# Unit-1

# **Chapter1: Crystal structure**

A solid is a group of atoms, ions or molecules possessing definite shape and volume. When a solid is subjected to forces (shearing forces), it resists the forces and under goes deformation. After removing the forces it regains its shape and volume. Such properties are not exhibited by liquids or gases.

The properties and performance of every engineering material depends on internal structure. .mechanical properties determine the behavior of engineering materials under applied forces and loads. The response of the material to applied force depends on the type of bonding, structural arrangement of atoms or molecules and type of number of imperfections, sensitive to manufacturing process and operations. (Stress, strain, brittleness, ductility, fatigue, toughness)

The atoms in solids have two types of energies.i.e

- (a) Potential energy
- (b) Kinetic energy

When the atoms are in free state (separated by infinite distance) then the potential energy becomes zero. And the P.E is inversely related to some power of distance of separation.

$$P.E \propto \frac{1}{r^n}$$

The P.E due to attraction is -ve; as the atoms do work of attraction.

The P.E due to repulsion is + ve; as the external work is done to bring the atoms together.

BONDING: the process of holding the atoms together.i.e the attractive and repulsive forces that tend to hold the adjacent atoms together at a particular distance in order to balance the opposite forces.

Nature of bonding forces:

To understand the nature of bonding forces, consider a system of two atoms. These two atoms exert attractive and repulsive forces on each other, such that the bonding force is 'F'

When the two atoms are present at distance of separation of 'r',

then the attractive force ' $F_A$ ' is given by

$$F_A = \frac{1}{r^M}$$

 $F_A = \frac{A}{r^M}$ , where A is proportionality constant, M= 2 as per Coulomb's law

Repulsive force ' $F_R$ 'is given by

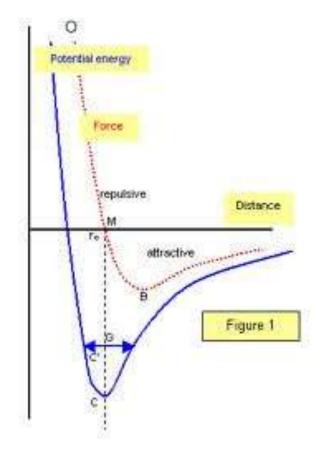
$$F_R = \frac{1}{r^N}$$

 $F_R = \frac{-B}{r^N}$ , B is proportionality constant and N=7-10 as per Coulomb's law.

When two atoms are present at equilibrium distance ' $r_0$ ',then magnitude of  $F_A$  and  $F_R$  are equal and opposite.

The sum of attractive and repulsive force is

$$F_{(r)} = F_A + F_R$$
$$F_{(r)} = \frac{A}{r^M} - \frac{B}{r^N}$$



#### Calculation of Cohesive energy of a solid:

"The amount of energy required to separate the atoms in a crystalline solid is known as cohesive energy also called as bonding cohesive energy

Or the amount of energy required to separate the atoms in a crystalline solid is known as cohesive energy or dissociation cohesive energy.

At equilibrium position the PE of either atom is given by

U= decrease in P.E due to F.A + increase in PE due to F.R

Since the work done on the system is stored as PE, it can be calculated by integrating the equation

$$F_{(r)} = \frac{A}{r^{M}} - \frac{B}{r^{N}}$$

$$U_{(r)} = \int F(r) dr...(1)$$

$$= A \int r^{-M} dr - B \int r^{-N} dr$$

$$= \frac{Ar^{-M+1}}{-M+1} - \frac{Br^{-N+1}}{-N+1} + C...(2)$$
Here  $\frac{A}{M-1} = a; \frac{B}{N-1} = b; m = M - 1; n - N - 1...(3)$  in (2)
$$U_{(r)} = \frac{-a}{r^{m}} + \frac{b}{r^{n}} + C...(4)$$

Here a and b are attractive and repulsive force constants and n are+ve integers and 'C' is a constant.

when  $r \to \infty$ ,  $V(r) = 0 \leftrightarrow C = 0$  in (4)

$$U_{(r)} = \frac{-a}{r^m} + \frac{b}{r^n} \dots (5)$$

The first term represents P.E due to force of attraction and second term represents P.E due to repulsion.

i.e when  $r \rightarrow r_0$ , at equilibrium distance of seperation

$$U_{(r_0)} = \frac{-a}{r_0^m} + \frac{b}{r_0^m} \dots (6)$$

By differentiating eqn(6)

$$\left(\frac{du}{dr}\right)_{r=r_0} = (-a)(-m)r_0^{-m-1} + b(-n)r_0^{-n-1}$$

$$= \frac{ma}{r_0^{m+1}} - \frac{bn}{r_0^{n+1}}$$

$$= \frac{ma}{r_0^{m+1}} = \frac{bn}{r_0^{n+1}}$$

$$= \frac{ma}{r_0^m} = \frac{bn}{r_0^n}$$

$$r_0^n = \frac{n}{m}\frac{b}{a}r_0^m \dots (7) \text{ in } (6)$$

$$U_{min} = \frac{-a}{r_0^m} + \frac{b}{n}\frac{b}{h}$$

$$r_0^{m} + \frac{n}{m} \frac{b}{a} r_0^{m}$$
$$= \frac{-a}{r_0^m} + \frac{m}{n} \frac{a}{b} \frac{b}{r_0^m}$$
$$= \frac{-a}{r_0^m} + \frac{m}{n} \frac{a}{r_0^m}$$

$$U_{min} = \frac{-a}{r_0^m} \left(1 - \frac{m}{n}\right)$$

This is the expression for cohesive energy of a molecule containing two atoms in a solid. The energy  $U_{min}$  is called Bonding energy or dissociation energy or cohesive energy.

#### Calculation of Lattice energy of Ionic crystals:

The lattice energy of an ionic solid will differ from the bond energy of diatomic soilds.in the former case there will be interactions between more atoms.

"The cohesive energy of an ionic crystal is the energy that would be liberated by the formation of the crystal from individual neutral atoms

In case of NaCl crystal, each sodium ion is subjected to attractive potential due to 6 chloride ions each at a distance 'r'.thus the attractive potential at the sodium ion by the chloride ion is

$$U_1 = -6\frac{e^2}{4\pi\epsilon_0 r}$$

The next nearest neighbors are 12 sodium ions at a distance of  $\sqrt{2}r$ .thus

$$U_2 = 12 \frac{e^2}{4\pi\epsilon_0 r(\sqrt{2})} \text{ ans so on}$$

Thus the total potential energy is

$$\begin{aligned} U_{attraction} &= -6\frac{e^2}{4\pi\epsilon_0 r} + 12\frac{e^2}{4\pi\epsilon_0 r(\sqrt{2})} - 8\frac{e^2}{4\pi\epsilon_0 r(\sqrt{3})} + \cdots \dots \\ &= -\frac{e^2}{4\pi\epsilon_0 r} \left(6 - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \frac{6}{2} + \cdots\right) \\ \text{Let} &\propto = \left(6 - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \frac{6}{2} + \cdots\right) = 1.75 \text{ is called Madelung constant} \\ \text{Thus } U_{att} &= -\frac{\alpha e^2}{4\pi\epsilon_0 r} \end{aligned}$$

The P.E due to short range repulsive forces can be expressed as

$$U_{rep} = \frac{B}{r^n}$$

Where B is a constant and  $U_{rep}$  is positive which increases rapidly with decreasing internuclear distance 'r'.thus the total P.E 'U' of each ion due to its interaction with all other ions in the crystal is

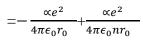
$$U_{(r)} = -\frac{\propto e^2}{4\pi\epsilon_0 r} + \frac{B}{r^n} \dots (1)$$

At the equilibrium spacing 'r<sub>0</sub>', U is min and hence  $\frac{du}{dr} = 0$ 

$$\left[\frac{du}{dr}\right]_{r=r_0} = -\frac{\propto e^2}{4\pi\epsilon_0 r_0^2} - \frac{nB}{r_0^{n+1}} = 0$$
$$\frac{\propto e^2}{4\pi\epsilon_0 r_0} = \frac{nB}{r_0^n}$$

 $B = \frac{\propto e^2 r_0^{n-1}}{4\pi\epsilon_0 n} \dots (2) \text{ in } (1) \text{ with } r=r_0 \text{, we get}$ 

$$U_{min} = -\frac{\propto e^2}{4\pi\epsilon_0 r_0} + \frac{\propto e^2 r_0^{n-1}}{4\pi\epsilon_0 n r_0^n}$$



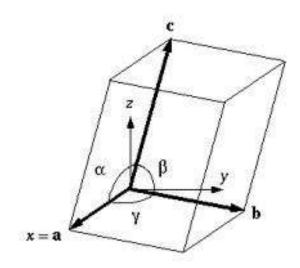
$$U_{min} = -\frac{\propto e^2}{4\pi\epsilon_0 r_0} \left[1 - \frac{1}{n}\right]$$

Thus for one KMol of the crystal, the energy is

$$U_{min} = -\frac{\propto e^2 N_A}{4\pi\epsilon_0 r_0} \left[ 1 - \frac{1}{n} \right]$$

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

Lattice parameters: the primitives (a,b,c) and interfacial angles ( $\alpha$ , $\beta$ , $\gamma$ ,) are the basic lattice parameters which determine the actual size of unit cell.

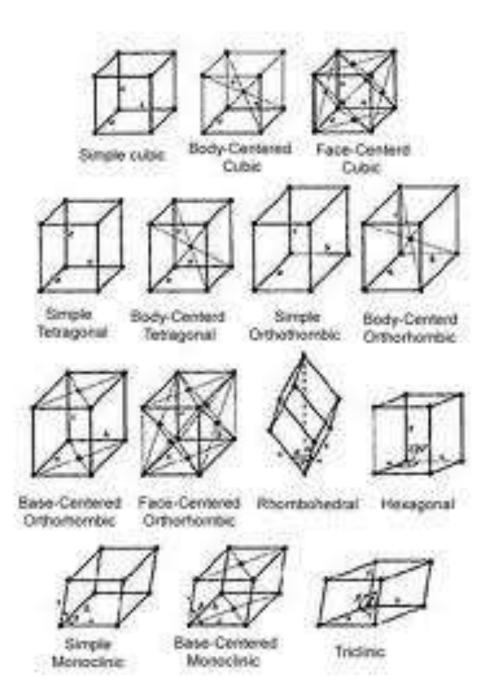


# Seven crystal systems with 14 Bravais points

S:no	Name of the crystal	Primitives	Interfacial angles	Bravais Lattice
	systems			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	α=β=γ≠90°	1(P)
7	Hexagonal	$a=b\neq c$	$\alpha=\beta=90^{\circ}and \gamma=120^{\circ}$	1(P)

P= simple, C= base centered , I= body centered, F= face centered



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

**Co-ordination number**-defined as the no: of equidistant neighbors that an atom has the given structure .Greater the co-ordination no: the atom are said to be closely packed.

**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

# Simple crystal structure

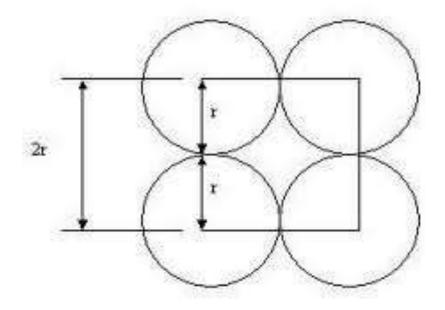
- 1. Simple cubic structure (SC)
- 2. Body centered structure (BCC)
- 3. Face centered structure (FCC)

# Packing factor of SC.BCC, FCC

1. Simple cubic

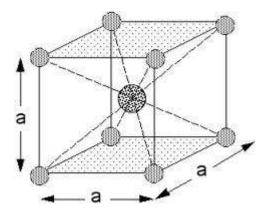
Packing fraction = <u>volume of all the atoms in unit cell</u>

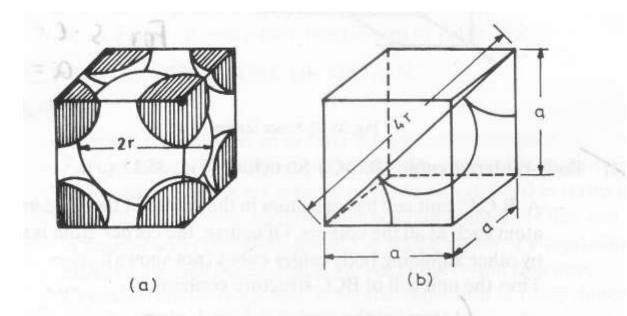
Volume of unit cell  
= 
$$\frac{1 \times 4/3\pi r^3}{a^3} = 56\%$$

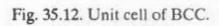


2. Body centered structure (BCC)

Packing fraction = 
$$\frac{2 \times 4/3\pi}{a^3}$$
 = 68%



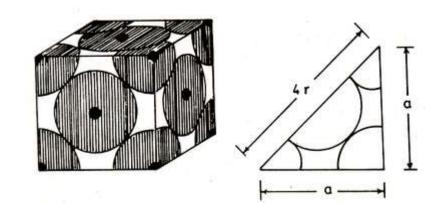




3. Face centerd structure(FCC)

Packing fraction= $4 \times (\pi a^3 \sqrt{2}/24)$  =74%

a<sup>3</sup>



# Chapter 2 **DEFECTS IN CRYSTALS**

# In a perfect crystal:

- 1. Atoms exist only in lattice sites.
- 2. Periodicity of lattice extends up to infinity.
- 3. Atoms do not loose electrons, no free electrons are present.
- 4. Atoms would be stationary.

Any deviation from the above four properties is known as defect.

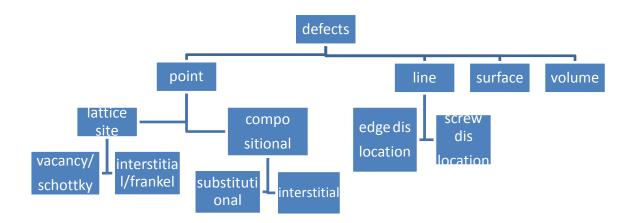
The properties of crystal are divided into two categories based on the presence of imperfections.

- 1. **Structure sensitive properties:** which are affected by the presence of imperfections. Ex: mechanical strength, electrical conductivity in semi conductors, magnetic hysteresis, dielectric strength.
- Structure insensitive properties: which are not affected by the presence of imperfections.
   Ex: stiffness.

## Defects are produced by various methods:

- 1. by heating
- 2. Rapid cooling
- 3. By applying external strength
- 4. By bombarding with high energy particles like neutrons or particles from cyclotron.

#### 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).

Point defects are:

**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.

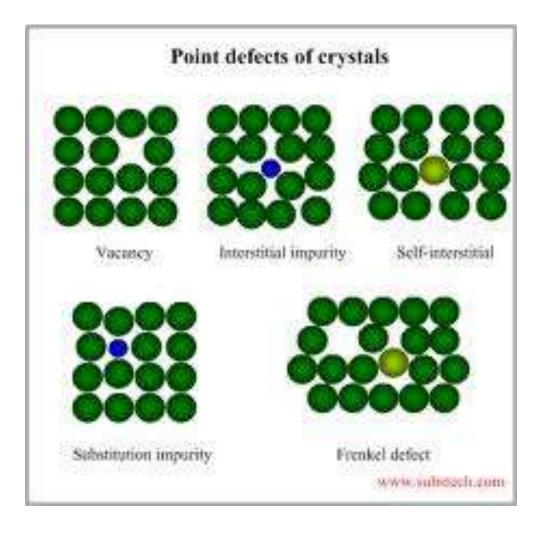
Impurity atom: an atom that does not belong to the parent lattice (original crystal).

**Substitutional defects:** this defect arises when an impurity atom replaces or substitutes parent atom.

Ex: in brass, zinc is a substitutional 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.



**Imperfections in ionic crystals:** 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.

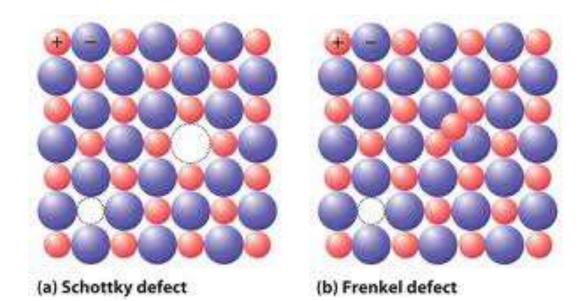
## Frenkel defect:

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.



Line defects (or) dislocations (one dimensional defect) dislocation is 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.

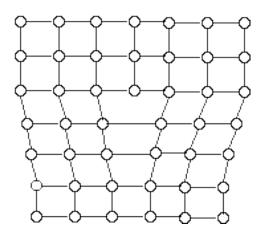
In imperfect crystal all the atoms above the dislocation plane are squeezed together and compressed there by the bond length decreases. And all the atoms below the dislocation plane are elongated by subjecting to the tension and thereby the bond length increases.

There are two types of edge dislocation. They are

- 1. Positive edge dislocation
- 2. Negative edge dislocation.

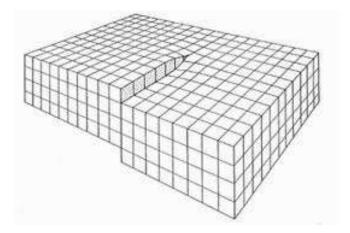
**Positive edge dislocation:** if the vertical plane starts from top of the crystal and never reaches to the bottom .

**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.



Burger's vector: gives the magnitude and direction of dislocation line.

### **Construction of Burger, s vector:**

Starting from a point 'p' move same number of steps left, right, up and down in the clockwise direction.

If the starting point 'p' and ending point 'p<sup>l'</sup> coincide, then the region enclosed in the Burger's circuit is free from imperfection.

If the starting point and ending point do not coincide i.e.  $pp^{l} = b$ . b is the quantity indicating magnitude.

Burgers' vector is perpendicular to edge dislocation plane and parallel to screw dislocation plane.

**Surface defects:** (two dimensional defects) ,grain, twin, twilt and stacking defects come under surface defects

**Volume defects:** (three dimensional defects) when group of atoms are missing and cracks arise in the crystal.

Expression for the number of vacancies at any temperature. Or energy of formation of vacancy.

Let 'N' be the number of atoms in a crystal, ' $E_v$ ' is the energy required to create 'n' vacancies.

