



# PIE Tech

**POLLACHI INSTITUTE OF ENGINEERING AND TECHNOLOGY**

(Approved by **AICTE** and Affiliated to **Anna University**)

*sky is the limit*

**DEPARTMENT OF SCIENCE HUMANITIES**

**REGULATION 2021**

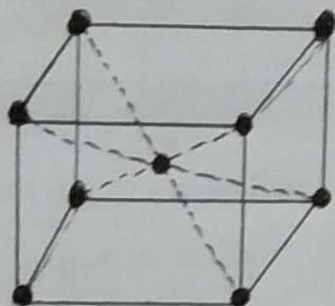
**I YEAR / II SEM**

**PH3251 MATERIAL SCIENCE**

Crystallography

Crystal Structures : BCC, FCC and HCP - directions and planes - linear and planar densities - crystal imperfections - edge and screw dislocations - grain and twin boundaries - Burgers vector and elastic strain energy - slip systems, plastic deformation of materials - Polymorphism - Phase changes - nucleation and growth - homogeneous and heterogeneous nucleation.

- ① calculate the number of atoms per unit cell, coordination number and packing factor, for BCC structure.



Number of atoms per unit cell

$$\begin{aligned} \text{All corner atoms} &= \frac{1}{8} \times 8 \\ &= 1 \text{ atom} \end{aligned}$$

$$\begin{aligned} \text{Total number of atoms in one} \\ \text{unit cell} &= 1 + 1 = \underline{2 \text{ atoms}} \end{aligned}$$

Coordination number

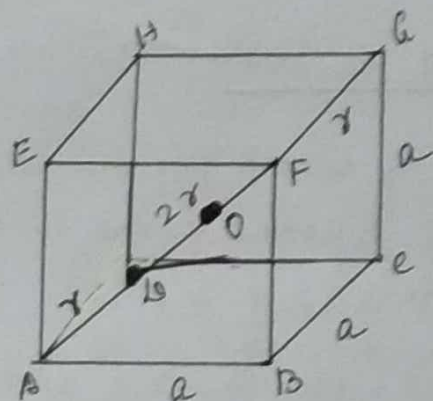
Coordination number of body centered cubic structure is 8

Atomic radius :

$$\begin{aligned} AG &= r + 2r + r \\ &= 4r \end{aligned}$$

Squaring on both sides

$$(AG)^2 = (4r)^2$$



From the right angled  $\triangle ABC$

$$AC^2 = AB^2 + BC^2$$

Substituting for AB and BC from the figure

$$AC^2 = a^2 + a^2$$

$$AC^2 = 2a^2$$

From the right angled  $\triangle ACG$

$$AG^2 = AC^2 + CG^2$$

Substituting for  $AG^2$ ,  $AC^2$  and  $CG^2$

$$\begin{aligned} (4r)^2 &= 2a^2 + a^2 \\ &= 3a^2 \end{aligned}$$

$$4^2 r^2 = 3a^2$$

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

Taking Square root on both sides

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

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

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

### Packing factor

Number of atoms per unit cell = 2

Volume of 2 atoms in the unit

cell,  $V = 2 \times \frac{4}{3} \pi r^3$

Atomic radius,  $r = \frac{\sqrt{3} a}{4}$

Volume of the unit cell

$$V = a^3$$

Packing factor =  $\frac{V}{V_{\text{cell}}}$

Substituting for  $v$  and  $V$ ,

$$PF = \frac{2 \times \frac{4}{3} \pi r^3}{a^3}$$

Substituting for  $r$

$$PF = \frac{2 \times \frac{4}{3} \pi \left( \frac{\sqrt{3} a}{4} \right)^3}{a^3}$$

$$= \frac{\frac{8}{3} \pi (\sqrt{3})^3 \cancel{a^3}}{4^3}$$

$$= \frac{\frac{8}{3} \pi \sqrt{3} \times \sqrt{3} \times \sqrt{3}}{4 \times 4 \times 4}$$

$$= \frac{\frac{8}{3} \pi \times 3\sqrt{3}}{64}$$

$$PF = \frac{\pi \sqrt{3}}{8}$$

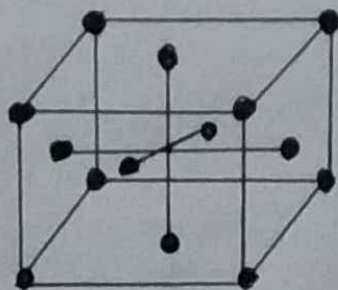
$$P.F = \frac{3.14 \times \sqrt{3}}{8} = 0.68$$

$$P.F = 0.68 \times 100\%$$

$$P.F = 68\%$$

Examples : Chromium, Tungsten

- ② Calculate the number of atoms per unit cell, Coordination number and packing factor for FCC structure.



Number of atoms per unit cell

Share of each unit cell =  $1/8$

Corner atoms

Number of atoms per unit cell from the contribution of

Corner atoms =  $1/8 \times 8 = 1$  atom

Share of each unit cell =  $1/2$  of face centered atoms

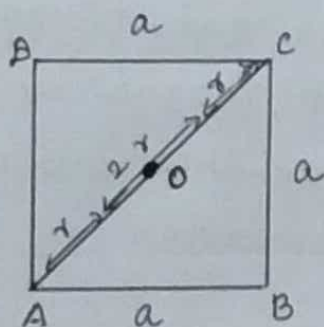
=  $1/2 \times 6 = 3$  atoms

Total number of atoms per unit cell =  $1 + 3 = 4$  atoms

Coordination number

Coordination number is 12

Atomic radius



The length of the face diagonal

$$AC = r + 2r + r = 4r$$

In right angled  $\Delta ABC$

$$AC^2 = AB^2 + BC^2$$

Substituting for  $AC^2$ ,  $AB^2$  and  $BC^2$

$$(r + 2r + r)^2 = a^2 + a^2$$

$$(4r)^2 = a^2 + a^2 \quad (\because AC = 4r)$$

$$4^2 r^2 = 2a^2$$

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

Taking square root on both sides

$$\begin{aligned} \sqrt{r^2} &= \sqrt{\frac{2a^2}{4^2}} = \frac{\sqrt{2a^2}}{\sqrt{4^2}} \\ &= \frac{\sqrt{2} \sqrt{a^2}}{4} \end{aligned}$$

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

Packing factor

Number of atoms per unit cell = 4

Volume of 4 atoms  $V = 4 \times \frac{4}{3} \pi r^3$

$$\text{Atomic radius } r = \frac{\sqrt{2}a}{4}$$

Side of the unit cell =  $a$

Volume of the unit cell  $V = a^3$

$$\text{Packing factor} = \frac{V}{V}$$

Substituting for  $V$ ,  $V$  and  $r$

$$\text{PF} = \frac{4 \times \frac{4}{3} \pi r^3}{a^3} = \frac{4 \times \frac{4}{3} \pi \left( \frac{\sqrt{2}a}{4} \right)^3}{a^3}$$



$$= \frac{4 \times \frac{4}{3} \pi (\sqrt{2})^3 a^3}{4^3}$$

$$= \frac{4 \times \frac{4}{3} \times \pi \times \sqrt{2} \sqrt{2} \times \sqrt{2} \times a^3}{4^3}$$

$$= \frac{\pi \times 2 \sqrt{2}}{3 \times 4}$$

$$PF = \frac{\pi \sqrt{2}}{6}$$

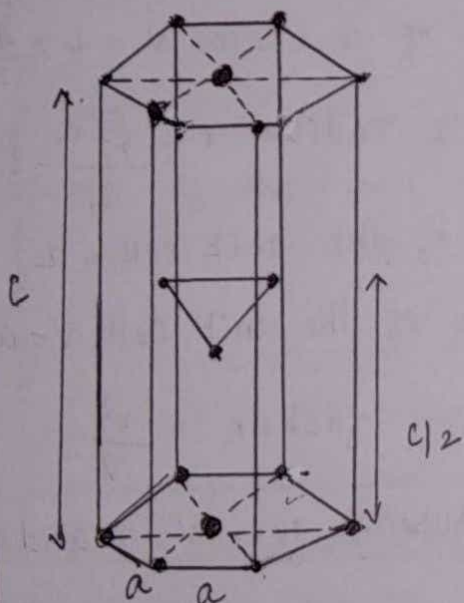
$$= \frac{3.14 \times \sqrt{2}}{6}$$

$$= 0.74 \times 100\%$$

$$PF = 74\%$$

Examples : Aluminium, Nickel, gold

③ What is Hexagonal closed Packed structure? Prove that the Packing factor of HCP is 0.74



closely packed structure has the highest packing factor of 0.74. Here the atoms are closely packed

leaving a small space as vacant in the crystal. Face centered cubic copper and hexagonal close packed magnesium are examples to this closely packed structure.

Number of atoms per unit cell

$$\text{upper corner atoms} = \frac{1}{6} \times 6 = 1$$

$$\text{lower corner atoms} = \frac{1}{6} \times 6 = 1$$

$$\text{Total number of central atoms in both upper and lower planes} = \frac{1}{2} \times 2 = 1$$

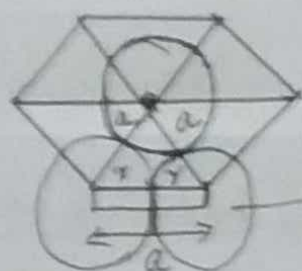
atoms completely inside the unit cell.

