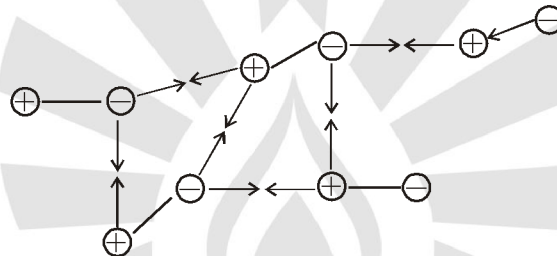
These bonds are having lesser bond energy as compare to primary bond.

Ex. Vanderwall bond, hydrogen bond.

Vanderwall Bond : Weak or secondary bond known as vander wall force can link molecules that posses a non symmetric distribution of charge.

Dipole interaction between molecules or atoms is due to presence of vanderwall force of attraction.

Ex. HF, H₂O, solid Ar, Solid He, solid hydrogen etc.



Hydrogen bond is a strong type of vanderwall's bond

1.2 | ATOM ARRANGEMENT IN MATERIALS

Arrangement of atoms in a material has significant effect on properties.

Depending on the manner of atomic grouping, materials are classified as

1.2.1 Molecular Structure

Molecular structure have a distinct number of atoms that are held together by primary bonds, but they have only relatively weak bonds with other similar group of atoms.

Ex. O₂, H₂O, C₂H₄ etc.

1.2.2 Crystal Structure

Crystal structure are assumed by solid materials and most minerals.

Atoms are arranged in a regular geometrical array known as space lattice.

1.2.3 Amorphous Structure

The atoms have a certain degree of local order but when viewed as an aggregate, have a more disorganized atoms arranged than the crystalline solid.

Ex. Glass

1.3 | ATOMS ARRANGEMENT IN SOLID

1.3.1 Crystalline Material

Atoms self-organize in a periodic manner is called crystalline material.

1.3.2 Single Crystal Material

Atoms are in a repeating or periodic manner over the entire extent of the material.

These material are anisotropic materials.

Ex. Quartz.

Anisotropic Material : The material in which properties depend on the direction in which they are measured is called anisotropic material.

Ex. Single crystal material

Isotropic Material : The material in which properties are independent of the direction in which they are measured is called isotropic material.

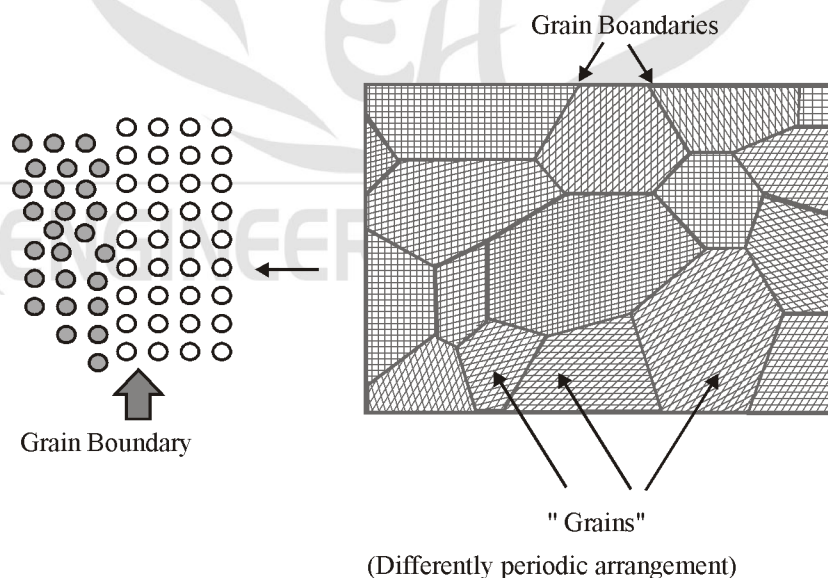
Ex. Polycrystalline material

1.3.3 Poly Crystalline Material

These material are divided into no. of small regions. These regions are called grain. within each grain. molecular arrangement is regular or periodic but this arrangement varies from are grain to another.