The total energy required for the creation of 'n' number of vacancies is called enthalpy and is given as

 $u=nE_v$ .....(1)

The number of ways of selecting 'N' atoms to create 'n' vacancies is p

$$p = Nc_n = \frac{N!}{n!(N-n)!}$$
-----(2)

Here 'p' is disorder parameter

In stastistical mechanics, the relation between disorder parameter 'p' and entropy's' is

s= k logp.....(3) where K= Boltzman constant

free energy (F) of the atoms in the crystal is given by

$$f = u - Ts \dots (4)$$

 $f = nE_V - KT \log p$ .....(5) from 1 and 3

$$f = nE_v - KT \log \frac{n!}{(N-n)!n!}$$
.....(6) substitute 2 in 5

By applying stirling's approximation, to eqn (6)

$$logx! = xlogx - x$$

$$f = nE_V - KT(logN! - log(N - n)! - logn!)$$

$$f = nE_v = KT(NlogN - N - (N - n)log(N - n) + (N - N) - nlogn + n)$$

$$F = nE_v - KT(NlogN - (N - n)log(N - n) - nlogn)....(7)$$

At thermal equilibrium, the free energy is minimum and constant.i.e.

$$\frac{dF}{dn} = 0 \text{ in } (7)$$

$$\frac{dF}{dn} = E_v - KT(0 - (N - n)\frac{1}{(N - n)}(-1) - \log(N - n)(-1) - n\frac{1}{n} - \log n)$$

$$0 = E_v - KT(1 + \log(N - n) - 1 - \log n)$$
$$0 = E_v - KT \left[ \log\left(\frac{N - n}{n}\right) \right]$$
$$E_v = KT \log\left(\frac{N - n}{n}\right)$$
$$\frac{E_v}{KT} = \log\left(\frac{N - n}{n}\right)$$

Taking exponential on both sides

$$e^{E_{v}/KT} = \frac{N-n}{n}$$
$$\frac{n}{N-n} = e^{-E_{v}/KT}$$

The number of vacancies in a crystal is very small when compared with the number of atoms  $N \gg n$ 

$$N - n \cong N$$

Therefore  $e^{-E_v/KT} \frac{n}{N}$ 

 $n = Nexp^{-E_{v}/KT}....(8)$ 

#### FRENKEL DEFECT:

Let 'N' be the number of atoms, 'N<sub>i</sub>'be the number of interstitial atoms, let 'E<sub>i</sub> 's the energy required to create 'n' number of vacancies and the total energy required is  $u = nE_1....(1)$ 

The total number of ways in which Frenkel defects can be formed is given by  $p = N_n^c \times N_{i_n}^c$ 

$$p = \frac{N!}{(N-n)!n!} \times \frac{N_i!}{(N_i-n)!n!}.....(2)$$

The increase in entropy (s) due to Frenkel defect is given by  $s = K \log p$ 

$$S = Klog\left[\frac{N!}{n!(N-n)!} \times \frac{N_i!}{(N_I - n)!n!}\right].....(3)$$

This increase in entropy produces change in Free energy F = u - TS.....(4) Substitute (1),(3) in (4)

$$F = nE_i - KTlog\left[\frac{N!}{n! (N-n)!} \times \frac{N_i!}{(N_i - n)! n!}\right]$$

Using Strling's approximation, logx! = xlogx - x

$$F = nE_i - KT \left[ \log \frac{N!}{n! (N-n)!} + \log \frac{N_i!}{(N_I - n)! n!} \right]$$

$$F = nE_i - KT[logN! - logn! - log(N - n)! + logN_i! - log(N_i - n)! - logn!]$$

$$\begin{split} F = nE_i - KT[(NlogN - N) - (nlogn - n) - [(N - n)log(N - n) - (N - n)] + N_i logN_i \\ & - N_I - [(N_i - n)log(N_i - n) - (N_i - n)] - (nlogn - n)] \end{split}$$

$$F = nE_i - KT[NlogN - N - nlogn + n - (N - n) log(N - n) + (N - n) + N_i logN_I - N_i - (N_i - n) log(N_i - n) + (N_i - n) - nlogn + n]$$

$$F = nE_I - KT[NlogN + N_i logN_i - (N - n) log(N - n) - (N_i - n) log(N_i - n) - 2nlogn]$$

Differentiating w.r.to 'n', and equating to 0, we get

$$\begin{split} \frac{dF}{dn} &= E_i - KT \left[ 0 + 0 - \left[ (N-n) \frac{1}{(N-n)} (-1) \right] + \log(N-n) (-1) \right] \\ &- \left[ (N_i - n) \frac{1}{(N_i - n)} (-1) + \log(N_i - n) (-1) \right] - 2 \left[ n \times \frac{1}{n} + \log n \right] \right] \\ &0 = E_i - KT [1 + \log(N-n) + 1 + \log(N_i - n) - 2 - 2\log n] \\ &0 = E_i - KT \left[ \log \frac{(N-n)(N_i - n)}{n^2} \right] \end{split}$$

$$E_{i} = KT \left[ log \frac{(N-n)(N_{i}-n)}{n^{2}} \right]$$

As  $n \ll N, N-n \cong N,$  similarly  $N_i-n \cong N_i$ 

$$E_{i} = KTlog\left(\frac{NN_{i}}{n^{2}}\right)$$

Thus  $E_i = KT[logNN_i - 2logn]$ 

$$\frac{E_i}{KT} = \log(NN_i) - 2\log n$$
$$2\log n = \log(NN_i) - \frac{E_i}{KT}$$
$$\log n = \frac{1}{2}\log(NN_i) - \frac{E_i}{2KT}$$

Taking exponentials on both sides

$$n = (NN_i)^{\frac{1}{2}} exp^{\frac{-E_i}{2KT}}$$

#### **SCHOTTKY DEFECT:**

In ionic crystals, the formation of paired vacancy is most favoured.i.e an equal number of positive and negative vacancy pairs are produced.

Let 'N' be the number of atoms,  $E_p$ ' is the energy required to create a pair of vacancies and 'n'be number of vacancies created. The total energy required to create vacancies is

 $U = nE_{p....(1)}$ 

The number of ways in which 'n' vacancies created is

$$p = N_n^c \times N_n^c = (N_n^c)^2$$
$$p = \left[\frac{N!}{(N-n)! n!}\right]^2$$

The relation between the disorder parameter 'p' and entropy 's' is given by

 $s = Klogp = klog \left[\frac{N!}{(N-n)!n!}\right]^2$ ....(2)

By applying Striling's approximation

$$\log \left[\frac{N!}{(N-n)! n!}\right]^{2} = 2[\log N! - \log(N-n)! - \log n!]$$
  
= 2[NlogN - N - ((N - n) log(N - n) - (N - n)) - (nlogn - n)]  
= 2[NlogN - N - (N - n) log(N - n) + N - n - nlogn + n]  
= 2[NlogN - (N - n) log(N - n) - nlogn]  
There fore s = 2K[NlogN - (N - n) log(N - n) - nlogn].....(3)

Free energy of the atoms in the crystal is given by F = U - TS....(4)Substitute (1),(3) in (4)

$$F = nE_p - 2KT[NlogN - (N - n) log(N - n) - nlogn]$$

Differentiating above equation w.r.to 'n' and equating it to zero ,we get

$$\frac{dF}{dn} = E_p - 2KT[\log(N - n) + 1 - \log n - 1 = 0]$$
$$E_p - 2KT\log\left(\frac{N - n}{n}\right) = 0$$
$$\frac{E_p}{2KT} = \log\left(\frac{N - n}{n}\right)$$

Taking exponentials on both sides

$$\frac{N-n}{n} = \exp^{\frac{E_p}{2KT}}$$

As nn  $\ll$  N, N = nexp  $\frac{E_{p}}{2KT}$ 

$$n = Nexp^{\frac{-E_p}{2KT}}$$

# **Chapter 3: PRINCIPLES OF QUANTUM MECHANICS**

De-Broglie Hypothesis –Matter waves: An electromagnetic wave behaves like particles, particles like electrons behave like waves called matter waves, also called de-Broglie matter waves.

The wave length of matter waves is derived on the analogy of radiation.

Based on Planck's theory of radiation, the energy of a photon is given by

$$\mathbf{E} = \mathbf{h}\boldsymbol{\vartheta} = \frac{\mathbf{h}\mathbf{c}}{\lambda}....(1)$$

c = Velocity of light

 $\lambda$  = Wavelength of the photon

According to Einstein's mass energy relation

$$\mathbf{E} = \mathbf{mc}^2 \dots \dots (2)$$

m= mass of the photon

Equating equations (1) and (2)

$$mc^2 = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc}{mc^2} = \frac{h}{mc} = \frac{h}{p}.....(3)$$

P = momentum of photon

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

 $\lambda = \frac{h}{mv} = \frac{h}{p}$ ... (4) is called de-Broglie's wave equation.

#### **Properties of matter waves:**

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

de-Broglie wavelength associated with an electron:

if a velocity 'v' is given to an electron by accelerating it through a potential difference 'V',then the work done on the electron is 'Ve',and the work done is converted into the kinetic energy of an electron.

$$eV = \frac{1}{2}mv^2$$
$$v = \sqrt{\frac{2eV}{m}}$$

 $mv = \sqrt{2meV}\dots(5)$  in (4)

$$\lambda = \frac{h}{\sqrt{2meV}}.....(6)$$

Ignoring relativistic corrections, m<sub>0</sub>= rest mass of electron

$$\lambda = \frac{h}{\sqrt{2m_0 eV}}....(7)$$

by substituting the values of h= $6.625 \times 10^{-34}$  Jsec

 $m_0$  = rest mass of electron = 9.1×10<sup>-31</sup>Kg and c= charge of electron=1.6×10<sup>-19</sup>C

$$\lambda = \frac{12.27}{\sqrt{V}} \mathbf{A}^0 \dots \dots (8)$$

where V= in volt and  $\lambda = in A^0$ 

Experimental verification of matter waves:

G.P Thomson experiment:

- 1. The electrons are produced from a heated filament 'F' and are accelerated through a high +ve potential (25-60 KV) given to anode 'A'.
- 2. The electron beam passes through a fine hole in a metal block 'B' and falls on a gold foil 'G' of thickness 10<sup>-8</sup> cm.
- 3. The foil consists of very large number of microscopic crystals oriented at random. The electrons after striking the gold foil diffracts according to Bragg's formula  $2d\sin\theta = n\lambda$ .
- 4. The electrons passing through the foil are received on a photographic plate 'P'

- 5. A central spot (position of undeflected electrons) surrounded by a series of concentric diffraction rings are obtained on a photographic plate 'P'.this pattern is similar to that of x-rays diffraction in powder method..
- 6. Since x-rays also produce same pattern, a magnetic test was performed: when a magnet is brought near the beam, electrons are displaced. Since x-rays are not deviated in the magnetic field, the pattern must be due to diffraction of electron beam only.
- 7. The whole apparatus is highly evacuated, so that electrons may not lose their energy in collisions with molecules of air.

Clearly this experiment demonstrated that the electrons behave like waves, since diffraction can be produced only by waves. The de-Broglie equation was verified by G.P Thomson by estimating the wavelength of the electrons with the knowledge of their velocity which depends on accelerating voltage.

From the fig, OA is the radius of the ring.'O' is the center of the ring, 'Q' is the point where the electron strikes a particular plane on the crystal in the metallic film. 'QO' is the distance between the metallic film and the photographic plate.' $\theta$ ' is the glancing angle of electrons with the foil.

From fig

 $\frac{r}{l} = tan \theta$ 

$$\theta = \frac{r}{l} \ (\theta \text{ being small})$$

from Bragg's equation

 $2d\sin\theta = n\lambda$ .

$$d = \frac{\lambda}{2\theta} if \ \theta \text{ is small}...(1)$$

From fig  $tan2\theta = 2\theta = \frac{r}{L}...(2)$  in (1)

$$\lambda = \frac{rd}{nL}$$

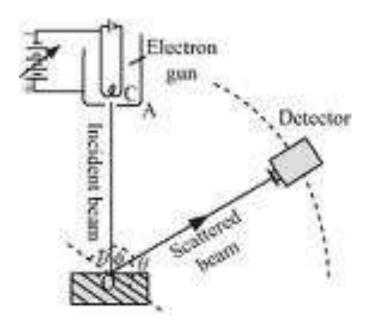
the wavelength of electrons was calculated from the above expression which matched well with the theoretical wavelength.

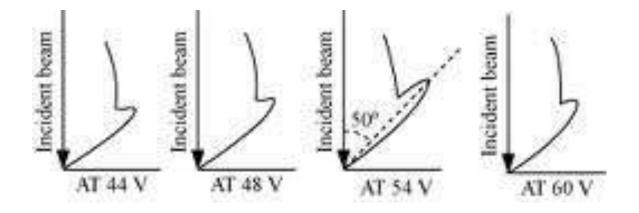
This experiment confirmed the existence of matter waves and dual nature of matter proposed by de-Broglie.

# **Division and Germer's experiment:**

The first experimental evidence of the wave nature of atomic particles was proved by C.J Division and L.H Germer in 1927.

They were studying scattering of electrons by a metal target and measuring the density of electrons scattered in different directions.





- 1. From fig, the electron beam from electron gun which consists of a tungsten filament 'F' heated by a low tension battery 'B<sub>1</sub>' are accelerated to a desired velocity by applying suitable potential from a high tension battery 'B<sub>2</sub>'.
- 2. The accelerated electrons are collimated into a fine beam by allowing them to pass thorough a system of pinholes in the cylinder 'C'.
- 3. The fast moving electron beam is made to strike the target (nickel crystal) capable of rotating about an axis perpendicular to the plane of diagram.
- 4. The electrons are scattered in all directions by atomic planes of a crystal and intensity of scattered electron beam in all directions can be measured by the electron collector and can be rotated about the same axis as the target.
- 5. The collector is connected to a sensitive galvanometer whose deflection is proportional to the intensity of electron beam entering the collector.
- 6. When electron beam accelerated by 54 V was directed to strike the given nickel crystal, a sharp max in the electron diffraction occurred at an angle of  $50^{0}$  with the incident beam.
- 7. The incident beam and the diffracted beam make an angle of 65<sup>0</sup> with the family of Bragg's planes.
- 8. The whole instrument is kept in an evacuated chamber.
- 9. The spacing of planes in Nickel crystal as determined by x-ray diffraction is 0.091nm

From Bragg's law

$$2d\sin\theta = n \lambda$$

$$2 \times 0.091 \times 10^{-9} \times sin65^{\circ} = 1 \times \lambda$$

 $\lambda = 0.615$ nm

Therefore for a 54 V electron beam, the de-Broglie wavelength associated with the electron is given by

$$\lambda = \frac{12.27}{\sqrt{54}} A^{\circ} = 0.166 nm$$

This wavelength agrees well with the experimental value. Thus division experiment provides a direct verification of de-Broglie hypothesis of wave nature of moving particles.

#### Schrodinger time independent wave equation:

According to de-Broglie ,a particle of mass 'm' moving with a velocity'v' is always associated with a wave whose wavelength is given by  $\lambda = \frac{h}{mv}$ 

Schrodinger describes the wave nature of a particle in mathematical form and is known as Schrodinger's wave equation.

Consider a plane wave moving along +ve x- direction with velocity 'v'. The equation of the wave is written in the from

$$y = asin\frac{2\pi}{\lambda}(x - \nu t)...(1)$$

Where  $\lambda$  = wavelength of the wave

a= amplitude of wave

y=displacement of wave in y- direction

x= displacement along x- axis at any instant of time 't'.

taking first order derivative w.r.to 'x' on both sides of eqn(1)

$$\frac{dy}{dx} = a\cos\frac{2\pi}{\lambda}(x-vt)\frac{2\pi}{\lambda}$$

$$\frac{d^2y}{dx^2} = -a\left(\frac{2\pi}{\lambda}\right)^2 \sin\left(\frac{2\pi}{\lambda}\right)(x-\nu t)\dots(2)$$

Substitute (1) in (2)

$$\frac{d^2y}{dx^2} + \left(\frac{2\pi}{\lambda}\right)^2 y = 0...(3)$$

This is known as differential plane wave equation.

In complex wave ,the displacement 'y' is replaced by ' $\psi$ ' and wavelength'  $\lambda$ ' is replaced by de-Broglie's wavelength  $\lambda' = \frac{h}{mv}$  in eqn(3)

$$\frac{d^2\psi}{dx^2} + \left(\frac{2\pi}{\lambda}\right)^2 \psi = 0$$

$$\frac{d^2\psi}{dx^2} + \frac{4\pi^2 m^2 v^2}{h^2} \ \psi = 0....(4)$$

For a moving particle, the\ total energy is E = U + V i.  $e U = E - V \dots (5)$ 

Where E= total energy

V= potential energy

U= kinetic energy  $=\frac{1}{2}mv^2$ 

 $2mu = m^2 v^2 \dots (6)$ , substitute (5) in (6)

 $2m(E - V) = m^2 v^2 \dots (7)$  substitute (7) in(4)

$$\frac{d^2\psi}{dx^2} + \frac{4\pi^2 2m(E-V)}{h^2} \ \psi = 0$$

 $\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m(E-V)}{h^2} \ \psi = 0....(8)$ 

This equation is known as Schrodinger's time independent wave equation in one dimension.