Total number of atoms in HCP unit cell =  $1+1+1+3$   
 $= 6$

Coordination number

Coordination number = 12

Atomic radius

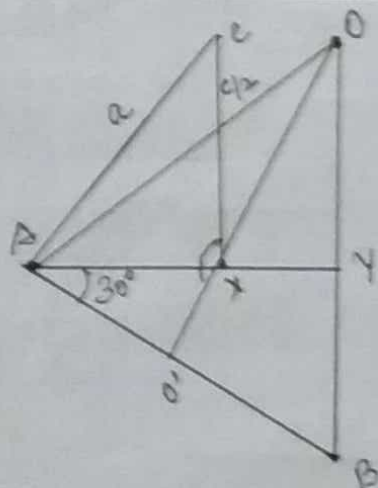


corner atom

$$a = 2r$$

$$r = a/2$$

Calculation of c/a ratio



Consider  $\triangle ABO$

$AY$  drawn  $\perp$  to  $BO$

$$\cos 30^\circ = \frac{AY}{AB}$$

$$AY = AB \cos 30^\circ$$

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

$$\left( \begin{array}{l} AB = a \\ \cos 30^\circ = \frac{\sqrt{3}}{2} \end{array} \right)$$

$$AY = \frac{a\sqrt{3}}{2} \rightarrow (1)$$

$X$  is a centre for  $\triangle ABO$

$$AX = \frac{2}{3} AY$$

Substituting for  $AY$

$$AX = \frac{2}{3} \times \frac{a\sqrt{3}}{2}$$

$$= \frac{2}{3} \times \frac{a\sqrt{3}}{2}$$

$$AX = \frac{a}{\sqrt{3}}$$

In  $\triangle AXC$ , Plane  $AXC \perp$  to  $ABO$

$$AC^2 = AX^2 + CX^2 \rightarrow (4)$$

$$AC = a, AX = \frac{a}{\sqrt{3}}, CX = c/2$$

Substituting the above values in eqn (4)

$$a^2 = \left( \frac{a}{\sqrt{3}} \right)^2 + \left( \frac{c}{2} \right)^2 \rightarrow (5)$$

$$a^2 = \frac{a^2}{3} + \frac{c^2}{4}$$

$$a^2 = \frac{a^2}{3} + \frac{c^2}{4}$$

$$\frac{c^2}{4} = a^2 - \frac{a^2}{3}$$

$$\frac{c^2}{4} = \frac{3a^2 - a^2}{3}$$

$$\frac{c^2}{4} = \frac{2a^2}{3}$$

$$\frac{c^2}{a^2} = \frac{2 \times 4}{3}$$

$$\frac{c^2}{a^2} = \frac{8}{3} \longrightarrow (6)$$

Taking square root on both sides

$$\sqrt{\frac{c^2}{a^2}} = \sqrt{8/3}$$

$$\frac{c}{a} = \sqrt{8/3} = 1.633$$

$$\boxed{\frac{c}{a} = 1.633} \longrightarrow (7)$$

### Packing Factor

Volume of all the atoms in a unit cell ( $V$ )

Number of atoms per unit cell  $n = 6$

Atomic radius  $r = a/2$

Volume of all 6 atoms in the unit cell

$$V = 6 \times \frac{4}{3} \pi r^3$$

Substituting for  $r$

$$V = 6 \times \frac{4\pi}{3} \left(\frac{a}{2}\right)^3$$

$$V = \frac{24\pi}{3} \frac{a^3}{2^3}$$

$$= \frac{24}{3} \frac{\pi a^3}{8}$$

$$\boxed{V = \pi a^3}$$

Volume of the unit cell

Area of the base of the hexagon  $= 6 \times \text{Area of } \triangle AOB$

Area of  $\triangle AOB = \frac{1}{2} \times \text{base}(BO) \times \text{height}(AY)$

Substituting for  $BO = a$

$$AY = a\sqrt{3}/2$$

$$\text{Area of } \triangle AOB = \frac{1}{2} \times a \times a\sqrt{3}/2$$

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

$$\text{Area of the base} = 6 \times \frac{a^2\sqrt{3}}{4}$$

$$= \frac{3\sqrt{3}a^2}{2}$$

Volume of the unit cell of the HCP = Area of the base  $\times$  height of the hexagon

$$V = \frac{3\sqrt{3}a^2}{2} \times c$$

$$\text{Packing factor} = \frac{V}{V}$$

$$P.F = \frac{\pi a^3}{\frac{3\sqrt{3}a^2c}{2}}$$

$$P.F = \frac{2\pi}{3\sqrt{3}} \left(a/c\right)$$

$$P.F = \frac{2\pi}{3\sqrt{3}} \left(3/8\right)^{1/2} \left(\because \frac{c}{a} = \left(\frac{8}{3}\right)^{1/2}\right)$$



$$= \frac{2\pi}{3\sqrt{3}} \frac{3^{1/2}}{8^{1/2}}$$

$$= \frac{2\pi}{3\sqrt{3}} \frac{\sqrt{3}}{\sqrt{8}}$$

$$= \frac{2\pi}{3\sqrt{4 \times 2}}$$

$$= \frac{2\pi}{3\sqrt{4} \times \sqrt{2}}$$

$$= \frac{2\pi}{8 \times 2 \sqrt{2}}$$

$$P.F = \frac{\pi}{3\sqrt{2}} = \frac{3.14}{3\sqrt{2}}$$

$$= 0.74$$

$$= 0.74 \times 100\%$$

Packing Factor = 74%

Examples :

Magnesium, Zinc

## ④ Explain about Miller Indices

### Definition

Miller introduced a set of three numbers to designate the orientation of a plane in a crystal. This set of three numbers is called Miller indices.

### Procedure for finding Miller

#### Indices

#### Step : 1

Intercepts of the plane along the coordinate axes x, y, z

#### Step : 2

Ratio of co-efficient of intercepts.

$$P : q : r \quad , \quad x = Pa, y = qb$$

$$z = rc \quad (7)$$

#### Step : 3

Ratio of reciprocal of numerical parameters

$$1/p : 1/q : 1/r$$

#### Step : 4

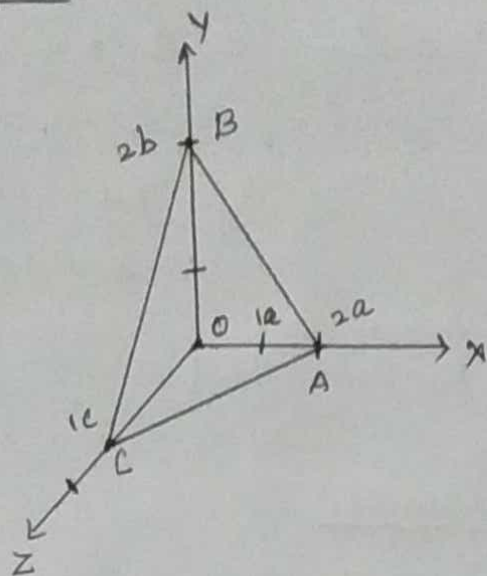
- Reduce the reciprocals into whole numbers.
- multiplying each reciprocal by a number, taking LCM of the denominators

#### Step : 5

Write these integers with in parentheses without commas to get Miller indices.



## Examples



- the Numerical Parameters of this plane 2, 2 and 1. Hence its orientation is  $(2, 2, 1)$

$$\left( \frac{1}{2} : \frac{1}{2} : 1 \right) \text{ or simply } (112)$$

- Intercepts are multiplied by 2

$$(112)$$

The general expression for Miller Indices of a plane is  $(hkl)$ .

- The symbol for a family of Parallel planes is  $\{hkl\}$

## ⑤ Explain crystal defects in detailed manner

### Definition

The disturbance occurred in the regular orientation of atoms is called crystal defect or imperfection.

### classification of crystal imperfections (or defects)

#### 1) Point Defects

- vacancies
- interstitials
- Impurities

#### 2) Line Defects

- Edge dislocation
- screw dislocation

#### 3) Surface Defects

- Grain boundaries
- Grain boundaries
- Twin boundaries
- Stacking faults

#### 4) Volume Defects

Cracks

#### 1) Point Defects

- Point defects are crystalline irregularities of atomic dimensions.

### Types of point defects

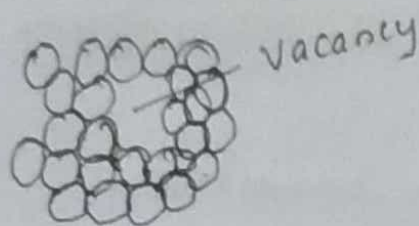
- vacancies
- interstitials
- Impurities

## Vacancies

• A vacancy is the simplest point defect in a crystal.

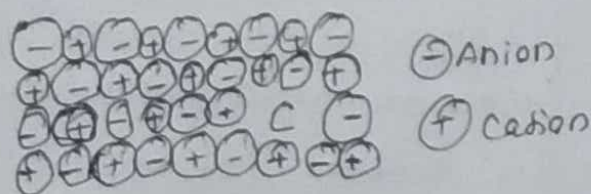
• It refers to a missing atom or vacant atomic site.

Whenever one or more atoms are missing from a normally occupied position, the defect caused is known as vacancy.



## Schottky defect :

missing of a pair of positive and negative ions in an ionic crystal.



## Frenkel defect

A vacancy associated with interstitial impurity is called Frenkel defect.

### b) Interstitial defect

When an extra atom occupies interstitial space within the crystal structure without removing parent atom, the defect is called interstitial defect.

## Types of interstitial defect

- i) Self interstitial
- ii) Foreign interstitial.

### i) Self interstitial

If an atom from same crystal occupies interstitial site, then it is called Self interstitial.

### ii) Foreign interstitial

If an impurity atom occupies interstitial site then it is called foreign interstitial.

### c) Impurities

When the foreign atoms are added to crystal lattices they are known as impurities. The defect is called impurity defect.

- i) Substitutional impurity defect.

- ii) Interstitial impurity defect.

### i) Substitutional impurity defect

A substitutional impurity refers to a foreign atom that replaces a parent atom in the lattice.

### ii) Interstitial impurity defect

An interstitial impurity is a small size atom occupying the empty space in the parent crystal without dislodging any of the parent atoms from their sites.



## Line defects or dislocations

The defects due to dislocation or distortion of atoms along a line are known as line defects. These defects are also called dislocations.

Types of line defects : 2 types

- a) Edge dislocation
- b) Screw dislocation

### a) Edge dislocation

Edge of a plane forms a line defect and it is called an edge dislocation.

### Classification of edge dislocation

There are two configurations

- a) Positive edge dislocation
- b) Negative edge dislocation

### a) Positive edge dislocation

If the extra plane of atoms is above the slip plane of the crystal then the edge dislocation is called positive edge dislocation.

It is denoted by the symbol  $\perp$

### b) Screw dislocation

Screw dislocation is due to a displacement of atoms in one part of a crystal relative to rest of the crystal.

## b) Negative edge dislocation

If the extra plane of atoms is below the slip plane than the edge dislocation is called negative. It is denoted by the symbol  $\top$ .

## Surface defects (Plane defects)

The defects on the surface of material are called surface defects or plane defects.

- i) Grain boundaries
  - ii) tilt and twist boundaries
  - iii) Twin boundaries
  - iv) Stacking fault
- ### i) Grain boundaries

Whenever the grains of different orientations separate the general pattern of atoms and exhibits a boundary the defect caused is called grain boundary.

### ii) Tilt and twist boundaries

Tilt boundary is another surface imperfection. It is an array of parallel edge dislocations of same sign, arranged one above other in an array or series.

low angle boundary is a low angle boundary.

$$\tan \theta = \frac{b}{\Delta}$$

$\Delta$  - dislocation spacing

$b$  - length of Burger's Vector

when  $\theta$  is very small

$$\tan \theta = \theta$$

$$\theta = \frac{b}{\Delta}$$

### Twist boundaries

Twist boundaries are another type of low angle boundaries

### (iii) Twin boundaries

Twin boundaries are another surface imperfections.