Ex. Polycrystalline silicon

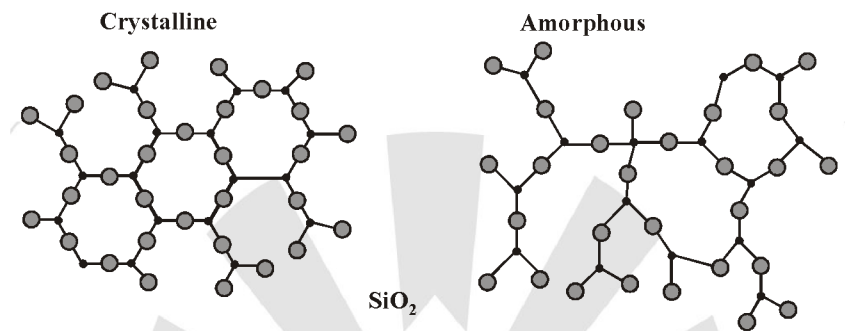
These materials are isotropic



1.3.4 Amorphous Material

In amorphous material, atoms upto first nearest neighbour are arranged periodically but atoms which are far away from nearest atoms are found to be arranged randomly.

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



Ex. Super cooled state of SiO_2 is called glass (amorphous material)

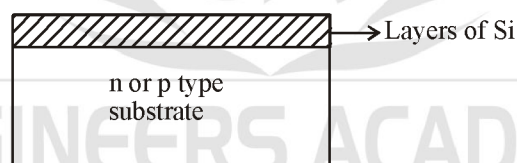
Note :

- On annealing (heating and cooling) SiO_2 crystallizes into Quartz.
- In some cases molecules may be extremely long and irregular in shape so that periodic or regular arrangement may not be obtained.

Ex. Polymers

1.3.5 Epitaxial Material

The process of growth of a layer of silicon over a substrate is called epitaxial and the material through layer is made is called epitaxial material.



1.4 | UNIT CELL

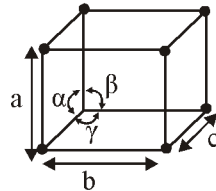
It is defined as the minimum area cell in 2-dimension or minimum volume cell in 3 dimension by repetition of which a crystal may be formed.

Parameters of unit cell :

- Unit cell dimension
- Angle between axis

- Number of atoms per unit cell
- Co-ordination number
- Atomic packing factor (APF)

Ex. $\angle \alpha : a, c$
 $\angle \beta : b, a$
 $\angle \gamma : c, b$



Co-ordination Number : The no. of atoms which are in physical contact with a particular atoms in a crystal structure is called co-ordination number.

Atomic packing factor (APF) : APF or packing efficiency indicates how closely atoms are packed in unit cell.

$$\text{APF} = \frac{\text{No. of atoms per unit cell} \times \text{Atomic volume}}{\text{Volume of unit cell.}}$$

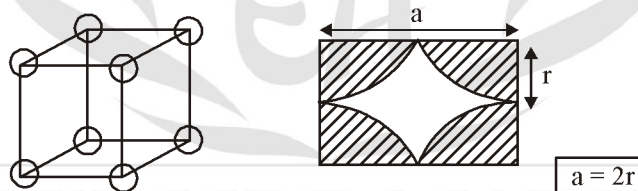
Lattice : Periodically or orderly arrangement of unit cell is called lattice.

1.5 | CUBIC CRYSTAL STRUCTURE

1.5.1 Simple Cubic

In a simple cubic there are 8 atoms at eight corner of a cube.

Atoms are in physical contact along edge of the cube.



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

$$\text{APF} = \frac{1 \times \frac{4}{3} \pi r^3}{a^3} = \frac{\frac{4}{3} \pi \left(\frac{a}{2}\right)^3}{a^3} = 0.52$$

Co-ordination no. = 6.