In three dimensions, it can be written as

$$\nabla^2 \psi + \frac{8\pi^2 m(E-V)}{h^2} \psi = 0...(9)$$
$$\nabla^2 \psi + \frac{2m(E-V)}{h^2} \psi = 0$$

For a free particle, the P.E is equal to zero i.e V=0 in equation (9)

Therefore the Schrodinger's time independent wave equation for a free particle is

$$\nabla^2 \psi + \frac{8\pi^2 mE}{h^2} \psi = 0$$

#### Physical significance of $\psi$ (wave function)

- 1. The wave function  $\psi$  enables all possible information about the particle.
- 2.  $\Psi$  is a complex quantity and has no direct physical meaning.
- 3. It is only a mathematical tool in order to represent the variable physical quantities in quantum mechanics.
- 4. Born suggested that, the value of wave function associated with a moving particle at the position co-ord(x,y,z) in space, and at the time instant 't' is related in finding the particle at certain location and certain period of time 't'.
- 5. If  $\boldsymbol{\Psi}$  represents the probability of finding the particle, then it can have two cases. Case 1: certainty of its Presence: +ve probability Case 2: certainty of absence :- ve probability, but -ve probability is meaningless, hence the wave function  $\boldsymbol{\Psi}$  is complex number and is of the form a+ib

- 6. Even though  $\psi$  has no physical meaning, the square of its obsolete magnitude  $|\psi^2|$  gives a definite meaning and is obtained by multiplying the complex number with its complex conjugate
- 7. Then  $|\Psi^2|$  represents the probability density 'p' of locating the particle at a place at a given instant of time. And has real and positive solutions.

$$\Psi\left(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{t}\right) = \mathbf{a} + \mathbf{i}\mathbf{b}$$

$$\psi^*(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{t}) = \mathbf{a} - \mathbf{i}\mathbf{b}$$
$$\mathbf{p} = \psi\psi^* = |\psi^2| = a^2 + b^2 as i^2 = -1$$

Where 'P' is called the probability density of the wave function.

8. If the particle is moving in a volume 'V', then the probability of finding the particle in a volume element dv, surrounding the point x,y,z and at instant 't' is Pdv

$$\int_{-\infty} |\Psi^2| dv = 1 \text{ if particle is present}$$
$$= 0 \text{ if particle does not exist}$$

This is called normalization condition.

#### Heisenberg's uncertainty principle:

•

- 1. According to Classical mechanics, a moving particle at any instant has fixed position in space and definite momentum which can be determined simultaneously with any desired accuracy. This assumption is true for objects of appreciable size, but fails in particles of atomic dimensions.
- 2. Since a moving atomic particle has to be regarded as a de-Broglie wave group, there is a limit to measure particle properties.
- 3. According to Born probability interpretation, the particle may be found anywhere within the wave group moving with group velocity.
- 4. If the group is considered to be narrow, it is easier to locate its position, but the uncertainty in calculating its velocity and momentum increases.
- 5. If the group is wide, its momentum is estimated easily, but there is great uncertainty about the exact location of the particle.

Heisenberg a German scientist in 1927, gave uncertainty principle which states that

# "The determination of exact position and momentum of a moving particle simultaneously is impossible".

In general, if  $\Delta x$  represents the error in measurement of position of particle along x-axis, and  $\Delta p$  represents error in measurement of momentum, then

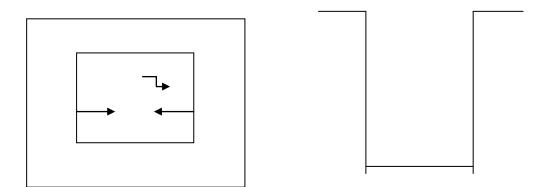
#### $\Delta x.\Delta p = h$

Or limitation to find the position and momentum of a particle is

$$(\Delta x). (\Delta p) \ge \frac{h}{4\pi}$$

i.e Heisenberg uncertainty principle states that both the position and momentum cannot be measured simultaneously with perfect accuracy.

#### Particle in 1-Dimensional potential box:



- 1. The wave nature of a moving particle leads to some remarkable consequences when the particle is restricted to a certain region of space instead of being able to move freely.i.e when a particle bounces back and forth between the walls of a box.
- 2. If one –dim motion of a particle is assumed to take place with zero potential energy over a fixed distance, and if the potential energy is assumed to become infinite at the extremities of the distance, it is described as a particle in a 1-D box, and this is the simplest example of all motions in a bound state.
- 3. The Schrodinger wave equation will be applied to study the motion of a particle in 1-D box to show how quantum numbers, discrete values of energy and zero point energy arises.
- 4. From a wave point of view, a particle trapped in a box is like a standing wave in a string stretched between the box's wall.
- 5. Consider a particle of mass 'm'moving freely along x- axis and is confined between x=0 and x= a by infinitely two hard walls, so that the particle has no chance of penetrating them and bouncing back and forth between the walls of a 1-D box.
- 6. If the particle does not lose energy when it collides with such walls, then the total energy remains constant.

- 7. This box can be represented by a potential well of width 'a', where V is uniform inside the box throughout the length 'a' i.e V= 0 inside the box or convenience and with potential walls of infinite height at x=0 and x=a, so that the PE 'V' of a particle is infinitely high V=∞ on both sides of the box.
- 8. The boundary condition are

v(x) = 0,  $\psi(x) = 1$  when 0 < x < a...(1) $v(x) = \infty$ ,  $\psi(x) = 0$  when  $0 \ge x \ge a...(2)$ 

Where  $\psi(x)$  is the probability of finding the particle.

The Schrodinger wave equation for the particel in the potential well can be written as

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E \psi = 0, \text{ as } V = 0 \text{ for a free particle}...(3)$$

In the simplest form eqn (3) can be written as

$$\frac{d^2\psi}{dx^2} + k^2 \psi = 0....(4)$$

Where k= propagation constant and is given by  $k = \sqrt{\frac{8\pi^2 mE}{h^2}}....(5)$ 

The general solution of equation (4) is

 $\psi(\mathbf{x}) = \operatorname{Asinkx} + \operatorname{Bcoskx}...$  (6)

where A and B are arbitrary constants, and the value of these constant can be obtained by applying the boundary conditions. Substitute eqn(1) in (6)

$$0 = Asink(0) + Bcosk(0)$$

Implies B=0 in eqn(6)

 $\psi(\mathbf{x}) = \operatorname{Asinkx...}(7)$ 

Substituting eqn(2) in (7)

$$0 = Asink(a)$$
  

$$\Rightarrow A = 0 \text{ or } sinka = 0$$

But 'A'  $\neq 0$  as already B=0 & if A= 0, there is no solution at all.

Therefore sinka=0( if sin $\theta$ =0,then general solution is  $\theta$ =n $\Pi$ )

Ka=nП

$$k = \frac{n\pi}{a}....(8)$$

Where n=1,2,3,4,... and  $n\neq0$ , because if n=0,k=0,E=0 everywhere inside the box and the moving particle cannot have zero energy.

From (8)  $k^2 = \left(\frac{n\pi}{a}\right)^2$ 

From (5)  $\frac{8\Pi^2 mE}{h^2} = \frac{n^2 \pi^2}{a^2}$ 

$$E = \frac{n^2 h^2}{8ma^2}$$

$$E_{n=}\frac{n^2h^2}{8ma^2}$$
 = the discrete energy level...(9)

The lowest energy of a particle is given by putting n=1 in the eqn (9)

 $E_{1=}\frac{h^2}{8ma^2}$  =lowest energy, minimum energy, ground state energy or zero point energy of the system.

$$E_{n=}n^2E_1$$

The wave functions  $\psi_n$  corresponding to  $E_n$  are called Eigen functions of the particle, the integer'n' corresponding to the energy  $E_n$  is called the quantum number of the energy level  $E_n$ .

Substituting (8) in (7)

$$\dots \psi_n = A \sin \frac{n\pi x}{a} \dots (10)$$

#### Normalization of wave function:

The wavefunctions for the motion of the particel are

$$\psi_n = Asin \frac{n\pi x}{a}$$
, for  $0 < x < a$ 

$$\psi_n = 0$$
, for  $0 \ge x \ge a$ 

According to normalization condition, the total probability that the particle is somewhere in the box must be unity.

$$\int_0^a p_x dx = \int_0^a |\psi_n|^2 dx = 1$$

From eqn(10)

$$\int_{0}^{a} A^{2} \sin^{2} \frac{n\pi x}{a} dx = 1$$

$$A^{2} \int_{0}^{a} \frac{1}{2} \left[ 1 - \cos \frac{2\pi nx}{a} \right] dx = 1$$

$$\left(\frac{A}{2}\right)^2 \left[x - \frac{a}{2\pi n}\sin\frac{2\pi nx}{a}\right] = 1$$

The second term of the integrand expression becomes zero at both the limits.

$$\frac{A^2}{2} = 1$$
$$A = \sqrt{\frac{2}{a}}$$

The normalized wave function is  $\psi_n = \sqrt{\frac{2}{a} \sin \frac{n\pi x}{a}}$ 

#### UNIT-2

#### **Chapter-1 ELECTRON THEORY OF METALS**

#### **FREE ELECTRON THEORY INTRODUCTION:-**

Drudge and Lorentz developed classical free election theory to explain many special properties like conduction of electricity, thermal conductivity, magnetic properties etc of metals later Somerfield improved the version by applying quantum principles next Bloch started band theory which consider the interaction between the positive ions centers and the free electrons. The band theory could explain the behavior of solids with respect to the conduction of electricity through them.

Free electron theory is required because only electrons are responsible for conduction in metals such electrons which responsible for conduction phenomenon are called free electrons or conduction electron.

Classical free electron theory or electron gas model

Drudge and Lorentz proposed free electron theory of metals on the basis of some assumptions

- In conductors (metals), there are large numbers of free electrons moving freely within the metal i.e. the free electrons or valence electrons are free to move in the metal like gaseous molecules, because nuclei occupy nearly 15% metal space and the remaining 85% space is available for the electrons to move.
- Since free electrons behave like gaseous molecules, applying the laws of kinetic theory of gases. The mean K.E of a free E is equal to that of a gas molecule at same temperature.
- In the absence of any electric field, the ES move randomly while undergoing scattering at +ve ion centers. The collisions are regarded as elastic (no loss of energy).
- The electron speeds are distributed according to the max well- Boltzmann distribution law.
- 5) When an electric filed is applied, the free electrons are accelerated in a direction apposite to that of the field.
- 6) The free electrons are cornfield to the metal due to surface potential.

7) The electrostatic force of attraction B/W the + ve ion cores and the free electrons is assumed to be negligible. The approximation is justified in the sense that the free electrons are move at a greater speed as they approach the electrons is also neglected in the concept of free electron theory.

#### **RMS VELOCITY OF FREE ELECTRONS:-**

RMS velocity  $C = \frac{\sqrt{3kt}}{m}$ 

Relaxation time (TR):

As the electric filed is switched off, the electron speed gradually decreases with time due to the scattering of free electrons in the metal by +ve ions.

According to the law of decay of velocities, the velocity of the electrons at any instance `+` is given by the expression,

$$V = voe^{-t/Tt}$$

Here Tr is called mean or relaxation time Vo is the initial velocity at += 0.

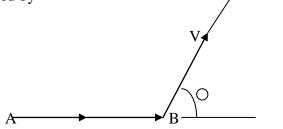
A++=Tr, the above equation becomes

V= Vo/e

i.e the relaxation time is defined as the time required for the electrons to reduce its velocity to 1/e of its initial value (directional velocity)

#### **RELATION BETWEEN RELAXATION TIME AND COLLISION TIME:-**

Consider a conduction electron travelling inside a metal in the direction AB with a velocity `V` let it be scattered by / C



an ion core located by `B` as a result, the electron travels along BC With the same velocity

making an angle Q with the Original Direction Q is called scattering angle.

The value of  $Q^$  is likely to be different for different collisions. The average value of coso taken avers Avery large number of collisions is represented by  $\langle \cos \phi \rangle$ . Then the relaxation time Tr is related to the mean collision time according to the relation.

$$\mathrm{Tr} = \frac{T}{1 - \langle coso \rangle}$$

If the scattering is equally possible is all directions (symmetric scattering) then the average scattering angle of a large number of scattering will be  $\cos \phi = 90^{\circ}$ , then  $\langle \cos \phi \rangle = 0$  and Tr = T. i.e. the mean collisions time can be treated as relaxation time itself.

#### MEAN FREE PATH (^):-

Let us consider S1, S2, and S3..... Etc are the free paths between the first, second, third etc. collisions, the mean free path  $\land$  is defined as the average of all the free paths.

$$\wedge = (s_1 + s_2 + s_3 + \dots + s_n)/n$$

Mean free path is obtained as the product of rms velocity and mean time Tr.

$$\lambda = C^{-} x T$$
  
i.e  $C^{-} = \frac{\sqrt{3kt}}{m}, T = \frac{m}{\sqrt{ne^2}}$ 
$$\lambda = \frac{\sqrt{3kt}}{m} x \frac{m}{\sqrt{ne^2}}$$
$$\lambda = \frac{\sqrt{3mkT}}{\sqrt{ne^2}}.$$

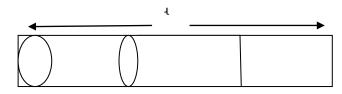
From the above expression, the resistibility `S` is Proportional to square root of temperature in according with classical theory. But experimentally it is no true.

Relation between relaxation time and mobility is

$$\mu = \frac{Tr}{m} = \frac{1}{\ln e}$$

#### **DRIFT VELOCITY OF AN ELECTRON IN A METAL:-**

When a current  $\Gamma$  is passed through a metallic wire, the electrons undergo multiple scattering with the + ve ions and move in a direction opposite to the current direction.



Let us consider a conductor of cross – sectional area `A` and length `'+', so that  $\lambda A$  is the volume of the conductor .if there are length `N` Number of electrons for unit volume of the metal, then the total number of electrons in the specimen in ` NLA`. If `E` is the charge of the electron, then the total charge `Q` due to all the free electrons in the sample.

$$q = nAle.$$

Let `t` be the time taken by the e<sup>-</sup> for moving from one end of the conductor to the other end. During this time, the charge crossed at any point in the conductor is q. the flowing through the conductor.

$$i = \frac{charge}{time} = \frac{q}{t} = \frac{nAle}{t}$$

If v is the drift velocity of the electron, then the time required for the electron to move from one end to the other end is t= distance / velocity = l/v.

Replace 
$$l/v = t$$
  
 $i = \frac{nAle}{(l/v)} = nAve.$   
 $\therefore$  Drift velocity  $V = \frac{i}{nAe}$ 

But the current density J is defend as current flowing per unit cross sectional area,

$$J = \frac{i}{A}$$
$$\therefore V = \frac{J}{ne}$$

The drift velocity increases with the increase of current density or current and decreases with the increase of electron concentration `n`

#### **RELATION BETWEEN DRIFT VELOCITY AND MOBILITY OF THE ELECTRON:-**

According to the ohm's law R = v/i, where 'v' is the potential difference between the ends of a conductor, 'i' is the current flowing though the conductor and 'R' is the resistance.

The ohm's law can otherwise be stated as E/J = P called microscopic ohm's law . here 'E' is the electric filed, 'J' is the current density flowing through the conductor and 'p' is the resistivity or specific resistance of the metal

$$V = j/ne$$
 and  $j = E/P$ 

Substitute J in the expression foe v we get

$$\mathbf{V}=\frac{E}{\int ne}\,.$$

i.e the drift velocity is proportional to applied electric field.

$$V \propto E \Longrightarrow V = \mu E$$

.

the proportionality constant  $\mu$  is called the mobility of

$$\mu = \frac{1}{\ln e}$$

when E = 1, then  $V = \mu$ , mobility is defined as the drift velocity of  $e^-$  when the applied electric field is unity.

Expression for resistivity  $\int = \frac{1}{\mu ne}$ 

Conductivity  $\sigma = \mu ne$ .

#### FAILURE OF THE CLASSICAL FREE ELECTRON THEORY:-

1) <u>Heat capacities :-</u> the internal energy of a molar substances

$$U = \frac{3}{2} KTN$$

Molar specific heat + c v =3/2kn=3/2R.

'N' is the Alvarado number, K is Boltzmann constant and 'R' is the universal gas constant .the molar specific heat is 1.5 R theoretically where as the experimental value obtained is too low . This is due to the fact that all free electrons do not contribute significantly to thermal or electrical conductivity.

There fore classical free e<sup>-</sup> theory can't hold good.

2) Mean free path :- It is calculated using the formula

$$\lambda = \mathbf{C}^{-} \mathbf{x} \mathbf{T}$$
$$\lambda = \frac{\sqrt{3kt}}{m} \mathbf{x} \frac{m}{\ln e^{2}}$$

$$\lambda = \frac{\sqrt{3kTm}}{\ln e^2} \, .$$

For cu at 20° c  $\int = 1.69 \times 10^{-8}$  ohm-m<sup>3</sup>

## **e**<sup>-</sup> **concentration** $n = 8.5 \times 10^{28} / m3$ .

The experimental  $\hat{x}$  was obtained nearly 10 times its theoretical value . so classical theory could not explain the large variability in  $\hat{x}$  values

3) **<u>RESISTIVITY:</u>** According to the classical free electron theory ,the resistivity is given by the equation.

$$\int = \frac{\sqrt{3mTk}}{ne^2}.$$

Which means the resistivity is proportional to the square root of absolute temperature. But according to the at room temperature it does not change up to 10K and in intermediate range of temperature  $\int$  is proportional to T<sup>5</sup>.

 The conductivity of semiconductors and Insulators can not be explained by the free electron theory.

#### **QUANTUM FREE ELECTRON THEORY:-**

In 1929, Somerfield stated to apply quantum mechanics to explain conductivity phenomenon in metal. He has improved the Drude  $\varepsilon$  Lorentz theory by quantizing the free electron energy and retaining the classical concept of free motion of electron at a random.

#### ASSUMPTIONS:-

- The electrons are free to move within the metal like gaseous molecules. They are confined to the metal due to surface potential.
- The velocity distribution of the free electrons is described by Fermi-Divac Statistics because electrons are spin half particles.
- The free electrons would be go into the different energy levels by following Pauli's exclusion Principle which states that no two electrons have same set of Quantum numbers.
- The motion of electrons is associated with a complex wave called matter wave, according to Debroglie hypothesis.
- 5) The electrons cannot have all energies but will have discrete energies according to

the equation  $E = n^2 h^2 / 8ma^2$ 

'a' is the dimensions of the metal 'h' is plank's constant and 'n' is the integer starts from 1.

#### Energy levels – Fermi Dirac Distribution:

According to the Quantum theory Quantization leads to discrete energy levels. The electrons are distribution among these energy levels according to Pauli's exclusions principle it allows a maximum number of two electrons with spins in opposite directors in any energy level. The pair of electrons, one with sign up and the other with sign down occupy the lowest energy level. The next pair occupies the next level. This process goes on until all the electrons in the metal occupy their position.

But there will be many more allowed energy levels available for occupation. The highest energy level that can be occupied at ok is called Fermi energy level. It is denoted by E f. When the metal is not under the influence of an external field, all the levels above the Fermi energy level are empty; those lying below are completely filled.