If the boundaries in which the atomic arrangement on one side of the boundary is some what a mirror image of the arrangement of atoms of the other side. The defect caused is called twin boundary.

### Stacking Faults

It is a kind surface imperfection.

Whenever the stacking of atoms is not in proper sequence

through out the crystal defect caused is called stacking fault.



## 6) write short notes in Polymorphism

• Many substances exist in more than one stable crystalline form.

• The various forms have the same composition but the crystal structures are different.

• The changes in crystal structure is caused due to either a change in temperature or pressure or both.

### Definition :

The ability of a material to exist in two or more crystal structure is called Polymorphism.

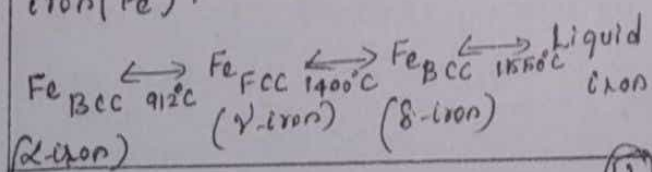
If the structural change is reversible, then the polymorphic change is known as allotropy.

### Example : 1

Cobalt at ordinary temperature has HCP structure, it is heated above  $477^{\circ}\text{C}$ , it changes to FCC structure.

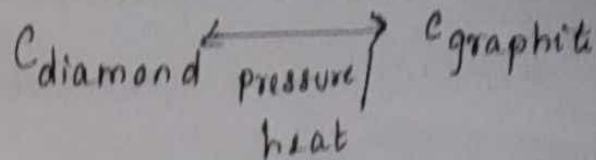
### Example : 2

A good example of Polymorphism and allotropy is iron (Fe).



### Example : 3

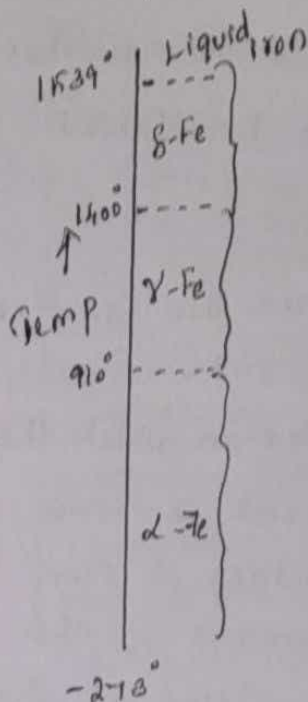
A similar reaction occurs in diamond and graphite.



• Carbon exists in either diamond

• Diamond is very hard, transparent

• Graphite is a good conductor.



Some of the properties which changes are

- |                             |                        |
|-----------------------------|------------------------|
| a) specific volume          | g) chemical Properties |
| b) Packing density          | h) physical Properties |
| c) Electricity Conductivity |                        |
| d) Thermal conductivity     |                        |
| e) Mechanical properties    |                        |
| f) Magnetic properties      |                        |

about notes in phase changes or transformation  
nucleation and growth in) Homogeneous or self nucleation  
ii) heterogeneous nucleation.

## 12 Phase changes or Transformations

Phase transformation is an important process in the production and treatment of metallic compounds and alloys.

- It involves nucleation and growth.

- Phase transformation occurs due to change of Pressure, temperature or Composition of the alloy.

### Different types of phase transformations

- i) Congruent transformation
- ii) Shear transformation

#### i) Congruent transformation

- A single component material crystallizes from liquid state with no change in composition.

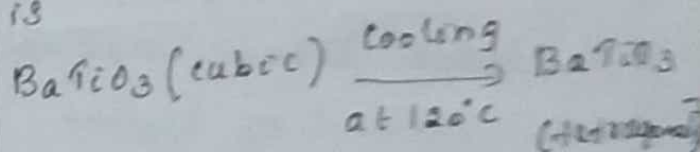
- Congruent transformation can be two types

- Reconstructive transformation
- Displacive transformation

- In reconstructive phase transformation the atoms diffuse across the  $\alpha$ - $\beta$  interface to transform  $\alpha$  phase into  $\beta$  phase.

- phase change occurs a gradual process in which the atomic coordination is altered.

- In displacive transformation arises from the cooperative movements of a large number of neighbouring atoms. The example of such transformation is

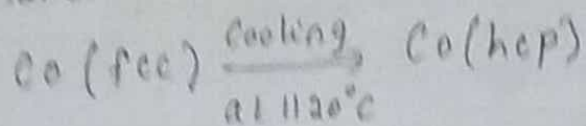


- occurs very rapidly
- No bonds are broken during the process.

#### ii) Shear transformation

- Shear like cooperative displacement of one layer of atoms with respect to the next layer

- Layers are close-packed planes



## Solidification of metals and alloys

- The Solidification of metals and alloys is an important industrial process.

- Two steps are taken place

- 1) The formation of stable nuclei in the melt
- 2) The growth of nuclei into crystals and the formation of a grain structure.

## ② Nucleation and Growth

- Nucleation is the beginning of phase transformation.

- It starts tiny regions called nuclei of new phase in the molten metal.

- Nucleation may involve

1. The assembly of atoms by diffusion
2. Structural change into one or more unstable intermediate structures.

3. Formation of critical particle called nuclei of new phase.

The process of Crystallization mainly consists of following stages

- a) Formation of Nuclei
- b) Growth of nuclei into Crystals
- c) Joining of crystals to form grains with grain boundaries.

- Two main mechanisms occurs

1. Homogeneous Nucleation / Self Nucleation
2. Heterogeneous Nucleation.

### Homogeneous or Self Nucleation

The formation of Nuclei in a melt without the aid of impurity foreign particles is called homogeneous or self nucleation.

- During the nucleation the molten metal must be cooled below its freezing temperature



atoms in a molten liquid and together to form a small crystal called embryo.

In homogeneous nucleation the stability of a nucleus is controlled by two factors.

- i) Free energy change during the liquid - solid transition.
- ii) Surface energy the nucleus thus formed.

As a result, the total free energy change, the embryo formation is

$$\Delta G = -\frac{4}{3} \pi r^3 \Delta G_0 + 4 \pi r^2 \gamma \quad \text{--- (1)}$$

$\Delta G$  - free energy change between liquid and solid per unit volume

$r$  - radius of an embryo

considered to be spherical.

$\gamma$  - Specific Surface energy

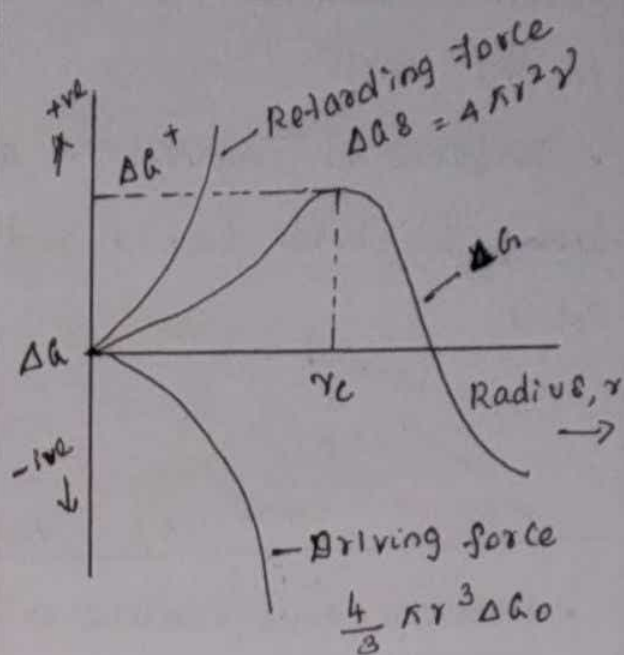
Below the melting temperature  $T_s$ ,  $\Delta G_0$  is negative and hence the first term on the right of eqn (1) is negative.

$\gamma$  is always positive

The term  $\frac{4}{3} \pi r^3 \Delta G_0$  - driving force for the creation of

Solid-liquid interface.

Surface energy which is the retarding force increases as  $r^2$  increases.



$$\frac{\Delta G}{dr} = -\frac{4}{3} \pi \times 3r^2 \Delta G_0 + 4 \pi \cdot 2r \gamma$$

$$\frac{\Delta G}{dr} = 0 \quad \text{when } r = r_c$$

$$0 = -\frac{4}{3} \pi \times 3r_c^2 \Delta G_0 + 4 \pi \times 2r_c \gamma$$

$$4 \pi r_c^2 \Delta G_0 = 8 \pi r_c \gamma$$

Rearranging above eqn

$$r_c = \frac{2\gamma}{\Delta G_0}$$

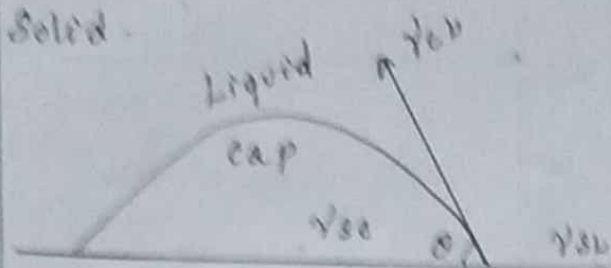
when  $r > r_c$  the free energy of the system decreases and initiating the formation of crystal.



## Heterogeneous Nucleation

• The source about which nuclei are formed on solid particles are always present in the melt.

• Surfaces or impurities are wet by both liquid and solid.



• Heterogeneous nucleus is considered as a spherical cap on a solid, flat substrate.

• Volume of the cap depends on the contact angle  $\theta$  at the nucleus - liquid - substrate junction.

$$\Delta G = V \Delta G_v + A_{CL} \gamma_{CL} + \pi r^2 \gamma_{SL} - \pi r^2 \gamma_{SV}$$

V - volume of the spherical cap (nucleus)

$A_{CL}$  - the interfacial surface area between liquid and cap.

$r$  - the radius of the cap (nucleus)

•  $\gamma_{CL}$ ,  $\gamma_{SL}$  and  $\gamma_{SV}$  are interfacial surface tension between cap and liquid, cap and substrate and substrate liquid respectively.

• In homogeneous nucleation the critical size of the nucleus is given by  $r_c = \frac{2\gamma_{CL}}{\Delta G_v}$

and it is independent of contact angle.

• The value of  $\gamma_{CL}$ , the interfacial surface tension surface energy is much smaller.

• Smaller amount of undercooling is required.