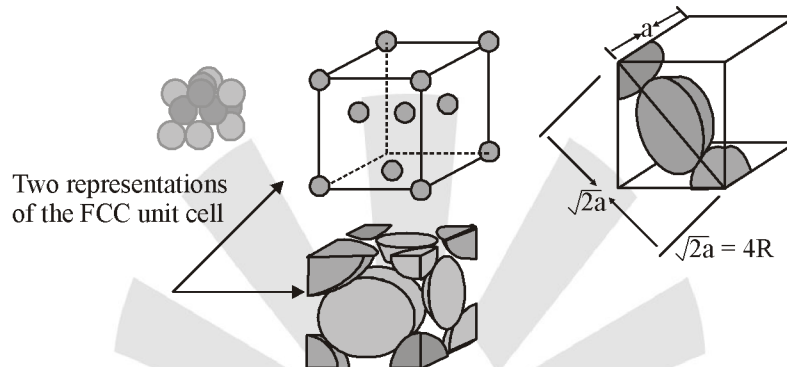
Ex. Mn, Polonium, Flourspar etc

1.5.2 Face Centered Cubic (FCC)

In FCC, there are 8 atoms at 8 corner of the cube and 6 atom at the centre of 6 faces of the cube.

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

Atoms are in physical contact along face diagonal



Cube length edge

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

$$\text{APF} = \frac{4 \times \frac{4}{3} \pi r^3}{a^3} = 0.74.$$

Co-ordination number = 12

Corner and face atoms in the unit cell are equivalent

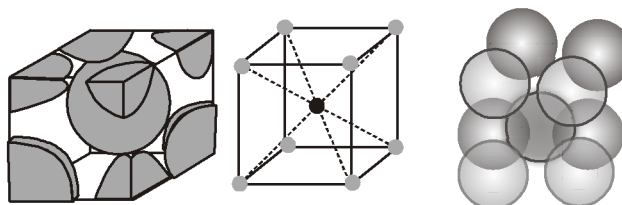
FCC crystal structure has APF of 0.74, the maximum packing for a system (FCC has closed pack structure).

Ex. Gold (Au), Ag, Pt, Cu, Ni, Pb, Fe (γ -type), Al etc.

1.5.3 Body Centered Cubic (BCC)

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

Atoms are in physical contact along body diagonal or in cubic diagonal.

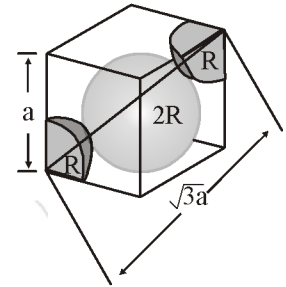


Cube edge length, $a = \frac{4R}{\sqrt{3}}$

Co-ordination number = 8

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

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



Body and corner atoms of unit cell are equivalent

Ex. Li, Na, K, Cr, Mn, Cb, W, Ti, Fe (α – iron, δ -iron) etc.

1.5.4 Diamond Cubic

Diamond cubic unit cell is having contribution of 18 atoms, out of 18 atoms

- (i) 8 atoms are corner atoms
- (ii) 6 atoms are face centered atoms
- (iii) Remaining 4 atoms are completely inside