#Energy levels and order of filling levels in a metal.

The energy associated with Ef is called Fermi Energy.

The speed of the electron occupying the Fermi level is called Fermi Velocity.

#### Fermi – Dirac Distribution:

When the material is at a temperature higher than OK, it receives thermal energy from surroundings i.e. electrons are thermally excited. As a result, they move into the higher energy levels which are unoccupied at OK. The occupation obeys a statistical distribution called Fermi – Dirac distribution law.

According to this distribution law, the probability f(E) that a given energy state E is occupied at a temperature T is given by  $\frac{1}{\exp(E-Ef)/KT + 1}$ 

Here f(E) is called Fermi – Dirac probability function. It indicates that the fraction of all energy state (E) occupied under thermal equilibrium 'K' is Boltzmann constant.

#### Expression for Fermi Energy level(Ef)

$$Ef = 3.65*10^{-19} n^{2/3}$$

Where n is concentration of electrons.

Drawbacks of Quantum free electron theory :

 Lorentz Number : The Lorentz number in the Quantum free electron theory is given by

$$\underline{\mathbf{L}} = \left( \frac{\pi^2}{3} \right) (\mathbf{K}/\mathbf{e})^2$$

Here 'K' is Boltzmann constant and 'e' is charge of electron the observed Lorentz number is greater than the theoretical value as calculated from the above expression. i.e the Lorentz number is found to be vary with temperature. When metals are heated, the positive ions cores vibrate about their mean position and generate photons. The Phonons along with the free electrons carry some of the heat supplied to the metal. This must be the cause of large difference between observed and theoretical Lorentz number.

(2) <u>Conductivity</u>: According to Quantum free electron theory, the conductivity of a metal is

 $\sigma = \mu ne$ 

Here ' $\mu$ ' is the mobility of electron, 'n' is the free electron concentration and 'e' is the electron charge.

According to the above equation, polyvalent metals like Aluminium (Al) should be more conductive than mono valent metals like copper (cu). But experimentally it is not so.

- (3) <u>Hall co efficient</u>: According to the free electron theory, the hall coefficients for all metals is negative where as there are certain metals like Be, Cd, Zn for which the Hall coefficient is + ve
- (4) Free electron theory could not explain why certain substances behave as insulators and some other substances as semiconductors, inspite of they have free electrons in them.

## **Chapter2:Band Theory of Solids**

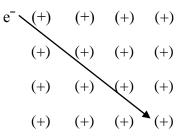
<u>Introduction:</u> According to Quantum free Theory of methods a conduction\_E in a metal experiences constant (or zero) potential and free to move within the crystal but will not come out the metal. This theory successfully explains electrical conductivity, specific heat etc but fails to explain many other physical properties, for example (I) Difference between conductors, insulators and semiconductors.

To overcome the above problems, the periodic potentials due to +ve ions in a metal have been considered.

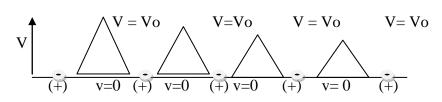
#### Electrons in a periodic potential –Bloch Theorem:

An E moves through + ve ions, it experiences varying potential. The potential of the E at the +ve ions site is zero and is maximum in between two +ve ions sites.

The potential experienced by an e<sup>-</sup>, then it passes though +ve ions shown in life.



i.e The potential experienced by an E's in shown in Fig known as real periodic potential variation



To study the motion of E in lattice and the energy states it can occupy, Schrodinger equation is necessary

For making simplicity, Koenig-penny introduced a simple model for the shape of potential variation. The potential inside the crystal is approximated to the shape of rectangular steps.

#### KRONIG PENNY MODEL:-

Kronig – penny consider a periodic management of potential walls and barriers to represent the potential variation exhibited by the E , Known as Ideal-periodic square well potential as shown in figure. New forms of boundary conditions are developed to obtain a simple solution known as cyclic or periodic boundary conditions.

Conclusion From Kronig –Penny Model:

1). The Energy spectrum of E consists of an infinite number of allowed energy bonds separated by intervals in which, there are no allowed energy levels. These are known as forbidden regions.

2). When  $\alpha$  a increase, the first term of eq(1) on LHS decrease, so that the width of the allowed energy bonds is increased and forbidden energy regions become narrow.

3). The width of the allowed bond decrease with the increase of p value. When  $p \rightarrow \alpha$ , the allowed energy regions become infinity narrow and the energy spectrum becomes line spectrum.

Validity : when  $p \rightarrow 0$ ,  $\cos \alpha a = \cos k a$ 

i.e 
$$x^2 = x^2$$
  
i.e  $\frac{8\pi^2 m}{h^2} = k^2$   
 $=> E = \frac{h^2 k^2}{8\pi^2 m}$   
Here  $k = \frac{2\pi}{\lambda}$ ,  $=> E = \frac{h^2}{8\pi^2 m} \frac{4\pi^2}{\lambda^2}$   
i.e  $E = (\frac{h^2}{2m}) \frac{1}{\lambda^2}$   
Here  $\lambda = \frac{h}{p}$ , ie  $E = (\frac{h^2}{2m}) \frac{p^2}{h^2}$   
Here  $p = mv_1 => E = (\frac{h^2}{2m}) \frac{m^2 v^2}{h^2}$   
 $E = \frac{1}{2} mv^2$ .

The wave functions associated with this model can be calculated by solving Schrödinger's eq for two regions 1 and 2.

(1) ie 
$$\frac{d^2 4}{dx^2} + \frac{8\pi^2 m}{h^2}$$
 E 4 = 0, 0 < x< a  
 $\frac{d^2 4}{dx^2} + x^2$  4 = 0,  $x^2 = \frac{8\pi^2 m}{h^2}$  E  
(2)  $\frac{d^2 4}{dx^2} = \frac{8\pi^2 m}{h^2} (v_0)$  4 = 0, -b < x < 0

(3) 
$$\frac{d^2 4}{dx^2} - \beta^2 4 = 0$$
,  $\beta^2 = \frac{8\pi^2 m}{h^2}$  ( $v_0 - E$ )

These two eq are solved by using Block and Koenig-penny models, and applying Boundary conditions the solution is

$$\frac{\beta^2 - \alpha^2}{2\alpha \beta} \sin \alpha a \sin h \beta b + \cos \alpha a \cosh \beta b = \cos k (a + b)$$

To provide simplest solution, Koenig-penny assumed that  $b \rightarrow o$ 

 $sin h \beta b \longrightarrow \beta b$ 

$$cos h \beta b \longrightarrow 1$$

i.e  $\frac{\beta^2 - \alpha^2}{2\alpha\beta} \sin \alpha \alpha \beta b + \cos \alpha a = \cos k a$ here  $\beta^2 - \alpha^2 = \frac{8\pi^2 m}{h^2} (v_0 - 2E) = \frac{8\pi^2 m}{h^2} v_0$ , since  $v_0 >> E$ i.e  $(\frac{8\pi^2 m}{h^2 2\alpha\beta} v_0) \sin \alpha \alpha \beta b + \cos \alpha a = \cos k a$ i.e multiplying this eq with  $\frac{\alpha a}{\alpha a}$  then  $\frac{mv_0 ba}{h^2} \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$ i.e  $p \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$ i.e  $p \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$ 

Here  $p = \frac{mv_0ba}{h^2}$  is scattering power

And ' $v_0$  b' is known as barrier strength.

The LHS and RHS of eq (1) are equal, then LHS of eq(1) on y-axis of a function of  $\alpha a$ , in value p=3 /2. The RHS of 1. i.e' cos ka can take values between +1to-1.so the LHS of each 1. Is also restricted to vary between =1.

## Chapter 3 SEMICODUCTORS

Energy bond Formation in solids:

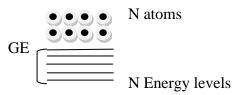
- In isolated atom, the e<sup>-</sup>s are tightly bond and have discrete, shape energy levels.

- When two identical atoms are brought closed the outermost orbits of these atoms overlap and intersects the wave functions of the E of the different atoms begin to overlap, then the energy levels corresponding to those wave functions split in to two.

$$\underbrace{\bullet}$$
  $E_1$ 

- If more atoms brought together more levels are formed and for a solid of N atoms, each of these energy levels of an atoms splits into N levels of energy.

 $----- E_2$ 



The levels are so close together that they form almost continuous bond.

-The E first occupies lower energy bonds and are no importance in determining many of the physical properties of solid.

-These E present in higher energy bonds are important in determining many of the physical of solids.

-These two allowed energy bonds are called as valence and conduction bonds.

-The bond corresponding to the outermost orbit is called conduction bond and the gap between those two allowed bonds is called forbidden energy gap are bond gap.

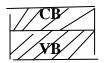
Classification of solids:

Solids are classified into three types based on energy gap.

- (1) Conductors(metal)
- (2) Insulators
- (3) Semiconductors

-In case of conductors, valence bond and conduction bond almost overlap each other and no significance in energy gap. The two allowed bond are separated by semi energy level.

-Here there is no role in Eg, as a result conducting is high.



-In case insulator, valence bond and conduction bond are separated by large energy gap, Hence conductivity is zero. -In case semiconductors, the valence bond and conduction bond are separated by relatively narrow energy gap, hence the conductivity lies in between conductors and insulators.

Effective mass of the E moving in a crystal lattice:

-Consider a crystal (metal) be subjected to an electric field 'E', so the experienced by an E of charge E is Ee.

-Acceleration of the E in the crystal is given by a=f/m=Ee/m

-But acceleration of the E is not constant because of the velocity changes i.e The E move faster near the +ve ions in the crystal. Since the electric field and charge of the E are invariant, the effective mass Mh of the E to change accordingly.

-Consider a particle velocity 'v' is equal to group velocity 'vg' of a wave packet, then

$$V=vg = \frac{dw}{dk}$$
, w= angular frequency, k= wave propagation vector

W= $2\pi v$  dw= $2\pi dv$ 

Frequency of the complex wave v=E/n dv=1/ndE

$$dw=2\pi de/h=de/h$$

:. V = dw/dk = 1/h de/dk

SO, 
$$a = \frac{dk}{dt} = (\frac{1}{h}) \frac{d^2 E}{dk dt}$$
$$a = \frac{1}{h} \frac{d^2 E}{dk^2} (\frac{dk}{dt})$$

Wove propagation vector  $k = \frac{2\pi}{\lambda}$ 

$$k = \frac{2\pi}{h} P = \frac{p}{h}$$

`P` is momentum, ` $\lambda$ ` is debrogle wave length  $\therefore \frac{dk}{dt} = \frac{1}{h} \left(\frac{dp}{dt}\right) = \frac{f}{h}$ 

Sings  $\frac{dp}{dt}$  is the rate of change of momentum, which is nothing but force F

$$a = \frac{1}{h} \frac{d^2 E}{dk^2} \frac{1}{h} F$$
$$a = \frac{f}{h^2} \left(\frac{d^2 E}{dk^2}\right)$$
i.e 
$$F = \frac{h^2}{\frac{d^2 E}{dk^2}} a - - -2$$

Compare 1 & 2

Effective mass 
$$m^{\nu} = \frac{h^2}{\frac{d^2 E}{dk^2}}$$

# **Chapter 3 Semi conductors**

## Introduction

Electrical conductivity of a semi-conductor:

In metals only the electrons participate in the conduction phenomenon where as in semiconductors both electrons and holes are responsible for conduction phenomenon. The electrons and holes more in opposite directions because of their opposite charges, they add conductivity to the semi-conductor.

In metals, the conductivity is given by expression  $\sigma = \mu n e^{-t} \mu n e^{-t}$  "is mobility, 'n'is electron Concentration and 'e' is charge of electron.

But in semi-conductors, contribution of () andholes re taken into account

i.e.,. Conductivity  $\sigma = ne\mu + pe\mu_p$ 

Where,

N = Electrons' concentration in conduction band

P =Holes concentration in valance bond

 $\mu_n = Mobility of electron$ 

 $\mu_P = mobility of holes$ 

e = effective charge

Semi-conductors are of two types:

1. Intrinsic and 2) Extrinsic

Extrinsic

N-Type

P-Type

## Intrinsic Semi conductors:

A semi conductor in which holes in the valance band and electrons in the conductions band are solely created by thermal excitations is called intrinsic semiconductors i.e.,.

A pure semi-conductor is considered as intrinsic semi conductor

The no. of electrons moving into the conduction band is equal to the no of holes created in the valence band

The Fermi Level lies exactly in the middle of forbidden energy gap.

The concentration of electrons and holes increases rapidly with temperature.

Intrinsic semi-conductors are not of practical use in view of their poor conductivity.

Carrier concentration in intrinsic semi-conductors

In the Conduction band, the level density D(E) at a energy E is given by the Expression.

$$D(E)dE = \frac{4\pi}{h^3} (2m)^3 / {}^2 E^1 / {}^2 dE$$

The probability of an energy level filled with electrons is given by Fermi-Dirac function

$$F(E) = \frac{1}{1 + \exp(\frac{E - EF}{KT})}$$

The no of E's 'n" filing into energy level between the energies E and E+dE is

$$n = \frac{4\pi}{h^3} (2me)^3 / {}^2 E^1 / {}^2 \frac{1}{1 + \exp(\frac{E - EF}{KT})} dE$$

In the Above expression, mass of the e" 'm" is replaced with effective mass me and factor '2' for the two possible spins of the electrons.

The number of electrons in the conduction band is obtained by making integration between the limits Ec to  $\infty$ .Since minimum energy in the conduction band is Ec and at the bottom of the conduction band we write E-Ec for E

$$n = \frac{4\pi}{h^3} (2me)^3 / {}^2 \int$$

For all possible temperatures E-Ef >>>> KT

Hence 
$$F(E) = \exp - \left(\frac{(E-Ef)}{KT}\right) = \exp \left(\frac{EF-E}{KT}\right)$$

Equation 1 becomes

n=
$$\frac{4\pi}{h^3} (2me^v)^3 / {}^2 \int (E-Ec)^{1/2} exp(\frac{EF-E}{KT}) dE$$
  
n= $\frac{4\pi}{h^3} (2me^v)^3 / {}^2 exp(E_F/KT) \int (E-Ec)^{1/2} exp(\frac{-E}{KT}) dE$ 

To solve this Integral Part

E-Ec = x

E = Ec + x

dE=dX

$$n = \frac{4\pi}{h^3} (2me^v)^3 / {}^2 \exp(E_F/KT) \int_{\chi} \frac{1}{2} \exp(-(\frac{Ec+x}{KT})) dx$$

$$n = \frac{4\pi}{h^3} (2me^v) \quad {}^3/^2 \exp(\frac{EF - Ec}{KT}) \int_{\chi} \frac{1}{2} \exp(-(\frac{-x}{KT}) dx$$

Using gamma function, it can be shown that

$$\int_{\chi} \frac{1}{2} \exp \left(-\left(\frac{-x}{KT}\right) dx d_{\chi} = (KT)^{3} / 2 \frac{\pi}{2} \frac{1}{2}^{\frac{1}{2}} \right)$$
  
Hence  $n = n = \frac{4\pi}{h^{3}} (2me^{v})^{-3} / 2 \exp\left(\frac{EF - Ec}{KT}\right) (KT)^{3} / 2 \frac{\pi}{2} \frac{1}{2}^{\frac{1}{2}}$ 

No of electrons per unit volume is given by

$$n=2(\frac{2\pi m e^{v} KT}{h^2}) \exp\left(\frac{Ef-Ec}{KT}\right)$$

The expression for no of holes in the valance bond is given by the expression

$$P=2(\frac{2\pi m p^{v} KT}{h^{2}}) \exp(\frac{Ev-Ef}{KT})$$

In Intrinsic semi conductor n=p then the Intrinsic carrier concentration is n=p=n;

ni<sup>2</sup> = 4 
$$\left(\frac{2\pi KT}{h^2}\right)^3 (m_e^v m_{p^v})^{3/2} \exp\left(\frac{Ev-Ec}{KT}\right)$$
  
ni<sup>2</sup> = 4  $\left(\frac{2\pi KT}{h^2}\right)^3 (m_e^v m_{p^v})^{3/2} \exp\left(\frac{-Eg}{KT}\right)$ 

Here Ec-Ev=Eg ( forbidden energy gap )

Hence ni =2 
$$\left(\frac{2\pi KT}{h^2}\right)^{3/2} \left(m_{e^v} m_{p^v}\right)^{3/4} \exp\left(\frac{-Eg}{KT}\right)^{3/4}$$

Fermi Level: In Intrinsic semi conductor n=p and assuming the effective mass of e and hole to be same, i.e.,. Me  $^v$ =Mp $^v$ 

$$\exp\left(\frac{Ef-Ec}{KT}\right) = \exp\left(\frac{Ev-Ef}{KT}\right)$$
  
Ef-Ec=Ev-Ef  
2Ef = Ev+Ec  
Ef =  $\frac{Ev+Ec}{2}$ 

Thus the Fermi level is located half way between the valance band and conduction band and its position is independent of the temperature.

Intrinsic semi conductor:

Impure semi conductors are called extrinsic semi-conductors .When pentavalent or trivalent impurities are added to Intrinsic (pure) semi-conductors, it becomes extrinsic semi-conductor. The phenomenon of adding impurities is called doping. The phenomenon of conductivity is increased by process of Doping.