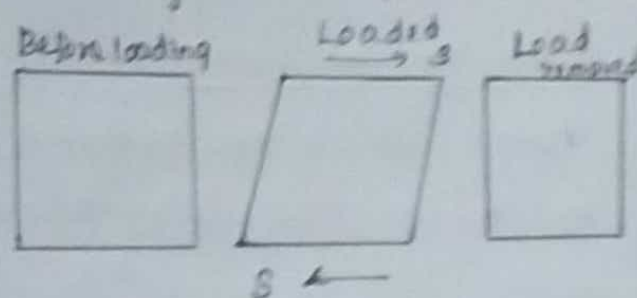
## ⑧ Explain about deformation of metals

• When metals or alloys are stressed they get deformed.

## Elastic deformation

If a metal is loaded a temporary deformation of the crystal takes place through displacement of the atoms.

As the deforming load is removed, the atoms return to their original position and the crystal recovers its original shape.



## Plastic deformation

- Follows elastic deformation
- If the deforming load is stresses in the metal piece cross the elastic limit, the specimen gets plastically deformed.

If the deforming load at this stage is removed, the metal piece does not regain its original shape.

- Depends on following factors
- Applied stress
- Temperature
- Strain rate

## Plastic deformation mechanisms

- Single crystal occurs in two ways
- a) Slip
- b) Twinning

### Slip

The deformation by slip takes place when one part of the crystal moves or glides over another part along certain planes.

The planes over which slip takes place are the planes of greatest atomic density and they are called slip planes.

### Mechanism of slip

- 4 stages during plastic deformation

#### Stage : 1

Perfect crystal with out slip

### Stage : 2

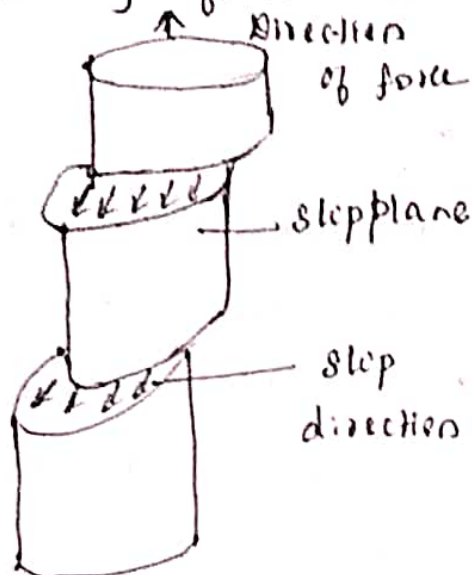
Deforming shear force is applied to the crystal

### Stage : 3

Slip taking place along the slip plane

### Stage : 4

Permanent deformation when deforming forces are removed.



Slip in a single crystal

The particular crystallographic planes where slip occurs are called slip planes

The direction along which slip occurs is called slip direction

### Twinning

Plastic deformation mechanism occurs in some metal known as twinning

The crystallographic plane of symmetry between the deformed and undeformed parts of the metal lattice is called the twinning plane.

• Twinning major deformation seen in HCP

• Types of twinning

1) Mechanical twins

2) Annealing twins

1) Mechanical twins

Twins which are produced by mechanical deformation are called mechanical twins

• BCC and HCP

2) Annealing twins

The twins which are produced by annealing are called annealing twins

• usually broader

• FCC metals form annealing twins

• Normal growth mechanism.

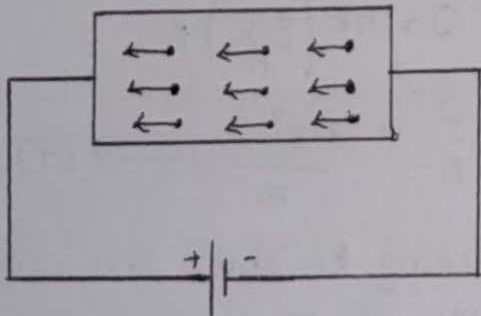


## UNIT : II

Electrical and Magnetic Properties of Materials

classical free electron theory - Expression for electrical conductivity. Thermal conductivity expression - Quantum free electron theory; Tunneling - degenerate states - Fermi-Dirac statistics - Density of Energy states - Electron in periodic potential - Energy band in solids - tight binding approximation - Electron effective mass - Concept of hole. Magnetic materials; Dia, Para and ferromagnetic effects - Paramagnetism in the conduction electron in metals - exchange interaction and ferromagnetism - quantum interference devices - GMR devices.

① Give the Assumptions or postulates of classical free Electron theory.



1. A solid metal has nucleus with revolving electrons. The electrons move freely like molecules in a gas.

2. The free electrons move in a uniform Potential field due to the ions fixed in the lattice.

3. In the absence of electric field ( $E=0$ ), the free electrons move in random directions and collide with each other.

• Since the collisions are elastic.

4. When the presence of electric field ( $E \neq 0$ ) the free electrons are accelerated in the direction opposite to the direction of applied electric field.

5. Electrons are assumed to be perfect gas, they obey the laws of classical theory of gases.

6. Classical free electrons in the metal obey Maxwell-Boltzmann statistics.

7. Electrons acquire a constant average velocity known as drift velocity.

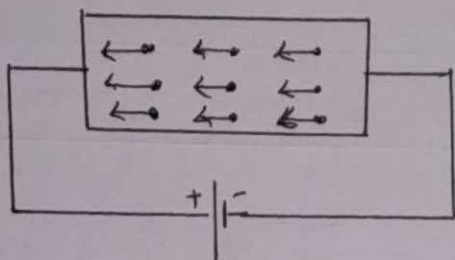
8. Free electrons can be assigned with mean free path, mean collision time and average speed.



② Derive the expression for electrical conductivity and then prove the conductivity metal based on classical free electron theory. State and prove Widemann - Franz law and Lorenz Number.

### 1) Expression for electrical conductivity [Based on Drude and Lorentz]

When an electrical field ( $E$ ) is applied to an electron of charge  $e$  of a metallic rod, the electron moves in opposite direction to the applied field with a velocity  $v_d$ . This velocity is known as drift velocity.



Force experienced by the electron

$$F = eE \rightarrow (1)$$

From Newton's second law of motion

$$F = ma \rightarrow (2)$$

From eqns (1) and (2)

$$ma = eE$$

$$a = \frac{eE}{m} \rightarrow (3)$$

From eqn (3) electron should be accelerated continuously due to the applied electric field.

• After each collision the velocity of electron increases until the next collision takes place.

Average drift velocity of electron = If  $\tau_c$  is collision time then acceleration

$$a = \frac{v_d}{\tau} \quad (\because \tau_c = \tau)$$

$$v_d = a\tau \rightarrow (4)$$

Substituting eqn (3) in eqn (4)

$$v_d = \frac{eE}{m} \tau$$

$$v_d = \left( \frac{e\tau}{m} \right) E \rightarrow (5)$$

The current density  $J$  is related to the drift velocity

$$J = ne v_d \rightarrow (6)$$

Substituting eqn (5) in eqn (6)

$$J = ne \left( \frac{e\tau}{m} \right) E$$

$$\frac{J}{E} = \frac{ne^2\tau}{m} \rightarrow (7)$$

According to ohm's law, Current density  $J$  is

$$J = \sigma E, \quad \sigma = J/E \rightarrow (8)$$

Comparing eqn (7) and eqn (8)

$$\sigma = \frac{ne^2\tau}{m} \rightarrow (9)$$

The eqn (9) is called electrical conductivity of the metal.

## Depression for Thermal Conductivity ( $\kappa$ ) of a metal

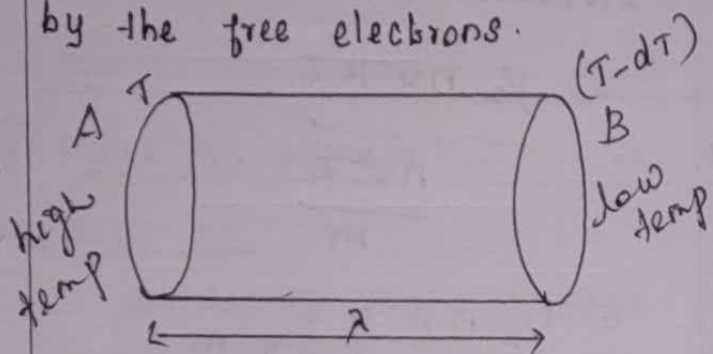
### Definition:

Thermal conductivity ( $\kappa$ ) of a metal is defined as the amount of heat ( $Q$ ) conducted per unit area ( $A$ ) per unit time ( $t$ ) maintained at unit temperature gradient.

Consider two cross-sections A and B of a metal rod separated by a distance  $\lambda$ .

- A be a high temperature ( $\tau$ )
- B at a low temperature ( $\tau - d\tau$ )

Now heat flows from A to B by the free electrons.



Conduction electron per unit volume =  $n$

Average velocity of the electrons =  $v$

• Elastic collision takes place

At A average kinetic energy of an electron =  $\frac{3}{2} kT$

$$\therefore K.E = \frac{1}{2} m v^2 = \frac{3}{2} kT \quad \rightarrow (1)$$

where

$k$  - Boltzmann's constant

$\tau$  = Temperature at A

At B, average K.E of the electron =  $\frac{3}{2} k(\tau - d\tau) \rightarrow (2)$

The excess of K.E carried by the electron from A to B

$$= \frac{3}{2} k\tau - \frac{3}{2} k(\tau - d\tau)$$

$$= \frac{3}{2} k\tau - \frac{3}{2} k\tau + \frac{3}{2} k d\tau$$

$$= \frac{3}{2} k d\tau \quad \rightarrow (3)$$

Number of electrons crossing per unit time from A to B

$$= \frac{1}{6} n v \quad \rightarrow (4)$$

The excess of energy carried from A to B per unit area in unit time

$$= \frac{1}{6} n v \times \frac{3}{2} k d\tau$$

$$= \frac{1}{4} n v k d\tau \quad \rightarrow (5)$$

The deficient of energy carried from B to A unit area per unit time

$$= - \frac{1}{4} n v k d\tau \quad \rightarrow (6)$$

The net amount of energy transferred from A to B per unit area per unit time

$$Q = \frac{1}{4} n v k d\tau - \left( - \frac{1}{4} n v k d\tau \right)$$

$$= \frac{1}{4} n v k d\tau + \frac{1}{4} n v k d\tau$$

$$\alpha = \left( \frac{1}{4} + \frac{1}{4} \right) n v k d\tau \rightarrow (7)$$

From the definition of thermal conductivity,  $\alpha = k d\tau / \lambda$

$$\frac{1}{2} n v k d\tau = k d\tau / \lambda \rightarrow (8)$$

For the metals

Relaxation time = Collision time

$$\tau = \tau_c = \lambda / v$$

$$\tau v = \lambda \rightarrow (9)$$

Substituting eqn (9) and eqn (8)

$$k = \frac{1}{2} n v k \tau v$$

$$k = \frac{1}{2} n v^2 k \tau \rightarrow (10)$$

The eqn (10) is the expression for the thermal conductivity of a metal.