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

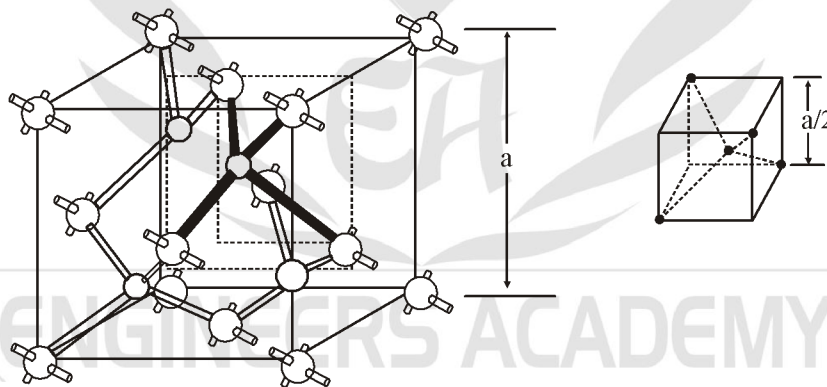


Fig. : Tetrahedral Structure of Closest Neighbor in Diamond Lattice

Length of cube $a = 8r/\sqrt{3}$ or $r = a \sqrt{3}/8$

$$\text{APF} = \frac{8 \times \frac{4}{3} \pi r^3}{a^3} = 0.34$$

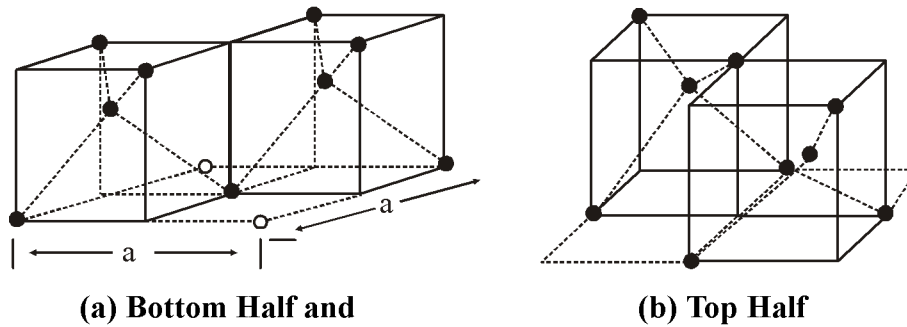


Fig. : Portions of the Diamond Lattice

Diamond cubic structure is similar to zinc blende structure

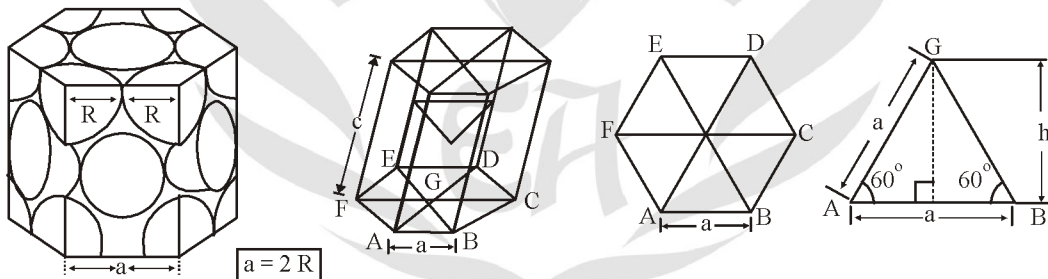
Group (III-V) compounds are having zinc blende structure

Ex. Diamond, C, Si, Ge, group II-V compounds

1.5.5 Hexagonal Close Packing (HCP)

HCP unit cell is having

- (i) 12 corner atoms
- (ii) 2 face centre atoms in top and bottom hexagon
- (iii) 3 atoms are inside

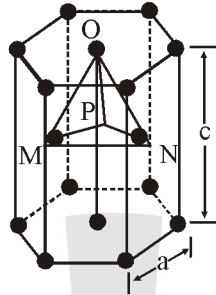


$$\text{No. of atoms per unit cell} = 3 + 2 \times \frac{1}{2} + \frac{1}{6} \times 12 = 6$$

$$\frac{c}{a} = \frac{\text{max}^m \text{ dimension}}{\text{min}^m \text{ dimension}} = 1.63$$

$$\begin{aligned} \text{Unit Cell Volume} &= \left(6 \times \frac{1}{2} \times a \times h \right) \times c \\ &= (3 \times a \times a \sin 60^\circ) \times c \\ &= 3a^2 c \sin 60^\circ \end{aligned}$$

The face-centered atom and the three mid-layer atoms from a tetrahedron MNOP which has sides equal to a (as atoms at vertices touch each other) and height of $c/2$. Using this tetrahedron it can be shown that for an ideal hexagonal crystal c/a ratio = 1.633.



$$\text{APF} = \frac{6 \times \frac{4}{3} \pi R^3}{3a^2 c \sin 60^\circ} = \frac{8\pi a^3}{3 \times 8 \times 1.414a^3} = 0.74$$

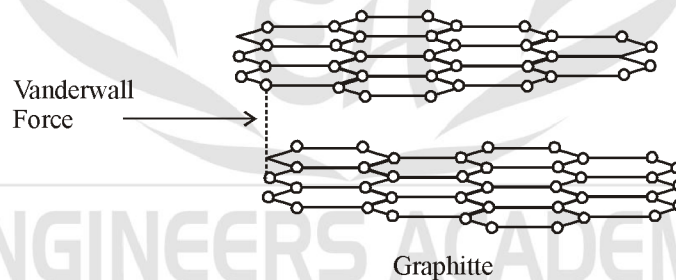
Co-ordination number of HCP unit cell is 12.

Ex. Be, Cd, Mg, Zn, Zr, etc.