N-Type semi – Conductors:

When pentavalent impurities like P. As, Sb is added to the intrinsic semi-conductors, resultant semi conductor is called N-Type semi-coductor.the concentration of free electrons is more when compared to concentration of holes carriers' concentration in N-type semi conductors:

In this type of semi conductor, there will be donor levels formed at an energy Ed

Nd represents no. of impurities per unit volume of semi conductor

At low temperature all donor levels are filled with electrons, with increase of temperature, more and more donor atoms gets ionized and the density of electrons in the conduction band increases

Density of electrons in the conduction band is given by

$$n=2(\frac{2\pi m e^{v} KT}{h^2})^{3/2} exp(\frac{Ef-Ec}{KT}) \rightarrow 1$$

The Fermi level (Ef) lies in between Ed & Ec

The density of empty donor levels is given by

Nd [ 1-F(E<sub>d</sub>)] 
$$\equiv$$
 N<sub>d</sub> [ 1-H exp( $\frac{Ed-Ec}{KT}$ )  
Nd [ 1-F(E<sub>d</sub>)]  $\equiv$  Nd exp( $\frac{Ed-Ec}{KT}$ )

At low temperature, there are no excitations of the electrons from donor level to the conduction band. Hence, density of empty donors and the electron desity in conduction band should be same

i.e., 
$$2\left(\frac{2\pi mp^{v}KT}{h^2}\right)^{3/2} \exp\left(\frac{Ef-Ec}{KT}\right) = N_d \exp\left(\frac{Ed-Ef}{KT}\right)$$

Taking lon on both the sides& rearranging

$$\left(\frac{\text{Ef}-\text{Ec}}{\text{KT}}\right) - \left(\frac{\text{Ed}-\text{Ef}}{\text{KT}}\right) - \log \text{Nd} - \log 2\left(\frac{2\pi \text{me}^{v}\text{KT}}{h^{2}}\right)^{3/2}$$

$$Ef - Ec - Ed/KT = \log \left(\frac{\text{Nd}}{2\left(\frac{2\pi \text{me}^{v}\text{KT}}{h^{2}}\right)^{3/2}}\right)$$

$$2\text{Ef} - (\text{Ec}+\text{Ed}) \text{ KT} \log \left(\frac{\text{Nd}}{2\left(\frac{2\pi \text{me}^{v}\text{KT}}{h^{2}}\right)^{3/2}}\right) \rightarrow 2$$

At absolute zero  $Ef = \frac{Ec+Ed}{2}$ 

i.e.,. Fermi level lies exactly at the middle of donor lvel Ed and the bottom of the conduction band E

Substituting equation 2 in eqn. 1 & re-arranging,

N = 
$$(2^{\text{Nd}}) \frac{1}{2} \left(\frac{2\pi \text{me}^{\nu}\text{KT}}{h^2}\right)^{3/4} \exp\left(\frac{\text{Ed}-\text{Ec}}{2\text{KT}}\right)$$

Hence the density of the electrons in the conduction band is proportional to the square root of the donor concentration

P-type semi conductors:

P-type semi-conductors are fabricated by addition of trivalent atoms like Al as impurity to the intrinsic semi-conductor

Hence, holes are majority charge carriers and free electrons are minority charge carriers.

Carrier concentration in P type semi-conductors

In this type of semi-conductor, there will be there will be acceptor levels formed at an enrgy Ea

Na represents no. of impurities per unit volume of semi-conductor.

At low temperatures, all the acceptor levels are empty

With increase of temperature, acceptor atoms gets integrated i.e., the electrons moves from valance band and occupy the vacant sites in the acceptor energy levels, there by leaving holes in the valence band

Density of holes in the valance band is given by

P =2 
$$\left(\frac{2\pi m p^{v} KT}{h^{2}}\right)^{3/2} \exp\left(\frac{Ev-Ef}{KT}\right)$$

Since Ef lies below the acceptor levels, the density of ionized acceptors is given by

$$N_a F (E_a) = N_a \exp(\frac{Ef-Ea}{KT})$$

Hence, density of holes in the valance band is equal to the density of ionized acceptors.

$$2\left(\frac{2\pi \mathrm{mp^{v}KT}}{h^{2}}\right)^{3/2} \exp\left(\frac{\mathrm{Ev}-\mathrm{Ef}}{\mathrm{KT}}\right) = \mathrm{N}_{\mathrm{a}} \exp\left(\frac{\mathrm{Ef}-\mathrm{Ea}}{\mathrm{KT}}\right)$$
  
Ie.,. 
$$2\frac{Ev-Ef-Ef+Ea}{KT} = \frac{\mathrm{Na}}{2\left(\frac{2\pi \mathrm{mp^{v}KT}}{h^{2}}\right)^{3/2}}$$
  
Taking log, 
$$\frac{Ev+Ea-2Ef}{KT} = \log \frac{\mathrm{Na}}{2\left(\frac{2\pi \mathrm{mp^{v}KT}}{h^{2}}\right)^{3/2}} \rightarrow 2$$
  
At 0° K, E f = 
$$\frac{Ev+Ea}{2}$$

i.e., at 0 o K, Fermi level lies exactly at the middle of the acceptor level and in the top of the valance bond

Sub. eqn. 2 in eqn. 1 & re-arranging

P=(2Na)  $\frac{1}{2} \left(\frac{2\pi mp * KT}{h^2}\right)^{3/4} \exp\left(\frac{Ev-Ea}{KT}\right)$ 

Thus the density of the holes in the valance band is proportional to the square root of the acceptor concentration

Equation of Continuity:

In the equilibrium, all the processes are balanced and there will not be any external force.

The Fermi level is constant throughout the volume of the solid.

Under equilibrium, there exists a steady state, in which the condition of the system does not change

In non-equilibrium conditions, the Fermi level will be varying through the volume of the solid. The Fermi level will not be exactly in the middle of the forbidden band. Hence, the electrons from the valance band can easily pass to the conduction band.

So the generation of charges will not be equal to the rate of recombination and there will be a net change in the concentration of excess electrons or holes.

The Condition will be changing with time.

The divergence of current density gives time rate of change of concentration of electrons or holes.

Number of electrons or holes generated =divergence of current density.

When electron concentration causes current

$$\frac{djn}{dx} = \frac{-dn}{dt}$$

This is one dimensional equation of continuity which is written as

$$\Delta \mathbf{J} + \frac{d\rho}{dt} = 0$$

J = Current density

 $\rho$ = charge density =Ne for electrons, 'n' is concentration of electrons.

$$\frac{d\rho}{dt} = \frac{1}{e} \Delta Jn$$

For electrons

$$\frac{1}{e}\Delta Jn - \frac{dn}{dt} = 0$$

For holes

$$\frac{1}{e}\Delta Jp - \frac{dp}{dt} = 0$$

Under equilibrium conditions the rate of generation of charges will be equal to the rate of recombination. But for non-equilibrium conditions, there is a net rate of change of generation

For Electrons  $\frac{dn}{dt} = \text{Gn-Rn} + \frac{1}{e} \Delta \text{Jn}$ For holes  $\frac{dp}{dt} = \text{Gp-Rp} + \frac{1}{e} \Delta \text{Jp}$ 

Gn, Gp =rate of generation of electrons/holes

Rn, Rp = rate of recombination of electrons/holes

Recombination rate Rn of electrons is

$$\operatorname{Rn} = \frac{n - no}{Tn}$$

 $n_0$ =Equilibrium concentration of electrons

n=Concentration of electrons.

Tn =Electron life time

$$\frac{dn}{dt} = \operatorname{Gn-}\frac{n-no}{Tn} + \frac{1}{e}\Delta \operatorname{Jn}$$

Electron current density Jn is sum of diffusion and drift currents due to electron is given by

$$Jn = n\mu_n eE + D_n e(\frac{dn}{dx})$$

Here the first term gives drift current of electrons with mobility Mu() due to application of the electric field

Second term gives diffusion current due to the concentration gradient of electrons,  $d^2$ 

$$\frac{dn}{dt} = \operatorname{Gn-} \frac{n-no}{Tn} + n\mu_n \frac{dE}{dx} + \operatorname{D_ne} \frac{d^2n}{dx^2}$$

For holes

$$\frac{dp}{dt} = \text{Gp-}\frac{p-po}{Tp} + p\mu_p \frac{dE}{dx} + D_p e \frac{d^2p}{dx^2}$$

Continuity equation is used to calculate the excess density of electrons and holes in time and space. This is the basic equation in describing the semi-conductors

## Hall-Effect

When a material carrying current is subjected to a magnetic field I a direction perpendicular to direction of current, an electric field is developed across the material in a direction perpendicular to both the direction of magnetic field and current direction. "this phenomenon is called "Hall-effect"

Explanation: Consider a semi-conductor, and a current passes along the X-axis and a magnetic field Bz is applied along the Z-direction, a field Ey is called the Hall field which is developed in the Y-direction

In P-tpe semi-conductor, holes move with the velocity "V" in the "+"ve X-direction. As they move across the semi conductor the holes experience a transverse force B() ev due to the magnetic field. This force drives the holes down on to face1, as shown in the figure. As a result, the lower face becomes +vely charged and –ve charge on the upper surface creating the hall field in the Y-direction.the Hall field exerts an upward force on holes equal to E().n the steady sate, two forces just balance and as a result, no further increase of + ve charge occurs on Face1.

If N type semi conductor, the majority charge carriers are electrons experiences a force in the downward direction and face1 gets – vely charged. As a result, Hall field will be in the Y – direction

Demonstration:

Consider a rectangular slab of n-type semi conductor carrying slab n-type semi conductor carrying a current in the + ve X- direction

If magnetic field "B' is acting in he X-direction shown in fig:

Under the influence of magnetic field, electrons experience a force Fl given by

 $F_{L} = -Bev$ 

e = Charge of electron

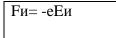
## V= Drift velocity

As a result of force FH acting on the electrons in the - ve Y - direction and electrons are tend to downwards.

As a consequence the lower face of the specimen gets – vely charged and upper surface is + vely charged

Hence a potential VH called the Hall Voltage present between the top and bottom faces of the specimen

The Hall field FH, exerts an upwrd force on the electrons is given by



The two opposing forces FL and FH establish an equilibrium under which

 $|F_{L}| = |F_{U}|$ 

-Bev =-е Еи

Еи=ВV

If 'd' is the thickness of th specimen

Eи = 
$$\frac{Vh}{d}$$
 (  $\therefore E = \frac{V}{d}$ )

Vи = Eиd

Vи = Bvd

If 'W' is the width of the specimen

$$\mathbf{J} = \frac{\mathbf{I}}{wd}$$

J= nev =PV

N= electron

P=charge density.

$$Pv = \frac{I}{wd}$$

&

$$V = \frac{I}{pwd}$$
$$=>V_{H} = \frac{Bid}{pwd} = \frac{Bi}{pw}$$
Bi

$$=> p = \frac{BI}{Vhw}$$

<u>Hall Coefficient :</u> Hall field Eh, for a given material depends on the current density J and the applied magnetic field B

i.e. Ен а JB  
Ен = Rн а JB  
SINCE, 
$$V_{\rm H} = \frac{{\rm Bi}}{pw}$$
,  ${\rm Eh} = \frac{{\rm Vh}}{d}$   
 $\Rightarrow {\rm Eh} = \frac{{\rm Bi}}{pwd}$   
 $\Rightarrow {\rm J} = \frac{{\rm i}}{wd}, \frac{{\rm Bi}}{pwd} = {\rm Rh} = (\frac{{\rm i}}{wd}) {\rm B}$   
i.e.  ${\rm Rh} = \frac{{\rm I}}{f}$ 

Applications :

1) Determination of the type of Semi-conductors:

The Hall coefficient Rh is \_ve for an n-type semiconductor and +ve for p-type semiconductor. Thus the sign of Hall coefficient can be used to determine whether a given Semi-conductor is n or p-type.

2) <u>Calculation of carrier concentration</u>:

$$R_{II} = \frac{I}{J} = \frac{I}{ne} \text{ (for e} \text{ s)}$$
$$R_{II} = \frac{I}{pe} \text{ (for holes)}$$
$$=> n = \frac{I}{eR_{II}}$$
$$=> p = \frac{I}{eR_{II}}$$

3) <u>Determination of Mobility</u>: It the conduction is due to one type carriers, ex: Es

 $\sigma = ne\mu n$ 

$$\mu n = \frac{\sigma}{ne} = \sigma R \mu$$
$$\mu = \sigma |R_{\mu}|$$

4) <u>Measurement of Magnetic Flux Density</u>: Hall Voltage is proportional to the magnetic flux density B for a given current I. so, Hall Effect can be used as the basis for the design of a magnetic flux density metal.

## UNIT3

## Chapter1 **DIELECTRIC PROPERTIES**

Dielectrics are non metallic materials of high specific resistance, negative temperature coefficient of resistance and large insulation resistance.

Dielectrics are of two types

(i) Polar dielectrics

(ii) Non polar dielectrics

(i) **Polar dielectrics:** these dielectric molecules will not have centre of symmetry here the centers of positive and negative charges will not coincide and hence it possess a net dipole moment in it.

Ex: H<sub>2</sub>o, N2o, Hcl

#### Effect of electric field:

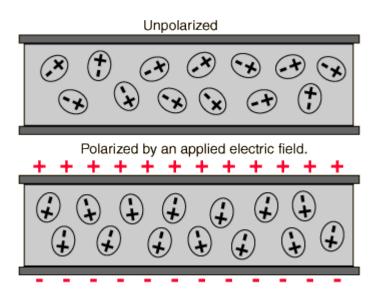
**In the absence of electric field:** in the absence of electric field the polar dielectric molecules themselves posses some dipole moment .but since these dipole are randomly oriented they cancel each other and the net dipole moment will be very very less

**In the presence of electric field:** now when an external electric field is applied to the polar dielectric molecule the dipole will align themselves parallel to the field direction and produce a net dipole moment.

(ii) **Non polar dielectricss:** these dielectric molecule posses centre of symmetry and hence the centres of positive and negative charges coincide. Therefore the net charges and net dipole moment of these molecule will be zero hence these non polar molecules will not posses any dipole moment in it.

Ex: N<sub>2,</sub> H2, O2, CO2

**Effect of electric field**: when non polar molecule is placed in an external electric field a force is exerted on each charge particle within the molecule i.e. the positive charges are pushed along the field direction and the negative charges are pushed opposite to the filed direction. Hence the positive and negative charges separated by some distance from their equilibrium position, creating a dipole and therefore net dipole moment will be produced in non polar molecule.



**Electric dipole**:two equal and opposite charges small in magnitude and separated by a small distance constitute a electric dipole.

**Dipole moment:** if two charges +q and –q are separated by a distance I than the dipole moment can be defined as product of magnitude of charges and distance between them.

μ =q.l

- it is a vector quantity
- the direction of  $\mu$  is from negative to positive

**Dielectric constant**  $\varepsilon_r$ : dielectric constant is the ratio between the permittivity of the medium and the permittivity of the free space

$$\varepsilon_r = \frac{\varepsilon}{\varepsilon_0}$$

• since it is the ratio of same quantity  $m{arepsilon}_r$  has no units

**Electric polarization** : let us consider an atom placed inside an electric field the centre of positive charge is displaced along the applied field direction while the centre of negative charge is displaced in the opposite direction.thus a dipole is produced when a dielectric material is placed inside an electricfield such dipoles are created .

This process of producing electric dipoles which are oriented along the field direction is called polarization in dielectrics.

**Polarizability**( $\alpha$ ) when the strength of the electric field E is increased the strength of the induced dipole  $\mu$  is also increases . thus the induced dipole moment is proportional to the intensity of the electric field

 $\mu = \alpha E$  where  $\alpha$  the constant of proportionality is called polarizability.

It is defined as induced dipole moment per unit electric field.

$$\alpha = \frac{\mu}{E}$$

**Polarization vector (P)** :the dipole moment per unit volume of the dielectric material is called polarization vector P

$$P = \frac{\mu}{V}$$

If  $\mu$  is the average dipole moment per molecule and N is the number of molecules per unit volume the polarization vector

$$P = N\mu$$

The diple moment per unit volume of the solid is the sum of all the individual dipole moment with in that volume and is called polarization P of the solid.

#### Electric displacement vector (D) or electric flux density

The electric displacement vector is a quantity which is a very convenient function for analyzing the electrostatic field in the dielectrics and is given by

$$D = \frac{Q}{4\pi r^2} \quad ---- 1$$

We know that electric field intensity

$$E = \frac{Q}{4\pi r^2} - ---2$$

From 1 and 2

D=εE

 $D = \varepsilon_0 \varepsilon_r E$ ------3

Relation between P and E  $D=\varepsilon_o E+P-----4$ From 3  $D=\varepsilon_o \varepsilon_r E$ Therefore equ 4 becomes  $\varepsilon_o \varepsilon_r E=\varepsilon_o E+P$  $P=\varepsilon_o E(\varepsilon_r-1)$ 

**Electricsusceptability** $\phi$  The polarization vector (P) is proportional to the applied electric field (E) and is in the same direction of E

P=ε<sub>0</sub>**φ**E-----1

Where the constant  $oldsymbol{arphi}$  is refered as the electric susceptibility

From 1  $\varphi = \frac{P}{\varepsilon_0 E}$ 

But  $P = \varepsilon_0 E(\varepsilon_r - 1)$ 

$$\boldsymbol{\varphi} = \frac{\varepsilon_{O} E(\varepsilon_{r} -)}{\varepsilon_{O} E} = \boldsymbol{\varphi} = (\varepsilon_{r} - 1)$$

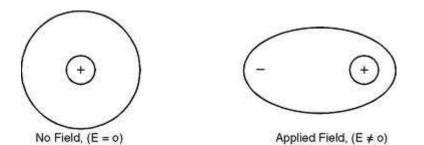
#### Various polarization process

Polarization occurs due to several atomic mechanisms. When the specimen is placed inside d.c electric field polarization is due to four types of process

- 1. Electronic polarization
- 2. Ionic polarization
- 3. Orientational polarization
- 4. Space charge polarization

## Electronic polarization and calculation of electronic polarizability

Electronic polarization occurs due to the displacement of positively charged nucleus and negatively charged electron in opposite direction when an external field is applied and there by creates a dipole moment in the dielectric



#### Therefore induced dipole moment $\mu = \alpha_e E$

Where  $\alpha_e$  is the electronic polarizability

- Electronic polarizability is proportional to the volume of atoms
- Electronic polarizability is independent of temperature.

#### Calculation of electronic polarizability

#### (i)Without field

Let us consider a classical model of an atom .assume the charges of the nucleus of that atom is

+Ze the nucleus is surrounded by an electron cloud of charge –Ze which is distributed in sphere of radius R

The charge density of the charged sphere = 
$$\frac{-Ze}{\frac{4}{3}\pi R^3}$$

Charge density  $\rho = \frac{-3}{4} \frac{Ze}{\pi R^3}$  ------1

(II) with field

When the dielectric is placed in a d.c electric field E two phenomena occur

- (a) Lorentz force due to the electrc field tends to separate the nucleus and the electron cloud from their equilibrium position.
- (b) After the separation an attractive coloumb force arises between the nucleus and electron cloud which tries to maintain the original equilibrium position.