### iii) Wiedemann - Franz law

Law:

The ratio between the thermal conductivity and electrical conductivity of a metal is directly proportional to the absolute temperature of the metal

$$\frac{k}{\sigma} \propto T$$

$$\frac{k}{\sigma} = L T$$

where,  $L$  - proportionality constant, and it is  $\frac{1}{6}$  as Lorentz number.

### Derivation

Thermal conductivity of a metal

$$k = \frac{1}{2} n v^2 k \tau \rightarrow (1)$$

Electrical conductivity of the metal

$$\sigma = \frac{n e^2 \tau}{m} \rightarrow (2)$$

$$\frac{\text{Thermal conductivity}}{\text{Electrical conductivity}} = \frac{k}{\sigma}$$

$$= \frac{\frac{1}{2} n v^2 k \tau}{\frac{n e^2 \tau}{m}}$$

$$= \frac{1}{2} \frac{n v^2 k \tau}{n e^2 \tau} \times m$$

$$\frac{k}{\sigma} = \frac{1}{2} \frac{m v^2 k}{e^2} \rightarrow (3)$$

The K.E of the electron is given by

$$\frac{1}{2} m v^2 = \frac{3}{2} k T \rightarrow (4)$$

Substituting the eqn (4) in eqn (3)

$$\frac{k}{\sigma} = \frac{3}{2} \frac{k T \times k}{e^2} = \frac{3}{2} \frac{k^2 T}{e^2}$$



$$\frac{1}{\sigma} = \frac{3}{2} \left( \frac{k^2}{e^2} \right) T$$

$$\frac{k}{\sigma} = LT \rightarrow (5)$$

where  $L = \frac{3}{2} \left( \frac{k^2}{e^2} \right)$  is constant and known as Lorentz number.

$$\frac{k}{\sigma} \propto T \rightarrow (6)$$

Hence it is verified

#### iv) Lorentz Number

The ratio of thermal conductivity to the product

of electrical conductivity and absolute temperature of the metal is constant.

It is known as Lorentz number and it is given by

$$L = \frac{k}{\sigma T}$$

$$L = \frac{3}{2} \left( \frac{k}{e} \right)^2$$

Boltzmann's constant

$$k = 1.38 \times 10^{-23} \text{ J K}^{-1}$$

charge of an electron

$$e = 1.602 \times 10^{-19} \text{ coulomb}$$

$$L = \frac{3}{2} \left( \frac{1.38 \times 10^{-23}}{1.602 \times 10^{-19}} \right)^2$$

$$L = 1.12 \times 10^{-8} \text{ W } \Omega \text{ K}^{-2}$$

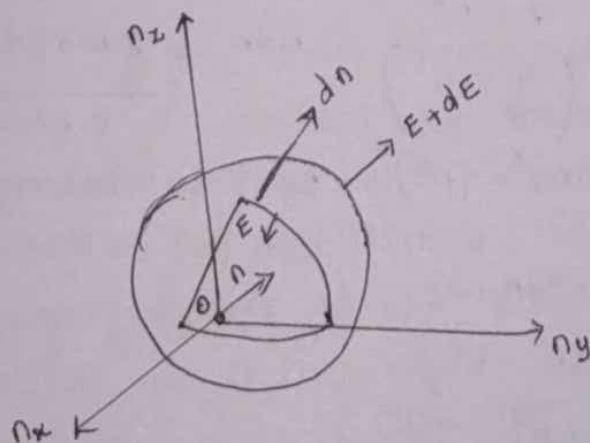
### 3) Derive an expression for the density of energy states.

#### Definition

Density of state  $Z(E)dE$  is defined as the number of energy states present per unit volume of a metal in an energy interval  $E$  and  $E+dE$ .

$$Z(E)dE = \frac{\text{Number of energy states in between energy } E \text{ and } E+dE \text{ in a metal piece } (N(E)dE)}{\text{Volume of the metal piece } (V)}$$

#### Derivation



- Consider a cubical metal of side 'a'.
- Number of energy states available between the energy  $E$  and  $E + dE$ .
- $n_x, n_y, n_z$  is the coordinate axes.
- Sphere is further divided into many shells.
- The number of energy states with in a sphere of radius

$$n = \frac{4}{3} \pi n^3 \rightarrow (1)$$

(Volume of the sphere)

- The quantum numbers  $n_x, n_y, n_z$  have only positive integer values.
- The number of available energy states with in one octant of the sphere of radius 'n' corresponding to energy.

$$E = \frac{1}{8} \left( \frac{4}{3} \pi n^3 \right) \rightarrow (2)$$

- The number of available energy states between within one octant of the sphere of radius ' $n + dn$ ' corresponding to energy

$$E + dE = \frac{1}{8} \left( \frac{4}{3} \pi (n + dn)^3 \right)$$

$\rightarrow (3)$

Subtracting eqn (2) from eqn (3)

$$N(E) dE = \frac{1}{8} \left( \frac{4}{3} \pi (n + dn)^3 \right) - \frac{1}{8}$$

$$\left( \frac{4}{3} \pi n^3 \right)$$

$$= \frac{1}{8} \left( \frac{4}{3} \pi \right) \left[ (n + dn)^3 - (n^3) \right]$$

$$= \frac{1}{8} \left[ \frac{4}{3} \pi \right] \left( n^3 + dn^3 + 3n^2 dn + 3n + dn^2 - n^3 \right)$$

Formula

$$[a + b]^3 = a^3 + b^3 + 3a^2 b + 3ab^2 \rightarrow (5)$$

Since the higher power of  $dn$  is very small,  $dn^2$  and  $dn^3$  terms can be neglected.

$$N(E) dE = \frac{\pi}{6} 3n^2 dn \rightarrow (6)$$

Number of available energy states between the energy interval and  $E + dE$  is given by

$$N(E) dE = \frac{\pi}{2} n^2 dn$$

$$N(E) dE = \frac{\pi}{2} n(n dn) \rightarrow (7)$$

The energy of an electron in a cubical metal piece of side 'a' is

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

$$n^2 = \frac{8ma^2 E}{h^2} \rightarrow (9)$$

$$n = \left[ \frac{8ma^2 E}{h^2} \right]^{1/2} \rightarrow (10)$$

Differentiating eqn (9)

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

$$n dn = \frac{8ma^2 dE}{2h^2} \rightarrow (11)$$

By substituting eqn (10) and eqn (11) in eqn (7)

$$N(E) dE = \frac{\pi}{2} n(n dn)$$

$$N(E)dE = \frac{\pi}{2} \left[ \frac{8ma^2E}{h^2} \right]^{1/2}$$

$$N(E)dE = \frac{\pi}{2} \cdot \frac{1}{2} \left( \frac{8ma^2E}{h^2} \right)^{1/2}$$

$$N(E)dE = \frac{\pi}{4} \left( \frac{8ma^2}{h^2} \right)^{3/2} E^{1/2} dE \rightarrow (12)$$

According to Pauli's exclusion Principle states that two electrons of opposite spins can occupy each state.

$$N(E)dE = 2 \times \frac{\pi}{4} \left( \frac{8ma^2}{h^2} \right)^{3/2} E^{1/2} dE$$

$$N(E)dE = \frac{\pi}{2} \left( \frac{8m}{h^2} \right)^{3/2} a^3 E^{1/2} dE$$

$$N(E)dE = \frac{\pi}{2} \left[ \left( \frac{2^2}{h^2} \right) 2m \right]^{3/2} a^3 E^{1/2} dE$$

$$N(E)dE = \frac{\pi}{2} \times 4 \times (2m)^{3/2} \left( \frac{a^3}{h^3} \right) E^{1/2} dE$$

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

Density of states is given by the number of energy states per unit volume.

$$Z(E)dE = \frac{N(E)dE}{V} \rightarrow (13)$$

on substituting  $N(E)dE$  and  $V$

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

$V = a^3 = 1$ , volume of the metal  
Density of states

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

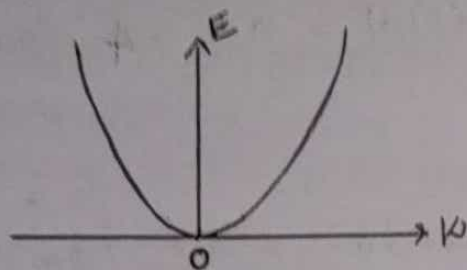
④ Explain with necessary diagram the Bloch theorem for the representation of electron in a periodic potential.

### Bloch Theorem

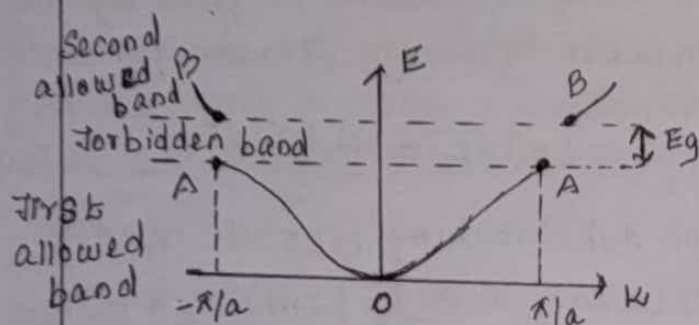
- According to the zone theory, the electrons move in a periodic field provided by the lattice.
- The potential of the solid varies periodically with the periodicity of the space lattice.
- The potential energy of the electron is zero near the nucleus of the positive ions in the lattice, and



maximum when it is half way between the adjacent nuclei which are separated by the interatomic spacing distance 'a'.



Classical free electron model energy curve



- This model was first postulated by Kronig and Penny
- If we use classical theory, we can get a parabola when we plot the curve between the electron's energy and its momentum.
- Since the curve is parabola the energy varies continuously.
- But in Kronig-Penney model, we can get a parabola with some discontinuities.

Consider the Schrodinger for one dimensional periodic potential field  $V(x)$  (Proposed by Kronig and Penny).