Note :

- HCP and FCC are also called closed pack structure as their packing efficiency is highest i.e., 74%

1.6 | GRAPHITE



Structure of graphite is hexagonal but it is not HCP as there is no centre atom in top and bottom hexagon.

Each carbon atom has 4 valence e^- , 3 of these valence e^- are used in forming covalent bond with adjacent atom in the same layer. The 4th e^- is free to move over the surface of the layer making graphite electrical conductor.

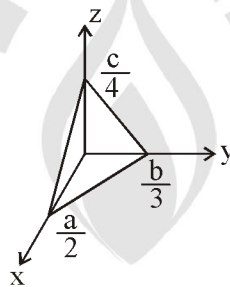
Weak bonding forces between layers are called vanderwall's force because this force is weak, the layers can slide on each other.

The sliding property of layers gives graphite its softness for writing and lubricating properties.

Comparison Between Diamond and Graphite		
	Diamond	Graphite
Hardness	Extremely hard	Soft
Transparency	Transparent	Opague
Electrical properties	Insulator	Conductor
Thermal properties	Conductor	Insulator
Structure	Tetrahedral	Hexagonal (not HCP)

1.7 | MILLER INDICES

Miller indices are used to determine the direction and planes in the unit cell and crystals.



Where a, b, c, are unit cell dimension along x, y, and z respectively.

Method to determine the Miller indices

- (i) Determine intercept made by plane among x,y and z axis respectively.

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

- (ii) Express intercept as multiples of unit cell dimension

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

- (iii) Get reciprocal of multiples

$$2, 3, 4$$

- (v) Reduce reciprocals to smallest set of integers

$$[2, 3, 4]$$

1.8 | INTERPLANAR SEPARATION

The distance between two adjacent parallel planes in a crystal structure is known as interplanar separation.

For a cubic crystal structure

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

Where

a = edge length of cube

$[l, m, n]$ → Miller indices of given plane.

1.9 | BRAVAIS LATTICE

The unit vectors a , b and c are called lattice parameters. Based on their length equality or inequality and their orientation (the angles between them α , β and γ) a total of 7 crystal systems can be defined. With the centering (face, base and body centering) added to these, 14 kinds of 3D lattices, known as Bravais Lattices, can be generated.

S.No.	Crystal Structure	Unit Cell Dimension	Angle Between Axis	Bravais Lattice
1.	Orthorhombic	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	P, I, C, F
2.	Monoclinic	$a = b \neq c$	$\alpha = \beta = 90^\circ \neq \gamma$	P, C
3.	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	P
4.	Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ,$ $\gamma = 120^\circ$	P
5.	Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	P, I
6.	Rhombohedral/Trigonal	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	P
7.	Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	P, I, F

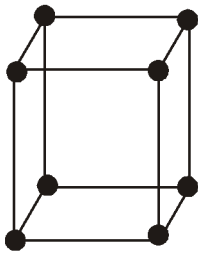
P : Simple cubic

I : Body centered cubic

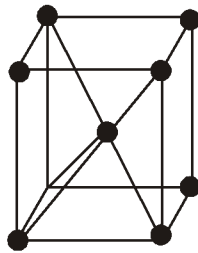
C : Base centered

f : Face centered

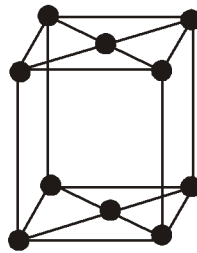
Orthorhombic : $a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$



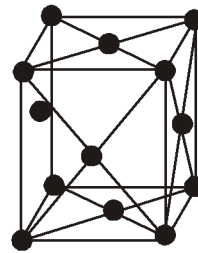
Simple



Body-centered

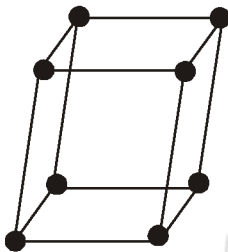


Base-centered

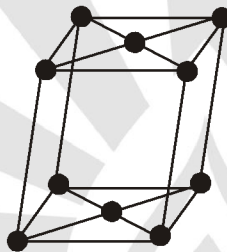


Face centered

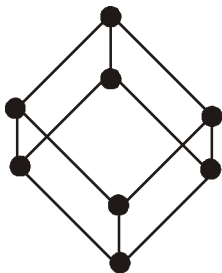
Monoclinic : $a \neq b \neq c, \alpha = \gamma = 90^\circ \neq \beta$