Let x be the displacement made by the electron cloud from the positive core .since the nucleus is heavy it will not move when compared to the movement of electron cloud here x<<R , where R is the radius of the atom.

Since the Lorentz and coloumb forces are equal and opposite in nature equilibrium is reached.

At equilibrium lorentzforce =coulomb force

Lorentz force = charge  $\times$  field

= -ZeE-----2

The negative sign indicates the repulsive forces

Coulomb force=charge  $\times$  field

= +Ze× $\frac{Q}{4\pi\varepsilon_0 x^2}$  the positive sign indicates the attractive force

Therefore coloumb force= charge  $\times \frac{total negative charges(Q)enclosed in the sphere of redius x}{4\pi\varepsilon_0 x^2}$ 

Here the total number of negative charges (Q) encloses in the sphere of radius

X=charge density of the electron × volume of the sphere ------4

Substitute  $\rho$  from 1 and 4 we get

$$Q = \frac{-3}{4} \frac{Ze}{\pi R^3} \times \frac{4}{3} \pi x^3$$
(a)  $Q = \frac{Zex^3}{R^3} - ---5$ 

Substitute Q from 5 in 3 we get

Coloumb force =  $\frac{Ze}{4\pi\varepsilon_0 x^2} \left(\frac{Zex^3}{R^3}\right)$ ------6

At equilibrium Lorentz force= coulomb force

$$-ZeE = \frac{Z^2 e^2 x}{4\pi\varepsilon_0 R^3}$$
$$X = \frac{4\pi\varepsilon_0 R^3 E}{Ze}$$

Therefore the displacement of electron cloud x is proportional to the applied electric fieldE

Dipole moment:now the two electrc charges +Ze and –Ze are displaced by a distance under the influence of the field and form a dipole.

Induced dipole moment =magnitude of charge × displacement

= Zex-----8

Substitute the value of x from 7 in 8 we have

 $\mu_e = \operatorname{Ze} \times \frac{4\pi\varepsilon_o R^3 E}{Ze}$  $\mu_e = 4\pi\varepsilon_o R^3 E$  $\mu_e = \alpha_e \operatorname{E------9}$ 

 $\alpha_e = 4\pi\varepsilon_o R^3$  is called electronic polarizability

## Chapter4 MAGNETIC PROPERTIES

**Magnetic dipole moment**: A system having two opposite magnetic poles separated by a distance d is called as a magnetic dipole. If m is magnetic pole strength and I is the length of the magnet then its dipole moment is

$$M = m \times l$$

**Magnetic induction (or)Magnetic flux density(B)=**The magnetic induction in any material is the number of lines of magnetic force passing through unit area perpendicularly.

Its nits is weber/ $m^2$  or tesla

**Magnetic field intensity(or)strength(H)=**Magnetic field intensity at any point in the magnetic field is the force experienced by an unit north pole placed at thet point.

```
Its units is ampere m^{-1}
```

The magnetic induction B due to a magnetic field of intensity (H) applied in vaccum is related by

 $B = \mu_0 H$ 

Where  $\mu_0$  is the permeability of free space (vaccum)= $4\pi imes 10^{-7}$  H  $m^{-1}$ 

Instead in vaccum if the field is applied in a medium the magnetic induction in the solids is given by

 $B{=}\mu H$  where  $\mu$  is permeability of the solid material through which the magnetic lines of force pass.

**Magnetic permeability**( $\mu$ )=magnetic permeability of any material is the ratio of the magnetic induction in the sample to the applied magnetic field intensity.

$$\mu = \frac{B}{H}$$

**relative permeability(**  $\mu_r$ )=it is the ratio between the permeability of the medium to permeability of the free space

$$\mu_r = \frac{\mu}{\mu_0}$$

**Magnetization (or)intensity of magnetization(I)**=the term of magnetization is the process of converting a non magnetic material into a magnetic material .it measures the magnetization of the magnetized

It is also defined as the magnetic moment per unit volume

 $I = \frac{M}{V}$  Its units is ampere  $m^{-1}$ 

**Magnetic susceptibility(x)**=the ratio of intensity of magnetization (I) produced to the magnetic field strength (H) in the which the material is placed

$$x = \frac{1}{H}$$
 Type equation here.

Relation between  $\mu_r$  and x

B= $\mu$ H or  $B = \mu_0 \mu_r$  H

 $B = \mu_0 \mu_r H + \mu_0 H - \mu_0 H$ 

 $B = \mu_0 \operatorname{H} + \mu_0 \operatorname{H} (\mu_r - 1)$ 

 $B = \mu_0 H + \mu_0 I$  where I= H( $\mu_r - 1$ )

So  $B = \mu_0(H + I)$ 

$$\mu_0 = \frac{B}{H+I}$$

Relative permeability  $\mu_r = \frac{\mu}{\mu_o}$ 

 $= \frac{B}{H} \times \frac{H+I}{B}$  $= 1 + \frac{I}{H}$ 

$\mu_r = 1 + \mathbf{x}$
--------------------------

#### Classification of magnetic materials:

By the application of magnetic field some materials will not show any effect that are called non magnetic materials and those which show some effects are called magnetic materials

All magnetic materials magnetized in an applied external magnetic field.

Depending on the direction and magnitude of magnetization and also the effect of temperature on magnetic properties, all magnetic materials are classified into dia, para and ferromagnetic materials.

Two more classes of material have structure very close to ferro magnetic materials, but posses quiet different magnetic properties. They are anti-ferro magnetic and ferromagnetic materials.

#### Diamagnetism:

The number of orientations of electronic orbits in an atom be such that vectoe sum of magnetic moment is zero

The external field will cause a rotation action on the individual electronic orbits this produces an induced magnetic moment which is in the direction opposite to the field and hence tenda to decrease the magnetic induction present in the substance. Thus the diamagnetic is the phenomena by which the induced magnetic moment is always in the opposite direction of the applied field.

## **Properties of diamagnetic materials**

1 Diamagnetic material get magnetized in a direction opposite to the magnetic field.

2 Weak repulsion is the characteristic of diamagnetism

3 permanent dipoles are absent

4 Relative permeability is less than one but positive

5 The magnetic susceptibility is negative and small. It is not effected by temperature.

6 Diamagnetism is universal i.e all materials when exposed to external magnetic fields, tend to develop magnetic moments opposite in the direction to the applied field.

7 When placed inside a magnetic field, magnetic lines of force are replaced as

## Paramagnetism

The number of orientations of orbital and spin magnetic moments be such that he vector sum of magnetic moment is not zero and there is a resultant magnetic moment in each atom even in the absence of applied field.

The net magnetic moments of the atoms are arranged in random directions because of thermal fluctuations ,in the absence of external magnetic field.Hence there is no magnetization.

If we apply the external magnetic field there is an enormous magnetic moment along the field direction and the magnetic induction will be increase. Thus induced magnetism is the source of paramagnetism.

## Preperties of paramagnetism materials:

**1** paramagnetic materials get magnetized in the direction of the magnetic field.

2 Weak attraction is characteristic of paramagnetism

3 paramgnetic material posses permanent magnetic dipoles.

4 Relative permeability is greater than one but small i.e this indicate that when paramagnetic substance is placed in a uniform magnetic field the field inside the material will be more than the applied field.

5 The magnetic susceptibility is small and positive the magnetic susceptibility of paramagnetics is inversely proportional to absolute temperature

i.e x=C/T this is called curie law ,c is calles curie constant

6 Paramagnetic susceptibility is independent of the applied field strength.

7 Spin alignment is random

8 When placed inside a magnetic field it attracts the magnetic lines of force

9 Some of the material which exhibit the paramagnetism are aluminium, manganese , oxygen.

#### Ferromagnetism:

Ferromagnetism arises when the magnetic moments of adjacent atoms are arranged in a regular order i.e all pointing in the same direction .The ferromagnetic substance thus posses a magnetic moment even in the absence of the applied magnetic field ,this magnetization is known as the spontaneous magnetization

There is a special form of interaction called "exchange "coupling occurring between adjacent atoms , coupling their magnetic moment together in rigid parallelism.

#### **Properties of ferromagnetic materials**

1 In ferromagnetism materials, large magnetization occurs in the direction of the field.

2 Strong attraction is the characteristic of ferromagnetism.

3 They posses spontaneous magnetization.

4 The relative permeability is very high for Ferro magnetic.

5 The magnetic susceptibility is positive and very high.

6 Magnetic susceptibility is fairly high and constant up to a certain temperature according the equation

 $X = \frac{C}{T - T_C}$  C= curie constant  $T_C$  = Curie temperature

7 Ferromagnetism is due to the existence of magnetic domains which can be spontaneously magnetized.

8 Exhibit hysteresis.



9 Spin alignment is parallel in the same direction

10 When placed inside a magnetic field it attracts the magnetic lines of forces very strongly

11 Permanent and electro magnetic are made using ferromagnetic materials.

12 Example iron, nickel, cobalt.

## Antiferro magnetism

Anti ferromagnetism arises when the spin magnetic moment of neighbouring atoms are oriented in an antiparllel order  $\mathbf{A} \mid \mathbf{A} \mid \mathbf{A}$ 

In the absence of external external magnetic field the magnetization of anti ferro magnetic specimen will be zero, because of anti parallel and equal spin magnetic moment.

By the application of the external magnetic field a small magnetization in the direction of the applied magnetic field takes place this magnetization varies with temperature as shown

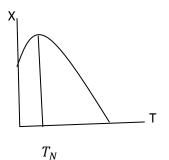
The susceptibility increases with an increase of temperature upto  $T_N$  called as neel temperature

At neel temperature the magnetization or susceptibility is maximum and above it the magnetization decreases with increasing temperature according to the relation

 $X = \frac{C}{T+\theta}$ , C = is curie constant  $\theta$  = paramagnetic curie temperature

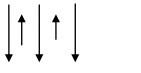
The decrease of magnetization with an increase of temperature is a property of of the paramagnetic substance, therefore the specimen becomes paramagnetic above  $T_N$ 

Examples Mno, Nio, Feo, Mns etc



## Ferrimagnetism and property of ferromagnetic materials(ferrites)

Ferrimagnetic substance are those in which the atomic or ionic dipoles in one diection are of unequal magnitudes ,this alignment of dipole gives a net magnetization and is the property of those magnetic substance which have two or more different kind of atoms.



In ferri magnetic materials there may be large net magnetization as compared to anti Ferro magnetic materials, due to the resultant of anti parallel alignment of neighboring dipoles of unequal magnitudes.

Ferrimagnetic materials generally known as ferrites consist of two or more different kind of atoms their formula is  $M_e^{++}Fe_2^{++}O_4^{--}$ 

Where  $M_e^{++}$  stands for a suitable divalent metal ion such as  $Fe^{++}$ ,  $CO^{++}$ ,  $Ni^{++}$ ,  $Mg^{++}$ , etc,  $Fe_2^{++}$  is a trivalent ferric ion. The magnetization of ferromagnetic material material can be understood by taking one of the materials as an example say ferrous ferrite

- (i) In ferrous ferrite we have two types of ions i.e.  $Fe^{+3}$ ,  $Fe^{+2}$
- (ii) here  $Fe^{+2}$  iona has six electrons in 3d sheels out of 6 electrons two electrons are paired with each other and hence left with 4 unpaired electrons Therefore  $Fe^{+2}$  gives rise to 4 Bohr magneton
- (iii)  $Fe^{+3}$  ions has five electrons in 3d shell and hence all these 5 are unpaired electrons

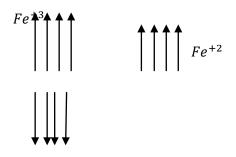
Therefore  $Fe^{+3}$  give rise to 5 Bohr magneton

Since we have two  $Fe^{+3}$ , totally the  $Fe^{+3}$  give rise to 2x5=10 bohe magneton

Therefore total magnetization of  $Fe^{+3} + Fe^{+3} = 4+10+14$  bohr magneton.

Theoretically we get 14  $\mu$ B(bohr magneton) but experimentally the total magnetic moment is only 4.08 $\mu$ B.The reason is if all the spins are aligned parallel then we get the total magnetization as 14 $\mu$ B

But in ferrites half of the magnetic spins of  $Fe_2^{3+}$  ions are parallel to one direction and the remaining half of  $Fe_2^{3+}$  ions are parallel in opposite direction as shown in fig hence they cancel each other.



Therefore net magnetic moment is only due to  $Fe^{+2}$  ions alone i.e .hence we get the total magnetization as 4µB which is a good agreement with the experimental value.

## Application of ferrites(ferromagnetic substance)

1 They are used to produce ultrasonics by magnetization principle.

2 Ferrites are used in audio and video transformers.

3 Ferrites rods are used in radio receivers to increase the sensitivity.

4 They are also used for power limiting and harmonic generation.

- 5 Ferrites are used in computers and data processing circuits
- 6 ferrites are used in switching circuits and in storage devices of computers.

7 Ferrites are not metals but their resistivity lies in the range of insulators or semiconductors.

#### Explanation of hysteresis curve based on domain theory of ferromagnetism:

#### Domain theory of ferromagnetism

According to Weiss a virgin specimen of ferromagnetic material consist of a number region or domains which are spontaneously magnetized .In each domain spontaneous magnetization is due to parallel alignment of all magnetic dipoles

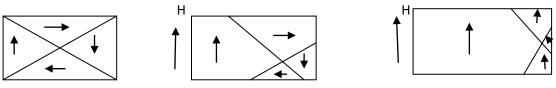
The direction of spontaneous magnetization varies from domain to domain

The resultant magnetization may hence br zero or nerly zero

When an external field is applied there are two possible ways of alignment of domains

(i)**By motion of domain walls:** the volume of domains that are favourably oriented with the respect to the magnetizing field increases at the cost of those that are unfavourably oriented fig(b)

(ii)**By rotation of domains**:when the applied magnetic field is strong rotation of the direction of magnetization occurs in the direction of the field.fig(c)

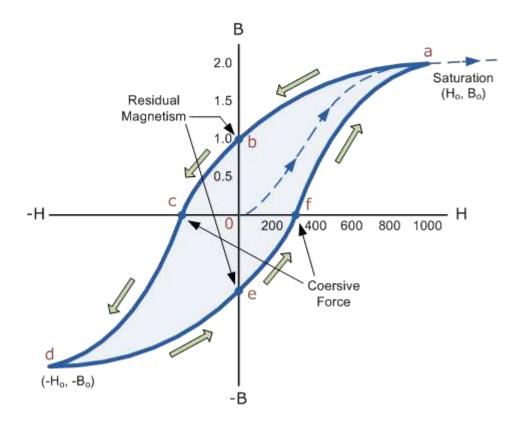


Fig(a)



fig(c)

Hysteresis curves



Hysteresis : lagging of magnetization behind the magnetizing field(H)

We know when the ferro magnetic material is subjected to external field ,there is increase in the value of the resultant magnetic moment due to two process

(i) the movement of domain walls

(ii)rotation of domain walls

When a weak magnetic field is applied the domains are aligned parallel to the field and in the easy direction of magnetization grow in size at the expense of the less favourably oriented domains.

This result in the bloch wall (or)domain wall movement and when the weak field is removed the domains reverse back to their original state .this reversible wall displacement is indicated by OA the magnetization curve.

When the field becomes stronger han the domain wall movement continues and it is mostly reversible movement .this is indicated by path AB of the graph .the phenomena of hysteresis is due to the irreversibility.

At the point B all domains have got magnetized along their easy direction

Application of still higher field rotates the domains into the field direction indicated by BC.

Once the domains rotation is complete the specimen is saturated denoted by C.

Thus the specimen is said to be attain the maximum magnetization .at this position if the external field is removed (H=0),the magnetic induction B will not fall rapidly to zero ,but falls to D rather than O this shows that even when the applied field is zero the material still posses some magnetic induction(OD)which is called residual magnetism or retentivity.

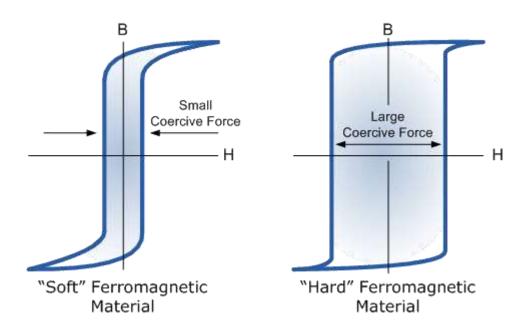
Actually after the removal of the external field the specimen will try to attain the original configuration by the movement of domain wall .But this movement is stopped due to the presence of impurities, lattice imperfections.

Therefore to overcome this a large amount of reverse magnetic field ( $H_c$ ) is applied to the specimen .the amount of energy spent to reduce the magnetization (B) to zero is called "coercitivity" represented by OE in the fig.

HSTERESIS: lagging of magnetization (B) behind the magnetizing field (H) is called hysteresis.

**Hysteresis loss:** It is the loss of energy in taking a ferromagnetic body through a complete cycle of magnetization and this loss is represented by the area enclosed by the hysteresis loop.

**Hard and soft magnetic materials:** Based on the area of hysteresis, magnetic materials can be classified into hard and soft magnetic materials.



S

Hard magnetic materials	Soft magnetic materials
(i) Hard magnetic materials have large hyster- due	(i)Soft magnetic materials have low hysteresis loss
esis loss due to large hysteresis is loop area	to small hysteresis loop area.
(ii)in these material the domain wall movemen relati-	(ii) in these materials the domain wall movement is

is difficult because of presence of impurities magnetizing	vely easier .even for small changes in the
and crystal imperfection and it is irreversible	field magnetization changes by large amount.
in nature	
(iii) The coercitivity and retentivity are large	(iii) )the coercitivity and retentivity aresmall .these
Hence these materials cannot be easily magne- demagnetized.	materials can be easily magnetized and
Tised and demagnetized	
(iv)In these materials because of the magnet	(iv)since these materials free from irregular the
presence of impuroties and crystal imperfection	ostatic energy is very small.
the mechanical strain is more hence magnetost	
atic energy is loss .	
(v)these materials have small values of permea and	(v)these materials have large values of permeability
Bility and susceptibility.	Susceptibility.
(vi)they are used to make permanent magnets.	(vi)there are used to make electromagnets.
(vii)eample copper nickel iron alloys,copper	(vii)examples:iron silicon alloys,ferrous nickel alloys,
nickel Cobalt alloys.	Ferrites.
(viii)applications:for production of magnetic	(vii)mainly used in electromagnetic machinery and
Detectors ,microphones,damping devices.	And transformer cores.used in switching circuits
	,microwave isolators.