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

The solutions of this eqn shown by Bloch in the form

$$\psi(x) = U_k(x) e^{ikx}$$

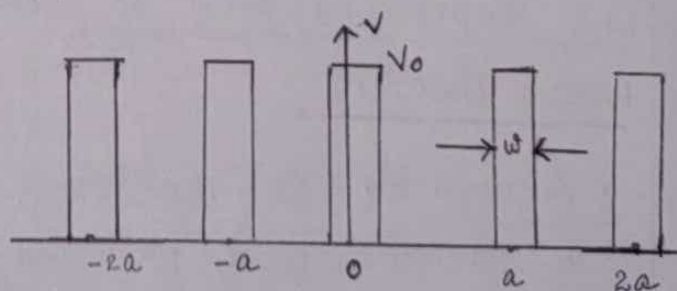
where,

$U_k(x)$  is periodic with the periodicity of the lattice.

$$U_k(x+a) = U_k(x)$$

The form of  $U_k(x)$  depends on the exact nature of the potential field.

- $\psi$  and  $\frac{d\psi}{dx}$  should be continuous throughout the crystal.
- In order to simplify the attendant computations, an assumption is made regarding the potential barrier.



one dimensional periodic potential

- $V_0$  increases, the width of the barrier decreases so that the product  $V_0$  remains constant

Reflections are possible only for energies given by the relation

$$\cos ka = \frac{dy}{dx} P \frac{\sin a}{a} + \cos a$$

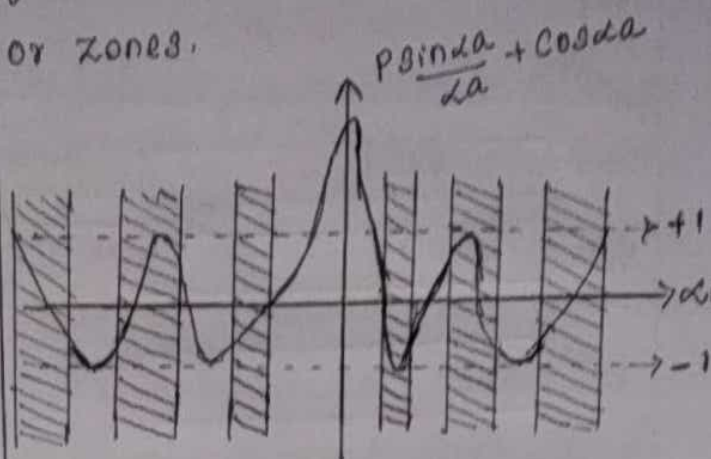
where

$$P = \frac{4\pi^2 m a V_0}{h^2}$$

$$a = \frac{2\pi}{h} \sqrt{2mE}$$

- only certain range values of  $\alpha$  are allowed.
- energy  $E$  is restricted to lie

within certain ranges which form the allowed energy bands or zones.



- Allowed energy bands are shaded.
- The energy spectrum of an electron moving in the presence of a potential field is divided into so called allowed zones and forbidden zones.

5. Discuss qualitatively how band theory of solids leads to the classification of solids in conductors, semiconductors and insulators.

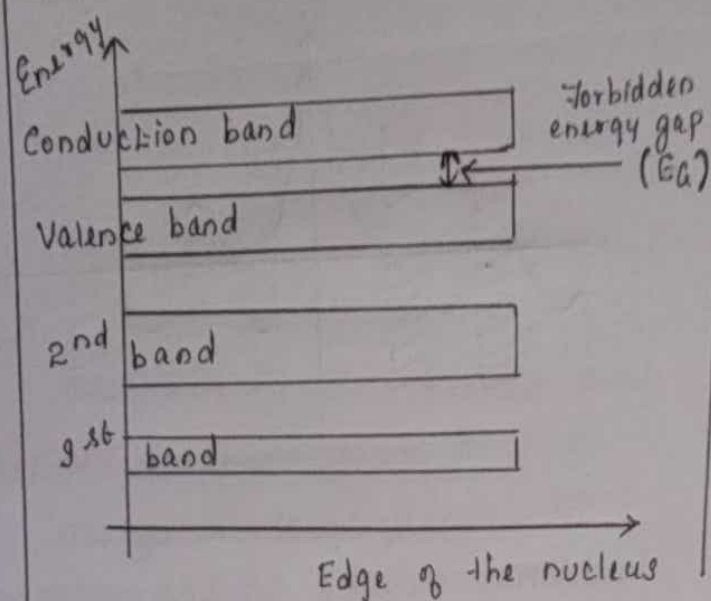
### Formation of Energy Bands in Solids

- Solid crystals are formed when isolated atoms are brought together.
- Various interactions occur between the neighbouring atoms.
- At a particular inter atomic spacing  $d$ , there is a proper balance between forces of attraction to form a crystal.

- The changes occur in the electron energy level configuration.
- In case of a single atom, there is a single energy for an electron orbit.
- When two atoms are brought close to each other, it leads to intermixing of electrons in the valence shell.
- The number of permissible energy levels is formed which is called an energy band.
- Three bands are important from the conductivity point



are valence band, Conduction band, Forbidden gap or energy gap.



• The electrons in the most shell are called electrons and the outermost shell is called valence shell.

• At higher temperature, electrons acquire energy and move to the conduction band as electron is not allowed to occupy any energy state in forbidden gap. These electrons are called free electrons.

## Classifications on the basis of Energy band Theory

The materials are classified as conductors, insulators and the semiconductors.

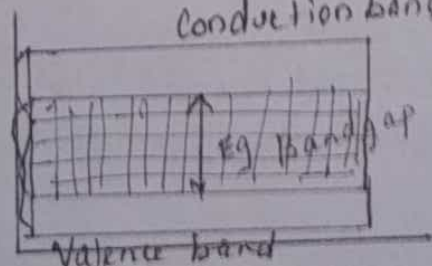
1) Conductors: Both valence and conduction bands overlap each other

• A material having large number of free electrons can conduct very easily.

Example: Copper - Good conductor

• In the metals like copper, aluminium there is no forbidden gap between valence band and conduction band.

• A large number of electrons are available for conduction



2) Insulators

• Forbidden energy band is very wide.

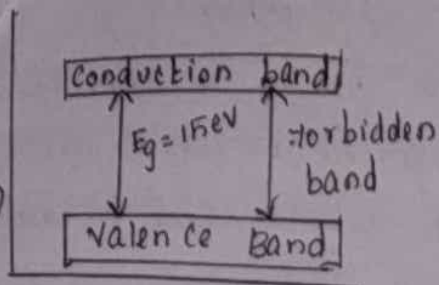
• Electrons cannot jump from valence band to conduction band.

• Valence electrons are bound very tightly to their parent atoms.

For example: Glass, the valence band is completely full at 0K and the energy gap between valence band and conduction band is the order of 10 eV.



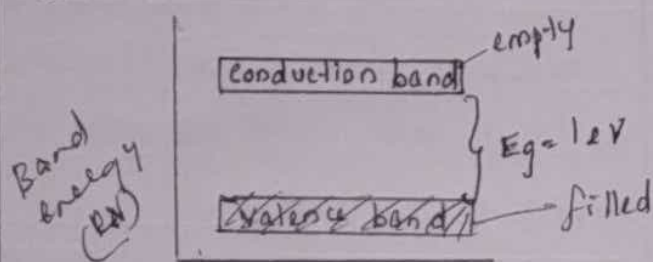
Electron Energy (eV)



- When a very large energy is supplied an electron may jump across the forbidden gap.
- The resistivity of insulators is of the order of  $10^7 \Omega m$ .

### Semiconductors.

- Forbidden gap is very small
- Germanium and Silicon are the best examples of semiconductors.



- In germanium, the forbidden gap is of the order of 0.7 eV
- In the case of Silicon, it is the order of 1.1 eV.
- A semiconductor is one whose electrical properties lies between those of insulators and conductors.
- At 0K there are no free electrons in conduction band and valence band is completely filled.
- Small amount of energy is supplied, the electrons can easily jump from valence band to conduction band.
- Forbidden gap is very small.
- Conductivities are of the order of  $10^2 \Omega m$ .

### 6) Describe tight binding approximation to explain the formation of energy band

For the explanation of band structures in solids two models are followed namely

- Free electron approximation
- Tight binding approximation

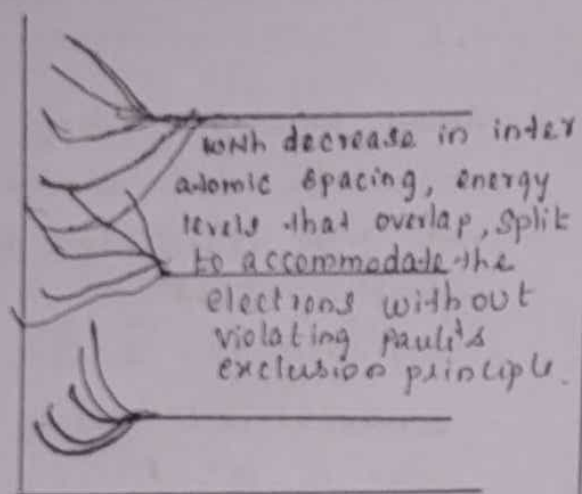
#### 1. Free electron approximation

- In solids ionic cores at fixed locations

- There is a free electron gas enveloping and enclosing these ionic cores.
- The solid already exists and the ionic cores are tightly bound to their lattice locations while the electrons are "free" to run through the extent of the solid. This is called the "free electron approximation"

### ii) Tight binding approximation

- Atoms are considered to be independent
- All the electrons are bound to their respective individual atoms to begin with.
- Atoms are free while the electrons are tightly bound



- when atoms are far apart, all of the bound electrons associated with each atom have fixed energy levels.
- when the atoms closer to each other to form the solid, as long as the inter atomic separation is large.
- Electrons will still maintain their original energy levels
- when the atoms get close enough, the outer shell electrons begin to overlap

with each other.

- Now the outer shell electrons are forced to split into levels above and below the energy level.
- The splitting of energy level occurs because electrons obey the Pauli's exclusion principle.
- only the outer shell electron overlap.
- At each energy level the level will split to enough new energy levels.

to the electron theory. Postulates, Merits and Demerits of Quantum Free Electron Theory.

• Theory uses quantum concepts and hence it is known as quantum free electron theory.

### Postulates of Quantum Free Electron Theory

- The potential energy of an electron is uniform or constant within the metal.
- The electrons have wave nature.
- The allowed energy levels of an electron are quantized.
- Free electrons obey Fermi-Dirac statistics.

### Merits of Quantum free Electron theory

- Theory treats the electron quantum mechanically rather than classically.
- It explains the electrical conductivity, thermal conductivity, specific heat capacity of metals, photoelectric effect

and Compton effect etc.