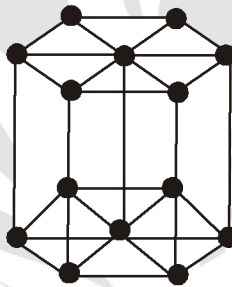
Simple Monoclinic



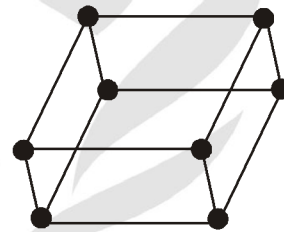
Base-centered Monoclinic



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

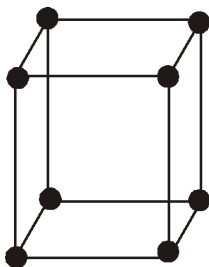


Hexagonal
 $a = b \neq c$
 $\alpha = \beta = 90^\circ \neq \gamma = 120^\circ$

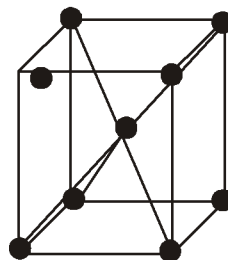


Triclinic
 $a \neq b \neq c$
 $\alpha \neq \beta \neq \gamma \neq 90^\circ$

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

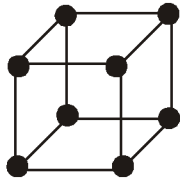


Simple Tetragonal

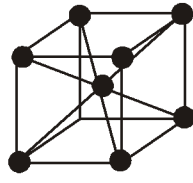


Body-centered Tetragonal (BCT)

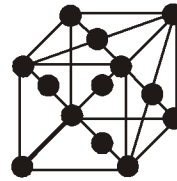
Cubic : $a = b = c, \alpha = \beta = \gamma = 90^\circ$



Simple Cubic



Body-centered cubic (BCC)



Face-centered cubic (FCC)

Crystal system	Example
Triclinic	$K_2S_2O_8, K_2Cr_2O_7$
Monoclinic	$As_4S_4, KNO_2, CaSO_4 \cdot 2H_2O, \beta-S$
Rhombohedral	Hg, Sb, As, Bi, $CaCO_3$
Orthorhombic	Ga, $Ge_3C, \alpha-S$
Tetragonal	In, $TiO_2, \beta-Sn$
Cubic	Au, Si, Al, Cu, Ag, Fe, NaCl

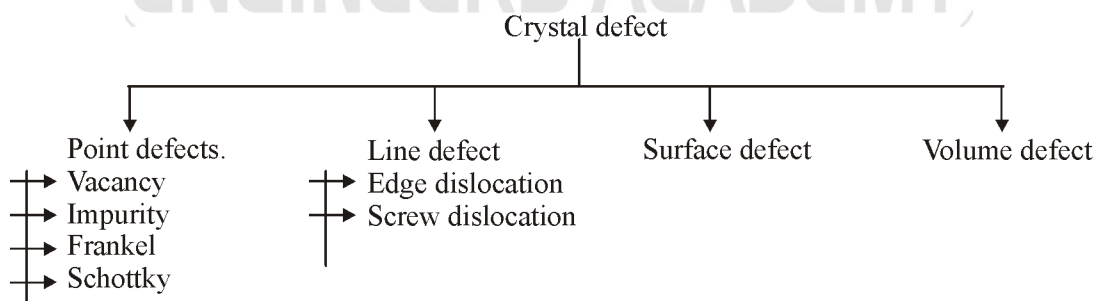
1.10 | CRYSTAL DEFECTS

In a real crystal, the lattice is not perfect, but contains imperfections or defects.

Such imperfections tend to alter the electrical properties of a material. In some cases, electrical parameters can be dominated by these defect.

Imperfections in crystalline solids

1. Point defect
2. Line defect
3. Surface or plane defect
4. Volume defect

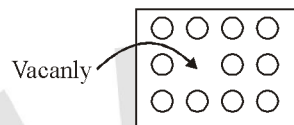


1.10.1 Point Defects

Point defects are where an atom is missing or is in irregular place in the lattice structure.