### Origin of magnetic moment.

In atoms the permanent magnetic moments can arises due to the following.

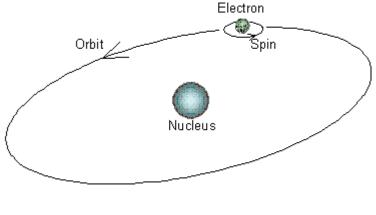
- 1 the orbital magnetic moment of the electrons
- 2 the spin magnetic moment of the electrons.
- 3 the spin magnetic moment of nucleus.

#### Orbital magnetic moment of the electrons and bohr magneton:

We know that in an atom electrons revolve round the nucleus in different circular orbits.let m be the mass of the electron and r the radius of the orbit in which it moves with angular velocity w

We can calculate the electric current due to the moving electron.

Current I=charge flow/unit time



= -e/T

Where T is the time taken for one revolution

$$I = \frac{-e\omega}{2\pi} \qquad (T = \frac{2\pi}{\omega})$$

We know that the current flowing through a circular coil produces a magnetic field in a direction perpendicular to the area of the coil and it is identical to a magnetic moment produced by such a dipole is

$$\mu_m = I.A$$
$$= \frac{-e\omega}{2\pi} \times \pi r^2$$
$$= \frac{e\omega r^2}{2} = \frac{e\omega r^2}{2} \times \frac{m}{m} = \frac{-e}{2m} L$$

Where L=  $mwr^2$  is the orbital angular moment of the electron

The possible orientation of the angular momentum vector when placed in an external magnetic field

$$L_{l,B} = m_l \times \frac{h}{2\pi}$$

$$\mu_m = \frac{-e}{2m} \times m_l \times \frac{h}{2\pi}$$

$$= \frac{-eh}{4\pi m} \times m_l =$$

$$\mu_m = -\mu_B \times m_l \qquad \mu_B = \frac{eh}{4\pi m} = \text{bohr magneton}$$

#### UNIT4

#### **Chapter1 LASERS**

Lasers: Laser means light amplification by stimulated emission of radiation.

#### **Specialty of Lasers:**

Any light beam is composed of photons, two photons are said to be coherent if they have same energy, phase and direction. Laser beam is composed of such coherent photos where as ordinary light contain incoherent photons. So the property of coherence adds special characteristics to LASER beam such as high directionality, high intensity, monochromacity and penetration.

Laser source is an electromagnetic radiation with absolute purity and high intensity which were never found in any other electromagnetic radiation.

#### Absorption:

When at atom absorbs an amount of energy 'hv' in the form of photon from the external agency and excited into the higher energy levels from ground state, then this process is known as absorption

$$atom + hv \rightarrow atom^*$$

#### **Spontaneous Emission:**

When an atom in the excited state emits a photon of energy 'hv' coming down to ground state by itself without any external agency, such an emission is called spontaneous emission.

$$atom^* \rightarrow atom + hv$$

Photons released in spontaneous emission are not coherent. Hence spontaneous emission is not useful for producing lasers.

#### **Stimulated Emission:**

When an atom in the excited state, emits two photons of same energy 'hv' while coming to down to ground state with the influence of an external agency, such an emission is called stimulated emission.

atom\*  $\rightarrow$  atom + 2hv

In the two photons one photon induces the stimulated emission and the second one is released by the transition of atom from higher energy level to lower energy level. Both the photons are strictly coherent. Hence stimulated emission is responsible for laser production .

#### **Laser Production Principle:**

Two coherent photons produced in the stimulated emission, interacts with other two excited atoms, resulting in four coherent photons. Thus, coherent photons are multiplied in a lasing medium. The continuous successive emission of photons results for the production of laser beam.

### **Characteristics of Laser Beam:**

Some of the special properties which distinguish lasers from ordinary light sources are characterized by:

- 1. Directionality
- 2. High Intensity
- 3. Monochromacity
- 4. Coherence

## **1. Directionality:**

Laser emits radiation only in one direction. The directionality of laser beam is expressed in terms of angle of divergence i.e., it is twice the angle that the outer edge of the beam makes with the axis of the beam with reference to emitting source.

The outer edge of the beam is defined a point at which the intensity of beam falls to 1/37 times to that of value at the centre.

**2. High Intensity:** Generally, light from conventional source spread uniformly in all directions. For example, take 100 watt bulb and look at a distance of 30 cm, the power enter into the eye is less than thousand of a watt. This is due to uniform distribution of light in all directions.

But in case of lasers, light is a narrow beam and its energy is concentrated within the small region. The concentration of energy accounts for greater intensity of lasers.

**3. Monochromacity:** The light emitted by laser is highly monochromatic than any of the other conventional monochromatic light. A comparison b/w normal light and laser beam, ordinary sodium (Na) light emits radiation at wave length of  $5893A^0$  with the line width of  $1A^0$ . But He-Ne laser of wave length  $6328A^0$  with a narrow width of only  $10^{-7} A^0$  i.e., monochromacity of laser is 10 million times better than normal light.

The degree of monochromacity of the light is estimated by line of width (spreading frequency of line).

**4.** Coherence: If any wave appears as pure sine wave for longtime and infinite space, then it is said to be perfectly coherent.

Practically, no wave is perfectly coherent including lasers. But compared to other light sources, lasers have high degree of coherence because all the energy is concentrated within the small region. There are two independent concepts of coherence.

i) Temporal coherence (criteria of time)

ii) Spatial coherence (criteria of space)

**Population Inversion:** Generally, number of atoms in the ground state is greater than the number of atoms in higher energy states. But in order to produce a laser beam, the minimum requirement is stimulated emission. Stimulated emission takes place only if the number of atoms in the higher energy level is greater than the number of atoms in the lower energy level.

Simply population inversion is nothing but number of atoms in higher energy level is greater than the number of atom in lower energy level.

So, if there is a population inversion there by only stimulated emission will able to produce laser beam.

Population inversion is associated with three Phenomenon.

- i) Stimulated emission
- ii) Amplification
- iii) Pumping Process

**Stimulated Emission:** If majority of atoms are present in higher energy state than the process becomes very easy.

**Amplification:** If 'N', represents number of atoms in the ground state and 'N<sub>2</sub>' represents number of atoms in the excited state than the amplification of light takes place only when  $N_2 > N_1$ .

If  $N_2 > N_1$ , there will be a population inversion so induced beam and induced emission are in the same directions and strictly coherent than the resultant laser is said to be amplified.

Boltzmann's principle gives the information about the fraction of atom found on average in any particulars energy state at equilibrium temperature as

$$\underline{N1} = \exp\left(\underline{E2 - E1}\right)$$
N2 KT

$$= \exp\left(\frac{\Delta E}{KT}\right)$$

$$\underline{N}_{\underline{1}} = Exp\left(\underline{hv}\right) \qquad \text{or} \qquad \underline{N}_{\underline{2}} = exp\left(\underline{-hv}\right)$$
$$\underline{N}_{\underline{2}} \qquad KT \qquad \underline{N}_{\underline{1}} \qquad KT$$

**Pumping Process:** This process is required to achieve population inversion.

pumping process is defined as: "The process which excites the atoms from ground state to excited state to achieve population inversion".

Pumping can be done by number of ways

i)	Optical Pumping	<b>→</b>	excitation by strong source of light (flashing of a
			Camera)
ii)	Electrical Pumping	<b>→</b>	excitation by electron impact
iii)	Chemical Pumping	<b>→</b>	excitation by chemical reactions
iv)	Direct Conversion	<b>→</b>	Electrical energy is directly converted into radiant
			Energy in devices like LED's, population inversion is achieved in forward bids.

### **Einstein's Theory of Radiation:**

In 1917, Einstein predicted the existence of two different kinds of processes by which an atom emits radiation.

Transition b/w the atomic energy states is statistical process. It is not possible to predict which particular atom will make a transition from one state to another state at a particular instant. For an assembly of very large number of atoms it is possible to calculate the rate of transitions b/w two states.

Einstein was the first to calculate the probability of such transition, assuming the atomic system to be in equilibrium with electromagnetic radiation.

The number of atoms excited during the time  $\Delta t$  in above process is given by:

$$N_{ab} = Q N_1 B_{12} \Delta t$$

Where  $N_1$  = number of atoms in state 'E<sub>1</sub>'

Q = Energy density of induced beam

 $B_{12}$  = Probability of an absorption transition coefficient

The number of spontaneous transitions  $N_{sp}$  taking place in time ' $\Delta$ t' depends on only no.of atoms  $N_2$  lying in excited state.

$$N_{sp} = A_{21}N_2\Delta t$$

Where  $A_{21}$  = probability of spontaneous transistion.

The number of stimulated transitions  $N_{st}$  occurring during the time  $\Delta t$  may be written as:

$$N_{sp} = B_{21}N_2\Delta t$$

Where  $B_{21}$  = probability of stimulated emission

Under the thermal equilibrium number of upward transitions = number of downward transitions per unit volume per second.

So, we can write:

$$\mathbf{A}_{21}\mathbf{N}_2 + \mathbf{B}_{21}\mathbf{N}_2\mathbf{Q} = \mathbf{B}_{12}\mathbf{N}_1\mathbf{Q} \rightarrow \mathbf{1}$$

The co-efficients A<sub>21</sub>, B<sub>12</sub>, B<sub>21</sub> are known as Einstein coefficients.

Note: Since we are applying same amount of energy (Q) and observing in the same time ( $\Delta t$ ), number of atoms excited into higher energy levels (absorption) = number of atoms that made transition into lower energy levels (stimulated emission)

 $B_{12} = B_{21}$  i.e. absorption = stimulated emission

#### **Classification of Lasers:**

Depending upon state of active material lasers are classified into 3 types

- i. Solid state lasers eg.: Ruby laser
- ii. Gaseous lasers eg.: He-Ne Laser, CO<sub>2</sub> laser
- iii. Semi conductor laser eg.: Gallium Arsenide

#### **Ruby Laser:**

When solid substances are used in laser device the concentration of active material is less than 1%. The bulk of the remaining material is not participating in laser action, it is called host material.

For laser action to be possible, the atoms (or) ions of the active material will have to be excited to proper upper levels which is done by pumping process. The first successful solid state laser was operated to Maimann in 1960 using a crystal of Ruby mixed with chromium as active material.

Ruby  $\rightarrow$  Crystalline Al<sub>2</sub>O<sub>3</sub> + Cr (0.05%)

Ruby is crystalline  $Al_2O_3$  doped with 0.05% of some of the chromium ions replaces the Al ions, responsible for laser action.

The energy levels of Cr<sup>+3</sup> ions in Al<sub>2</sub>O<sub>3</sub> lattice is show in figure

The pumping of Cr ions is performed with flashed lamp to achieve population inversion. The Cr ions absorb radiation around the wave lengths 5500A (green light) & 4000 A (blue light) and are excited to the levels  $E_1 \& E_2$ . The levels  $E_1 \& E_2$  are known as pump bands.

The Cr ions in turn, reach to the metastable state (M) during the process of stimulated emission. The level 'M' contains a pair of energy levels which are known as upper energy level (2A) & lower energy level (E). The lifetime of Cr ions in metastable is  $3\mu$  sec.

Laser emission occurs b/w the level 'M' and ground state 'G' at an o/p wavelength of  $6943A^0$ . The laser action is obtained from both  $2A \rightarrow G \& E \rightarrow G$  transitions with corresponding wavelengths  $6929A^0$  (R<sub>2</sub> i.e., Rayleigh line 2) and  $6943A^0$  (R<sub>1</sub> i.e., Rayleigh line 1).

But the actual laser will be produced from  $E \rightarrow G$  transition lying nearer to the wavelength of red light and travels less distance to get high intensity.

#### **Experimental Arrangement:**

The Ruby is taken in the form of rod and is enclosed in a discharge tube whose length is 4 cm and diameter is 1.5 cm. Both the ends of the ruby rod are polished and one end of the rod is completely coated with silver for getting perfect transmission.

A helical flash lamp filled with xenon (Xe) provides white light in the form of flash for every 1/1000 of a second to achieve population inversion. This type of pumping process is known as optical pumping. Because of pumping, population inversion takes place in the higher energy levels, than stimulated emission can able to produce laser beam.

An intense red laser beam comes out from the end of ruby rod with divergence of about  $\frac{1}{2}$ " and output power is 10 KW.

### **He-Le Laser:**

The first gas laser to be operated successfully was the He-Ne laser in 1961 by the scientist A. Jawan.

In this method, two gases helium & Neon were mixed in the ratio 10:1 in a discharge tube made of quartz crystal. The dimensions of the discharge tube are nearly 80 cm length and 1.5 cm diameter, with its windows slanted at Brewster's angle i.e.,

$$\theta = \operatorname{Tan}^{-1}(n)$$

Where n = refractive index of the window substance.

The purpose of placing Brewster windows on either side of the discharge tube is to get plane polarized laser output. Two concave mirrors  $M_1 \& M_2$  are made of dielectric material arranged on both sides of the discharge tube so that their focci lines within the interior of discharge tube.

Note: There are 3 types of polarization for light

- i) Plane Polarized straight lines
- ii) Circularly Polarized arcs
- iii) Elliptically Polarized ellipse

One of the two concave mirrors  $M_1$  is thick so that all the incident photons are reflected back into lazing medium. The thin mirror  $M_2$  allows part of the incident radiation to be transmitted to get laser output.

#### Working:

The discharge tube is filled with Helium at a pressure of 1 mm of Hg & Neon at 0.1mm of Hg. The gas discharge is established by the application of large potential difference b/w the two electrodes of the discharge tube. Being large in number. He atoms are easily excited to higher energy levels by colliding with each other. Neon atoms present in less concentration, to excite the Ne atoms pumping process must be required.

The excited He atoms collide with Ne atoms and transfer the excitation energy to the Ne atoms. Because both the atoms having higher energy levels very close to each other i.e., 20.61 ev & 20.66 ev for He & Ne respectively. Here Ne is the lazing medium & He is the pumping medium.

Neon atoms undergo a radiative transfer through 18.7 ev energy level by emitting photons of wavelength 6328  $A^0$ .

The released photons are transmitted through the concave mirror  $M_2$  there by producing lasers. A continuous laser beam of red colour at a wavelength of 6328A<sup>0</sup>. By the application of large potential difference, Ne atoms are pumped into higher energy levels continuously. Laser beam of power 5 to 50 MW comes out from He-Ne laser.

#### **Description of Energy Levels:**

When electric discharge is set-up in the tube, collisions b/w the atoms raises the amount of He & Ne atoms to the higher energy levels  $F_1$ ,  $F_2$  and  $E_4$ ,  $E_6$  respectively. Ne has two energy levels  $E_4$ ,  $E_5$  at nearly same energy level of  $F_2$  to He.

The Ne atoms drop down to the levels  $E_3$ ,  $E_5$  a radiative transfer (St. emission) and reaches to the level  $E_2$  through non-radiative transfer (sp. Emission).

From level  $E_2$  Ne atoms are brought back to the ground state through collisions with walls of the discharge tube. The transitions from  $E_6 \rightarrow E_5$ ,  $E_4 \rightarrow E_3$  and  $E_6 \rightarrow E_3$  emit radiations corresponding to the wavelengths 3390A<sup>0</sup>, 1150A<sup>0</sup>, & 6328A<sup>0</sup>, respectively. 6328A<sup>0</sup> is the wall known red light of He – Ne laser because other two wavelengths are not in the region of electro magnetic radiation (visible region).

### Semi Conductor Laser:

#### **Principle & Working:**

- 1. After the invention of semi conductor leaser in 1961, laser have become at common use.
- 2. In conventional lasers, lasers are generated due to transition of  $\theta$ 's from higher to lower energy level.
- 3. but in semi-conductor lasers the transition takes place from conduction band to valence band.
- 4. The basic mechanism responsible for light emission from a semi conductor laser is the recombination of e's and holes at Pn-junction when current is passed through the diode.
- 5. Stimulated emission can occur when the incident radiation stimulates an e in conduction band to make a transition into valence band in that process radiation will be emitted.
- 6. When current is passed through PN junction under forward bias, the injected e's & holes will increase the density of e in CB & holes in VB. At some value of current the stimulated emission rate will exceed the absorption rate.
- 7. As the current is further increased at some threshold value of current the amplification will takes place and laser begin to emit coherent radiation.
- 8. The photon releasing zone is narrow and the method of use is simple.
- 9. The properties of semi conductor laser depends upon the energy gap i.e., the induced radiation must have a frequency greater than the value of the energy gap in order that transition will takes place.
- 10. The e's are pumped to conduction band by passing forward current through semi conductor and there is no role of metastable states.
- 11. Population inversion can be achieved by producing a large current to PN junction, causing stimulated emission.

### Fabrication:

- 1. Ga As is heavily doped with impurities in both P & N regions. N region is doped with tellurium & P region by Zn.
- 2. The concentration of doping is of the order of  $10^{17} + 10^{19}$  impure atoms per cm.
- 3. The size of the diode is small i.e., 1mm each side & the depletion layer's thickness varies from 1 to  $100 \mu$ Am.

These values depend on diffusion condition and 40 mp at the time of fabrication.

### Working:

When a forward bias with de source is applied to a semiconductor, e from N-region & holes from P-region move to cross the junction in opposite directions.

In natural region the e's & holes combine recombination is possible due to transition of e from CB to VB.

For low currents the P.I does not take place hence only spontaneous emission takes place and photon released are not coherent.

When forward current is further increased beyond the certain threshold value P.I. takes place and choereri photons are released.

The energy gap of Galium Arsendia (Ga-As) is 1.487 ev and corresponding wavelength of radiation is  $6435 \text{ A}^0$  which is responsible for laser emission.

#### **Applications of Lasers:**

Lasers have wide applications in different branches of science and engineering because of the following.