### Demerits of Quantum Free Electron Theory.

- This theory explains most of the physical properties of the metals, it fails to state the difference between conductor, semiconductor and insulator.
- It also fails to explain the positive value of Hall Coefficient and some of the transport properties of the metals.



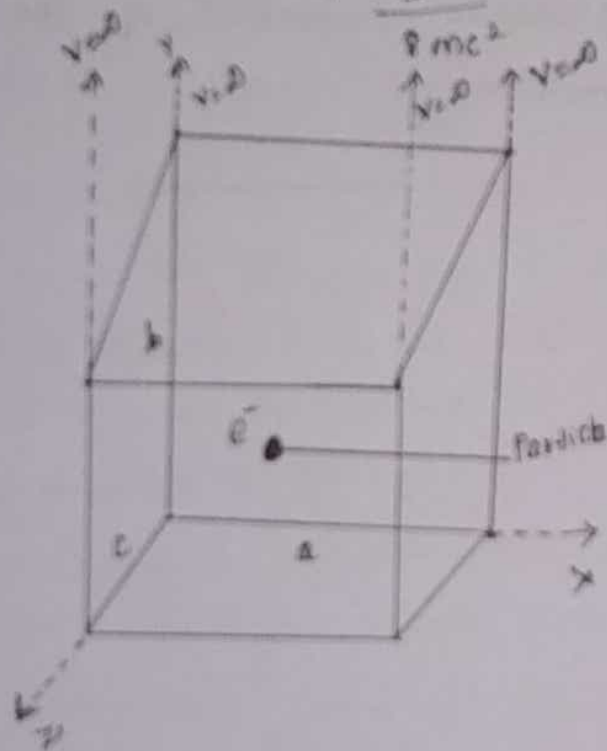
⑧ Derive an expression for Particle in a three dimensional box

The Solution of one dimensional Potential well is extended for a three-dimensional Potential box.

- Three quantum numbers  $n_x, n_y$  and  $n_z$
- Coordinate axes  $x, y, z$
- $a, b, c$  are the lengths

Energy of the particle  
 $= E_x + E_y + E_z$

$$E_{n_x n_y n_z} = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8mb^2} + \frac{n_z^2 h^2}{8mc^2}$$



If  $a = b = c$  as for a cubical box

$$E_{n_x n_y n_z} = \frac{h^2}{8ma^2} [n_x^2 + n_y^2 + n_z^2]$$

→ (1)

Normalised wave function of an electron in a cubical box

$$\psi_{n_x n_y n_z} = \sqrt{\frac{2}{a} \times \frac{2}{a} \times \frac{2}{a}} \sin \frac{n_x \pi x}{a}$$

$$\sin \frac{n_y \pi y}{a} \sin \frac{n_z \pi z}{a}$$

$$\psi_{n_x n_y n_z} = \sqrt{\frac{8}{a^3}} \sin \frac{n_x \pi x}{a}$$

$$\sin \frac{n_y \pi y}{a} \sin \frac{n_z \pi z}{a}$$

→ (2)

From the eqns (1) & (2)

Several combinations of the three quantum numbers ( $n_x, n_y$  and  $n_z$ ) lead to different energy eigen values and eigen functions.

Example

$$n_x = 1, n_y = 1, n_z = 2$$

$$n_x^2 + n_y^2 + n_z^2 = 6$$

$$n_x = 1, \quad n_y = 2, \quad n_z = 1$$

$$n_x = 2, \quad n_y = 1, \quad n_z = 1$$

$$n_x^2 + n_y^2 + n_z^2 = 6$$

$$\therefore E_{112} = E_{121} = E_{211} = \frac{6h^2}{8ma^2}$$

→ (3)

The corresponding wave functions are written as

$$\psi_{112} = \sqrt{\frac{8}{a^3}} \sin \frac{\pi x}{a} \sin \frac{\pi y}{a} \sin \frac{2\pi z}{a}$$

$$\psi_{121} = \sqrt{\frac{8}{a^3}} \sin \frac{\pi x}{a} \sin \frac{2\pi y}{a} \sin \frac{\pi z}{a}$$

$$\psi_{211} = \sqrt{\frac{8}{a^3}} \sin \frac{2\pi x}{a} \sin \frac{\pi y}{a} \sin \frac{\pi z}{a}$$

$$\sin \frac{\pi z}{a}$$

### Write notes in Tunneling

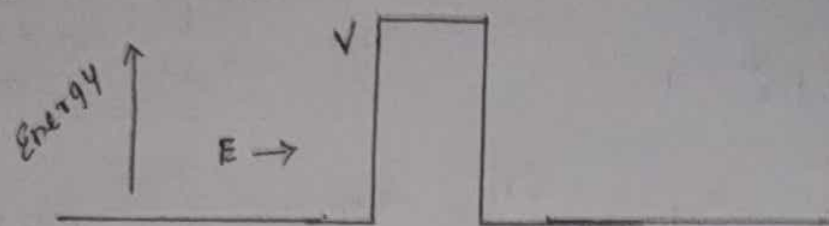
- According to classical ideas, a particle striking a hard wall has no chance of leaking through it.
- The behaviour of a quantum particle is different due to the wave nature associated with it.
- When an electromagnetic wave strikes at the interface of two media, it is partly reflected and partly transmitted through the interface and enters the second medium.
- De Broglie wave also has a possibility of getting partly reflected from the boundary of the potential well and partly

penetrating through the barrier.

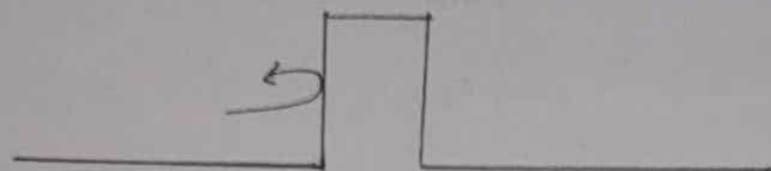
- $E < V$  approaching potential barrier of height  $V$ .
- From classical physics electron would be reflected from the barrier because its energy  $E$  is less than  $V$ .
- For the particle to overcome the potential barrier, it must have an energy equal to or greater than  $V$ .
- Quantum mechanics leads to an entirely new result. It shows that there is a finite chance for the electron

to leak to the other side of the barrier.

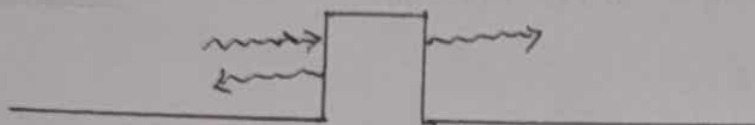
The transmission of electrons through the barrier known as barrier penetration.



a)  $E < V$



b) Particle not reflected by barrier



c) Probability of Penetrating & tunneling.

Q Derive an expression for effective mass

Effective mass of electron

The mass acquired by an electron when it is accelerated in a periodic potential is called effective mass of an electron. It is denoted by  $m^*$ .

Derivation

According to wave mechanics, a particle moving with a velocity  $v$  is equivalent to a wave packet moving with a

group velocity  $v_g$ .

$$v_g = \frac{d\omega}{dk} \rightarrow (1)$$

$\omega$  - angular frequency of the electron

$k \rightarrow$  wave vector

$$E = h\nu$$

$$E = \frac{h\omega}{2\pi}$$

$$E = \hbar\omega$$

$$\omega = \frac{E}{\hbar} \rightarrow (2)$$

Substituting (2) in (1)

$$\left[ \begin{aligned} \therefore \omega &= 2\pi\nu \\ \nu &= \frac{\omega}{2\pi} \\ \hbar &= h/2\pi \end{aligned} \right]$$



$$\vec{v}_g = \frac{d}{dk} \left( \frac{E}{\hbar} \right)$$

$$v_g = \frac{1}{\hbar} \frac{dE}{dk} \rightarrow (3)$$

The acceleration 'a' experienced by the electron is given by

$$a = \frac{d(v_g)}{dt}$$

$$= \frac{d}{dt} \left[ \frac{1}{\hbar} \left( \frac{dE}{dk} \right) \right]$$

$$= \frac{1}{\hbar} \frac{d^2E}{dk^2} \cdot \frac{dk}{dt} \rightarrow (4)$$

Momentum (P) of an electron inside the crystal.

$$P = \hbar / \lambda \quad [\text{from De-broglie's eqn}]$$

$$= \frac{\hbar}{2\pi} \frac{2\pi}{\lambda}$$

$$= \hbar k \rightarrow (5) \quad \left[ k = \frac{2\pi}{\lambda} \right]$$

Differentiating the eqn (5) with respect to 't'

$$\frac{dP}{dt} = \hbar \frac{dk}{dt} \quad \left( F = \frac{dP}{dt} \right)$$

$$\text{(or)} \quad F = \hbar \frac{dk}{dt}$$

$$\text{(or)} \quad \frac{dk}{dt} = \frac{F}{\hbar} \rightarrow (6)$$

Substituting eqn (6) in (4)

$$a = \frac{1}{\hbar} \frac{d^2E}{dk^2} \cdot \frac{F}{\hbar}$$

$$= \frac{1}{\hbar^2} \frac{d^2E}{dk^2} \cdot F$$

$$\text{(or)} \quad F = \left[ \frac{\hbar^2}{\left( \frac{d^2E}{dk^2} \right)} \right] a \rightarrow (7)$$

$$a = \frac{eE}{m^*} = \frac{F}{m^*}$$

$$F = m^* a$$

$$(\because F = eE)$$

Comparing eqns (7) and (8)

$$m^* a = \left[ \frac{\hbar^2}{\left( \frac{d^2E}{dk^2} \right)} \right] a$$

$$m^* = \frac{\hbar^2}{\left( \frac{d^2E}{dk^2} \right)}$$

Special cases

Case (i) If  $\frac{d^2E}{dk^2}$  is positive,

then  $m^*$  is also positive

Case (ii) If  $\frac{d^2E}{dk^2}$  is negative

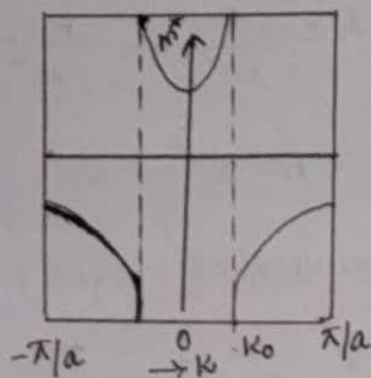
then  $m^*$  is also negative

Case (iii) If  $\frac{d^2E}{dk^2}$  is more,

then the electrons behave as light particle

Case (iv) If  $\frac{d^2E}{dk^2}$  is very small then the electrons behave as heavy particle.