Point defect is of three types

- (i) Vacancy
- (ii) Impurity
- (iii) Frankel
- (i) **Vacancy Defect** : In this type of defect an atom or molecule is absent in the crystal.

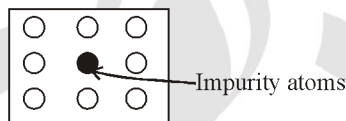


In an ionic crystal, if there is a missing pair of +ve and -ve ions within a crystal structure, then it is called a Schottky defect.

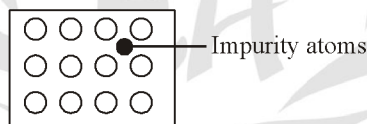
- (ii) **Impurity Defect** : Impurity defect arises when an impurity atom is introduced into the crystal structure either as an 'interstitial' or 'substitutional'.

It is of two types.

- (a) **Substitutional Type Impurity Defect** : In this type, impurity atoms replace parent atoms of the crystal.



- (b) **Interstitial Type Impurity Defect** : In this type, impurity atoms occupy free space or void space in the crystal structure.



- (iii) **Frankel Defect** : Combination of a vacancy and interstitial is called a Frankel imperfection.

1.10.2 Line Defect

Line defects are commonly known as dislocations.

Any deviation from the perfectly periodic arrangement of atoms along a line is called a line imperfection.

Dislocations are generated and more when a stress is applied.

There are two types of dislocation

1. Edge dislocations
2. Screw dislocations.

□□□

OBJECTIVE SHEET

1. In a Si crystal, the arrangement of atoms repeats periodically, this type of material is classified as
 - (a) Amorphous and non crystalline
 - (b) Non crystalline and epitaxial
 - (c) Amorphous and single crystal
 - (d) Epitaxial and single crystal
2. When BCC iron is heated, it changes to FCC iron resulting
 - (a) Increase in volume
 - (b) Contraction in volume
 - (c) No Change in volume
 - (d) Crack in the in material
3. Consider statements related to FCC structure
 1. Co-ordination number is 12
 2. APF is 0.74
 3. There is an atom at the body center of the unit cell.
 Which of the following statement are correct
 - (a) 1 and 2
 - (b) 2 and 3
 - (c) 1 and 3
 - (d) 1, 2, 3
4. Consider statement related diamond structure
 1. Co-ordination number is 4
 2. Packing efficiency is 34%
 3. Crystallizes into diamond structure
 Which of the following statement are correct
 - (a) 1 and 2
 - (b) 2 and 3
 - (c) 3 and 1
 - (d) 1, 2, 3
5. **Assertion (A)** : Atomic number of sodium is 11
Reason (R) : Sodium has a body centred cubic lattice
 - (a) Both A and R are true and R is the correct explanation of A
 - (b) Both A and R are true, but R is not the correct explanation of A
 - (c) A is true, but R is false
 - (d) R is true, but A is false
6. A material has FCC structure with atomic radius 1.06\AA . calculate interplanar separation for $\{1, 1, 0\}$ planes.
 - (a) 3.12\AA
 - (b) 1.12\AA
 - (c) 2.12\AA
 - (d) 4.13\AA
7. For Rhombohedral structure, the lattice parameters are
 - (a) $a = b = c, \alpha = \beta = \gamma \neq 90^\circ$
 - (b) $a = b = c, \alpha = \beta = 90^\circ; \gamma \neq 90^\circ$
 - (c) $a = b \neq c, \alpha = \beta = 90^\circ; \gamma = 120^\circ$
 - (d) $a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$
8. Read the following statements with respect to Single crystalline materials
 1. Periodic and repeated arrangement of atoms is perfect
 2. They are not existed naturally, they produced only artificially
 3. Electronic micro circuit is made up of single crystalline material
 Of the above the correct statements are:
 - (a) 1, 2
 - (b) 1, 2 & 3
 - (c) 1, 3
 - (d) 2, 3
9. Which of the following statements is/are true for the diamond structure?
 1. Coordination number is four.
 2. Packing fractions is 0.34
 3. Copper crystallizes into diamond structure
 4. Lattice is FCC.
 - (a) 1 only
 - (b) 1, 2 and 4
 - (c) 2 and 3
 - (d) 2, 3 and 4