- 1. Very narrow band width
- 2. High directionality
- 3. Extreme brightness

The following are the important uses of lasers

- 1. Lasers are used in optical communications, due 40 narrow band width
- 2. The laser beam can be used for the communication b/w earth & moon (or) other satellites due to the narrow angular speed.
- 3. By the use of lasers, the storage capacity of information in computers is greatly improved.
- 4. The lasers have industrial applications. They can make holes in diamond and hard steels.
- 5. Lasers have wide medical applications.
- 6. Lasers are widely used military purposes
- 7. Lasers have wide chemical applications. They can initiate or fasten chemical reactions.
- 8. Lasers can be used to find the size & shape biological cells such as erythrocytes.
- 9. Lasers can be used in air pollution control by analyzing the size of dust particles.

# Chapter2 OPTICAL FIBRES

- Optical fibers are the waveguides through which electromagnetic waves of optical frequency range can be guided through them to travel long distances.
- An optical fiber works on the principle of total internal reflection (71R).
- When light enters through one end of optical fiber it undergoes successive total internal reflections and travel along the fiber in a "zig-zag" path.
- Optical fibers are made up of glass, plastic or SiO<sub>2</sub> as thin as size of human heir.
- An optical fiber consists of three (3) co-axial regions.
- The inner most region is the light-guiding region known as "Core". It is surrounded by a middle co-axial regional known as "cladding". The outer most region which completely covers the core & cladding regions is called "sheath or buffer jacket".
- Sheath protects the core & cladding regions from external contaminations, in addition to providing mechanical strength to the fiber.
- The refractive index of core  $(n_1)$  is always greater than the refractive index of cladding  $(n_2)$  i.e.,  $n_1 > n_2$  to observe the light propagation structure of optical fiber.

# Expressions for acceptance angle (QA) & Numerical Aperture (NA)

Acceptance Angle (QA): All right rays falling on optical fiber are not transmitted through the fiber. Only those light rays making  $\theta_i > \theta_c$  at the core-cladding interface are transmitted through the fiber by undergoing T1R. For which angle of incidence, the refraction angle is greater than 90<sup>0</sup> will be propagated through T1R. There by Acceptance Angle is defined as:

The maximum angle of incidence to the axis of optical fiber at which the light ray may enter the fiber so that it can be propagated through T1R.

Consider the optical fiber with core refractive index  $n_1$  and cladding refractive index  $n_2$ . Light is incident on the axis of optical fiber at an angle  $\theta_1$ . It can produce an angle of refraction  $\theta_2$ .

The relationship at the interface is given by snell's law as:

At air-core interface (A)

 $n_o sin \theta_1 = n_1 sin s \theta_2$  - 1

At core-clad interface (B), for T1R

 $n_1 sin (90-\theta_2) = n_2 sin 90^0$  $n1 cos\theta_2 = n_2$  $cor\theta_2 = n_2/n_1 - 2$ 

This gives max value of external incident angle for which light will propagate in the fiber.

### Numerical Aperture (NA):

The main function of optical fiber is to accept and transmit as much of light as possible.

The light gathering ability of optical fiber depends on two factors i.e.,

- 1. Core diameter
- 2. NA

NA is defined as sine of the acceptance angle

i.e.,  $NA = Sin \theta A$ 

 $NA = \sqrt{n_1^2 - n_2^2}$ 

The efficiency of optical fiber is expressed in terms of NA, so it is called as figure of merit of optical fiber.

# NA is also expressed like this:

 $NA = \sqrt{n_1^2 - n_2^2} = \sqrt{(n_1 - n_2) (n_1 + n_2)}$ 

Fractional index change  $\Delta = n_1 - n_2 / n_1$ 

$$= \mathbf{n}_1 - \mathbf{n}_2 = \Delta \mathbf{n}_1$$
$$= \mathbf{N}\mathbf{A} = \sqrt{\Delta \mathbf{n}_1 (\mathbf{n}_1 + \mathbf{n}_2)}$$

Let  $n_1 = n_2$ , then  $n_1 + n_2 = 2n_1$ 

$$= \mathbf{N}\mathbf{A} = \sqrt{\Delta}\mathbf{n}_1 - 2\mathbf{n}_1 = \mathbf{n}_1\sqrt{2\Delta}$$

$$=$$
 NA  $=$  n<sub>1</sub> $\sqrt{2\Delta}$ 

### **Classification of Optical Fibers:**

- Based on variation in the core refractive index (n<sub>1</sub>), optical fibers are divided in to two types
  - 1. Step index fiber
  - 2. Graded index fiber
- Based on mode of propagation, fibers are further classified in to
  - 1. Single mode propagation
  - 2. Multi mode propagation
- Step index fibers have both single & multimode propagations.

- Graded index fibers have multimode propagation only
- All together in total three (3) types of fibers
  - 1. Single mode step index fiber
  - 2. Multi mode step index fiber
  - 3. Multi mode graded index fiber

# **Transmission of Signal in Optical Fibers**

# 1. Step Index Fiber:

The refractive index of core material is uniform through out and undergoes a sudden change in the form of step at the core-clad interface.

# a) Single Mode Step Index Fiber:

# Longitudinal cross section

The variation of the refractive index of a step index fiber as a function of distance can be mathematically represented as

Note: Mode of propagation: It is defined as the number of paths available for the light ray to transfer through the optical fiber.

### **Structure:**

- i) Core Diameter: 8 to 12 µm, usually 8.5µm
- ii) Cladding Diameter: Around 125µm
- iii) Sheath Diameter: 250 to 1000  $\mu$ m
- iv) NA : 0.08 to 0.15 usually 0.10

### **Performance Characteristics:**

### i) Band Width:

Greater than 500 MHZ Km

### ii) Attenuation:

2 to 5 dB / Km with a scattering limit of around 1 dB/Km at a wave length of  $0.85 \mu m$ 

#### iii) Applications:

These fibers are ideally suited for high band width applications using single mode injection coherent (LASER) sources.

### b) Multi Mode Step Index Fibers:

- These fibers have reasonably large core diameters and large NA to facilitate efficient transmission to incoherent or coherent light sources.
- These fibers allow finite number of modes.
- Normalized frequency (NF) is the cut off frequency, below which a particular mode cannot exist. This is related to NA, Radius of the core, and wave length of light as

### **Structure:**

- i) Core Diameter: 50 to 200 µm
- ii) Cladding Diameter: 125 to 400 µm
- iii) Sheath Diameter: 250 to 1000 µm
- iv) NA: 0.16 to 0.5

## **Performance Characteristics:**

## i) Band Width:

6 to 50 MHZ Km

### ii) Attenuation:

2.6 to 50 db/km at a wave length of 0.85  $\mu$ m, limited by absorption or scattering.

### iii) Applications:

These fibers are ideally suited for limited band width and relatively low cost applications.

# Multi Mode Graded Index Fibers:

- In case of graded index fibers, the refractive index of core is made to vary as a function of radial distance from the centre of the optical fiber.
- Refractive index increases from one end of core diameter to center and attains maximum value at the centre. Again refractive index decreases as moving away from center to towards the other end of the core diameter.
- The refractive index variation is represented as ......
- The number of modes is given by the expression

### **Structure:**

- i) Core Diameter: 30 to 100  $\mu m$
- ii) Cladding Diameter: 105 to 150  $\mu m$
- iii) Sheath Diameter: 250 to 1000  $\mu$ m

iv) NA : 0.2 to 0.3

### **Performance Characteristics:**

#### i) Band Width:

300 MHZ Km to 3 GHZ Km

# ii) Attenuation:

2 to 10 dB/km at a wave length of  $0.85\mu$ m is a scattering limit.

### iii) Applications:

These are ideally suited for medium to high band width applications using incoherent and coherent multimode sources.

Distinction b/w step & graded index fibers

Step Index	Graded Index
1. RI of core is uniform through out except at one stage	1. Refractive index varies gradually with radial distance.
2. Single & multimode propagations exist	2. It is a multi mode fiber
3. Used for short distance applications	3. Used for long distance applications
4. Attenuation losses are of the order 100	4. 4. Attenuation losses are of the order 10

dB/km
5. Skew rays propagation takes place
6. Difficult to manufacture

Distinction b/w single mode & multi mode

Single Mode	Multi Mode
1. Core diameter is small	1. Core diameter is large
2. Signal entry is difficult	2. Signal entry is easy
3. Exists in step index fiber	3. Exists in both step & graded index fibers
4. Light must be coherent	4. Light source may be coherent or incoherent source

# Advantages of optical fibers over metallic cables

- 1. Optical fibers allow light signals of frequencies over a wide range and hence greater volume of information can be transmitted either in digital form or in analog form with in a short time.
- 2. In metallic cables only 48 conversations can be made at once without cross talks where as in optical fibers more than 15000 conversations can be made at once without cross talks.
- 3. Light cannot enter through the surface of the optical fiber except at the entry interface i.e., interference b/w different communication channels is absent. Hence purity of light signal is protected.
- 4. Optical signal do not produce sparks like electrical signals and hence it is safe to use optical fibers.
- 5. External disturbances from TV or Radio Stations power electronic systems and lightening can not damage the signals as in case of metallic cables.
- 6. Materials used in the manufacture of optical fibers are SiO<sub>2</sub>, plastic, glasses which are cheaper & available in plenty.

#### **Optical Fiber Communication Link**

Optical fiber is an ideal communication medium by systems that require high data capacity, fast operation and to travel long distances with a minimum number of repeaters.

### **Encoder:**

It is an electronic system that converts the analog information signals, such as voice of telephone user, in to binary data. The binary data consists of series of electrical pulses.

## **Transmitter:**

Transmitter consists of a driver which is a powerful amplifier along with light source. The o/p of amplifier feeds to light source, that converts electrical pulses in to light pulses.

#### Source to Fiber Connector:

It is a special connector that sends the light from sources to fiber. The connector acts as temporary joint b/w the fiber and light source, misalignment of this joint, leads to loss of signal.,

### **Fiber to Detector Connector**

It is also temporary joint, which collects the source from fiber.

### **Receiver:**

Receiver consists of a detector followed by amplifier. This combination converts light pulses in to electrical pulses.

# **Decoder:**

Electrical pulses containing information are fed to the electronic circuit called decoder. Decoder converts binary data of electrical pulses in to analong information signals.

#### UNIT5

## Sciences & Technology of Nano Materials

- Nano means 10<sup>-9</sup> i.e., A Nanometer (nm) is one thousand millionth of the meter (i.e. 10<sup>-9</sup> m)
- 2. Atoms are extremely small and the diameter of a single atom can vary from 0.1 to 0.5 nm depending on the type of the element. The radius of the atom can be half the distance between neighboring atoms when they present in the solid phase.
- 3. At the Nano-scale, materials exhibit different or New Properties, changed properties include grater material strength, enhanced reactivity, better catalytic functioning and higher conductivity.
- 4. The first concept related to nano technology was proposed by the scientist Richard Feynman in 1959, made a statement "There is plenty of room at the bottom".
- 5. According to Feynman, all materials are composed of grains, which in turn comprise of many atoms. Depending on the site, these grains varying from hundreds of microns to centimeters. Any bulk material, its site can be expressed in three dimensions. Any planar material, its area can be expressed in two dimensions. They linear material, its length can be expressed in one dimension.
- 6. Nano materials can be defined as the materials which have structured components with site less than 100 nm at least in one dimension.
- 7. Nano Science can be defined as the study and manipulation of materials at atomic, molecular and micro molecular scales, where the properties different from those at a layer scale.
- 8. Nano Technology can be defined as the design characterization, production and application of structures, devices and system by controlling shape and size at the nano meter scale.
- 9. Various forms of nano materials
  - 1. One dimension surface coatings and films
  - 2. Two dimensions nano wires, nano tubes
  - 3. Three dimensions nano particles i.e. precipitates, colloids, quantum dots etc
- 10. Approaches of nano technology:

Two main approaches are used in nano technology

1. Bottom up : Materials and devices are built from molecular components

Which assemble chemically using principles of molecular recognition.

- 2. Top down : Nano objects are constructed from larger entities without atomic level control.
- 11. Basic Principles of Nano Technology
  - It uses a basic unit of measure called a "Nano Meter" (nm), indicates a billion the part 10<sup>-9</sup>. There are one billion nm's to a meter. Each nm is only three to give atoms wide. They are very small, about 40,000 times smaller than the width of an average human hair.
  - 2. B Bed on nano meters, i.e., considered as basic principle manufacturing, chemistry, health sciences, material science, space programs and engineering applications are designed.
  - 3. Materials referred as "Nano Materials" are divided in to two categories.
    - 1. Organic nano materials (fullerenes)
    - 2. Inorganic nano materials
- 12. Fabrication a production of Nano Materials:Fabrication of nano materials can be done by using any one of the two approaches
  - 1. Bottom up approach
  - 2. Top down approach

There are many methods to produce Nano materials

- 1. Gas condensation
- 2. Vacuum deposition and vaporization
- 3. Chemical vapor deposition (CVD)
- 4. Mechanical attrition
- 5. High energy mills include: Ball Milling
  - Attrition ball mill
  - Planetary ball mill
  - Vibrating ball mill

- How energy tumbling mill
- 6. Sol-gel Techniques: Sol-gel formation occurs in four stages
  - Hydrolysis
  - Condensation
  - Growth of particles
  - Agglomeration of particles
- 7. Electro Deposition
- 8. Physical Vapour Synthesis (PVS)
- 9. Nano Arc Synthesis (NAS)
- 10. Nano Particle Coatings
- 11. Nano Particle Dispersions
- 12. Catalysis
  - Using nano metal colloids
  - Using metal and gold nano clusters
  - Using metal nano particles
- 13. Plasma arcing

The entire range of fabrication (or) production methods are basically divided in to three basic methods.

- 1. Chemical Methods
- 2. Mechanical Process
- 3. Physical Methods

# Chemical Methods

- Sol-gel processes
- Chemical combustion
- Spray pyrolysis

# Mechanical Process

- Grinding
- Milling
- Mechanical alloying

# Physical Methods

- Electrical wire explosion method
- Chemical vapour deposition

• Label ablation

# Physical and chemical properties of nano materials

Nano materials have properties that are different from those of bulk materials. Most of nano structures are crystalline. Nano materials properties are depends on their site & structure.

- 1. Physical Properties:
  - a) Starting from the bulk, the first effect of reducing particle site is to create more surface sites i.e., surface to volume ratio increases. This charges the surface pressure and results a change in the interparticle spacing.
  - b) The interatomic spacing decreases with size. This is due to competition between long-range electrostatic forces and the short range core-core repulsion.
  - c) The change in interparticle spacing and the large surface to volume ratio in particles have a combined effect on material properties.
  - d) As a result, the thermodynamic properties may change for example melting point decreases with site.
- 2. Chemical Properties:
  - a) Increase in surface to volume ratio & variations in geometry have a strong effect on catalytic properties i.e., increases the chemical activity of the material
  - b) Due to increase in chemical activity, nano-materials can be used as catalyst.
  - c) Nano materials contains small particles may be useful in hydrogen storage devices in metals.
- 3. Electrical Properties:

The change in electrical properties in nano materials is electrical conductivity increases with reduction in particle size.

- 4. Optical Properties:
  - a) Depending upon the particle site, different colours are seen i.e., gold nano spheres of 100 nm appears orange in colour while 50 nm nano spheres appears green in colour.
  - b) The linear and non linear optical properties of materials can change with its size i.e., nano crystalline systems have novel optical properties.

- 5. Magnetic Properties:
  - a) The strength of the magnet, coercively and saturation magnetization values increases with decrease in the grain site.
  - b) Small particles are more magnetic than the bulk material.
- 6. Mechanical Properties:
  - a) Metals mode up of with small grains will greatly increase the strength.
  - b) Because of the nano site, many of the mechanical properties such as hardness, elastic modules, scratch resistance, fatigue strength are modified.
  - c) Super plasticity is achieved with help of nano technology (i.e. poly crystalline materials exhibit very large texture deformations without necking or fracture)

## Carbon Nanotubes (CNT)

- Carbon nano tubes first observed by Sumio Iijima in 1991
- Up to now we know only three forms of carbon, namely diamond, graphite and amorphous carbons.
- But there exist a whole family of other forms of carbon known as carbon nanotubes which are related to graphite.
- Usually graphite has the sheets of carbon are stacked on top of one another. They can easily slide over each other. So graphite is not hard.
- When graphite sheet are rolled in to a cylinder and there edges joined, they from carbon nanotubes i.e., carbon nanotubes are extended tubes of rolled graphite sheets.
- Simply carbon nano tubes are molecular scale tubes of graphitic carbon with outstanding properties like stiffest and strongest and have outstanding electrical properties.

### **Structure:**

The bonding CNT is SP2, with each atom joined to three neighbours, as in graphite. The tubes can be considered as rolled up graphite sheets. There are three dishinet ways in which a grapheme sheat can be rolled in to a tube.

- 1. Armchair
- 2. Zig-zg
- 3. Chiral

There may be single walled nano tubes and multi walled nano tubes.

In single walled nano tube, a nano tube consists of one tube of graphite of one atom thick.

In multi walled nano tubes, number of concentric tubes are arranged.

## **Production:**

There are number of methods of making carbon nanotubes. Out of those most widely used methods are

- 1. Arc method
- 2. Laser method
- 3. Chemical vapor deposition (CVD)

Carbon nanotubes have novel chemical and physical properties

- 1. Very high chemical reactivity
- 2. Electrical conductivity is improved
- 3. Enhanced optical activity
- 4. Mechanical strength is increased

# **Application of Nano Materials**

Nano materials possess unquie, beneficial chemical, physical and mechanical properties; they can be used for a wide variety of applications.

- 1. Manufacture of efficient computer clips.
- 2. used in kinetic energy (KE) penetrators with enhanced lethality
- 3. Used in production of better insulation materials
- 4. Used ion high definition plasma TV, to improve the pixel site.
- 5. Used in the manufacture of low-cost flat panel displays.
- 6. Cutting tools made of nano materials are to usher and harder
- 7. Nano science is useful in crimination of pollutants.
- 8. Nano technology is used for the manufacture of high energy density batteries.
- 9. Nano materials are sued to produce high power magnets.

- 10. Used to improve fuel efficiency in auto mobiles.
- 11. Used to manufacture aerospace components
- 12. Used to produce longer lasting satellites
- 13. Used to produce medical implants
- 14. Used to killing cancel calls
- 15. Used in the preparation of nano drugs.