Variation of  $m^*$  with  $k$



Near,  $k=0$  the mass approaches  $m$ .

As the value of  $k$  increases  $m^*$  increases reaching its maximum value at the point of inflection on the  $E-k$  curve.

Above the point of inflection  $m^*$  is negative and  $k$  tends to  $\pi/a$ , it decreases to a small negative value.

① Explain dia, para, ferro magnetic effect

### Diamagnetic Effect

Diamagnetism is exhibited by all the materials.

- The atoms in diamagnetic materials do not possess permanent magnetic moments.
- When the diamagnetic material is placed in an external magnetic field, the electrons in the atomic orbits tend to counteract the external magnetic field. the atoms acquire an induced magnetic moment.

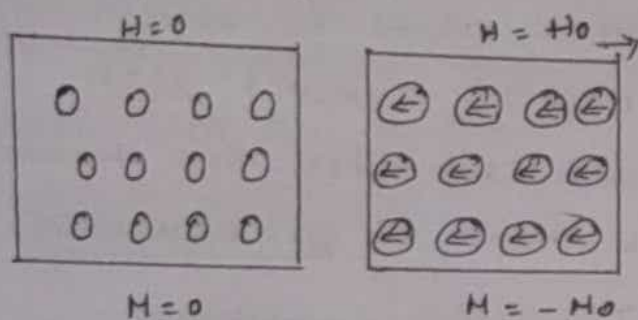
• As a result, the material becomes magnetised.

• The direction of the induced dipole moment is opposite to that of externally applied magnetic field.

Due to this effect, the material is very weakly repelled in magnetic field. This phenomenon is known as diamagnetism.

When the magnetic field  $H$  is zero, the atoms possess zero magnetic moment.

When a magnetic field  $H_0$  is applied in the direction, the atoms acquire an induced magnetic moment in the direction opposite to that of the magnetic field.



- The susceptibility of the diamagnetic material is negative
- Weakly repelled in the magnetic field.

#### Diamagnetic materials:

The materials which exhibit diamagnetism are called diamagnetic materials.

#### Properties

- repel the magnetic lines of force.
- No permanent dipole moment.
- Magnetic susceptibility is negative

Example: Gold, germanium, Silicon

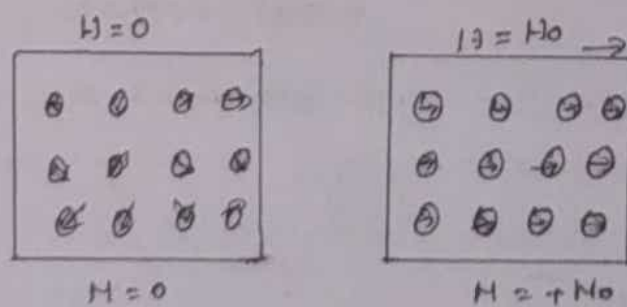
#### 1) Paramagnetic Effect

In certain materials, each atom or molecule possesses a net permanent magnetic moment even in the absence of an external magnetic field.

• The magnetic moments are randomly oriented in the absence of the external magnetic field.

• Net magnetic moment zero and magnetisation of the material is zero.

• When external magnetic field is applied the magnetic dipoles tend to align themselves in the direction of the magnetic field. Material becomes magnetized. This effect is known as paramagnetism.



• Paramagnetic susceptibility varies inversely with temperature

$$\chi \propto 1/T$$



$$\chi = C/T$$

This is known as Curie's law of paramagnetism.

### Paramagnetic materials

The magnetic materials which exhibit paramagnetism are called as paramagnetic material.

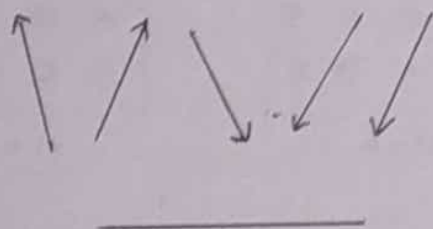
#### Properties

- i) Paramagnetic materials attract the magnetic lines of force.
- ii) They possess permanent dipole moment.
- iii) Value of susceptibility is positive.

$$\chi = \frac{C}{T - \theta}$$

Example: Ferric oxide, nickel sulphate

iv) The spin alignment is



### iii) Ferromagnetic Effect

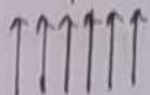
Certain metals like Iron (Fe), Cobalt (Co), Nickel (Ni) and certain alloys exhibit high degree of magnetisation. These materials show the spontaneous magnetization. There is a strong internal field within the material which makes the atomic magnetic moments align with each other. This phenomenon is known as ferromagnetism.

### Ferromagnetic materials

The materials which exhibit the ferromagnetism are called ferromagnetic materials.

#### Properties

- All the dipoles are aligned parallel to each other due to the magnetic interaction between the dipoles.
- Permanent dipole moment.
- Exhibit hysteresis.
- On heating lose their magnetisation slowly.
- The dipole alignment is



$$\chi = \frac{C}{T - \theta}, \quad C = \text{Curie Constant}$$

$\theta = \text{ferromagnetic Curie temperature}$

# plain paramagnetism in the conduction electrons in metals

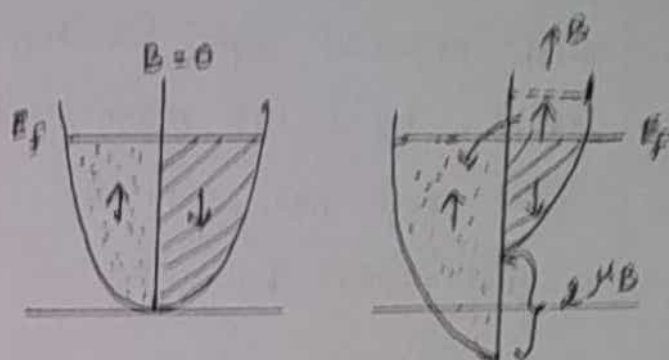
## paramagnetism of free electrons

• According to Langevin's theory the paramagnetic susceptibility is inversely proportional to the temperature.

• Curve may be split into two parts with spins pointing in the +ve z direction and other with spin in the opposite direction.

• In the absence of an external magnetic field, the distribution of electrons with spins parallel to z-direction is equal to the number of electrons with opposite spins and hence the net magnetic moment of the electron gas is zero.

• When a magnetic field ( $B$ ) is applied along the z-direction, the energy of the spins aligned parallel to  $B$  is lowered by the amount  $\mu_B$ , while the energy of the spins opposite to  $B$  is raised by the same amount.



• Fermi level for the two spins distributions shift with respect to each other and give rise to energetically unstable situation.

• The number of electrons which effectively change their direction is equal to the density of states at the energy level ( $Z(E_F)$ ) in one of the spin distribution times the change in energy

$$N_{eff} = \frac{1}{2} Z(E_F) \mu_B B \rightarrow (1)$$

where the factor  $\frac{1}{2}$  is due to the fact the density of states of one spin distribution is half of the total density of states.

•  $\mu_B$  is magnetic moment of electron.

- Number of electrons with spins parallel to the field is greater than the electrons with opposite spin by  $N_{\text{eff}}$  leading to a net magnetization.

- Each flip increases the magnetization by  $2\mu_B$

The net magnetization is given by

$$M \approx N_{\text{eff}} \times 2\mu_B = Z(E_F) \mu_B^2 B \quad \rightarrow (2)$$

Pauli spin susceptibility of the electron gas

$$\chi_p = \mu_0 \mu_B^2 Z(E_F) \quad \rightarrow (3)$$

According to eqn (3),  $\chi_p$  is essentially temperature independent.

$$Z(E_F) = \frac{3N}{2E_F}$$

$N$  - No of electrons per unit Volume

eqn (2) becomes

$$\chi_p = \frac{3\mu_0 N \mu_B^2}{2E_F} = \frac{3\mu_0 N \mu_B^2}{2kT_F}$$

$$E_F = kT_F$$

Eqn can be rewritten in terms of classical susceptibility

$$\chi_p = \frac{3}{2} \chi \frac{T}{T_F} \quad \rightarrow (5)$$

$$\chi = \frac{\mu_0 N \mu_B^2}{kT}$$

### 13) Discuss quantum interference devices

#### SQUID

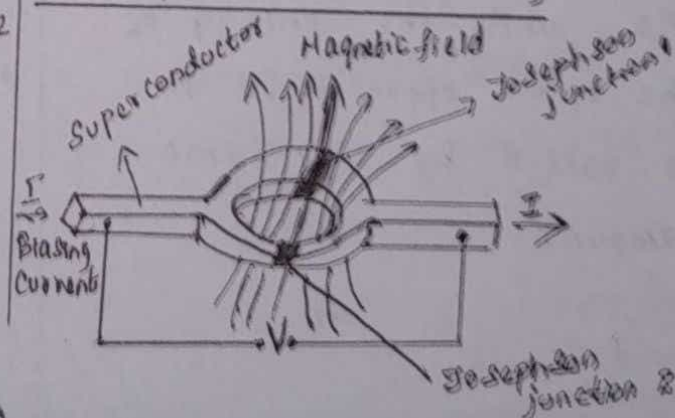
- SQUID stands for Superconducting Quantum Interference Device.

- An ultra-sensitive instrument used to measure very weak magnetic field of the order of  $10^{-14}$ .

#### Principle

Small change in magnetic field produces variation in the quantum flux.

#### Description and Working





SQUID consists of a superconducting ring which can have magnetic fields of quantum values of flux placed in between two Josephson junctions.

- When the magnetic field is applied perpendicular to the plane of the ring, the current is induced at the two Josephson junctions.

- Currents produce interference pattern and it flows around the ring.

- Magnetic flux in the ring can have the quantum value of magnetic field applied.

### Application

i) SQUID can be used to detect the variation of very minute magnetic signals in terms of quantum flux.

ii) It can also be used as storage device for magnetic flux.

iii) SQUID is useful in the study of earth quakes, removing paramagnetic impurities, brain, heart, etc.

### Q. Describe working of magnetic hard disc based on GMR

#### Sensor

#### Definition : (GMR)

The effect is observed as a significant change in the electrical resistance depending on whether the magnetization of adjacent ferromagnetic layers are in a parallel or an anti parallel alignment.

Two geometries are commonly used in GMR

a) Current in plane (CIP) of layers

b) Current perpendicular to plane (CPP) of layers.

- A device that works on the principle of the GMR is a Spin valve.

- Device is used in magnetic hard discs for high density data storage.
- There are 4 layers altogether in a Spin valve.
- Two ferromagnetic layers are separated by a thin spacer layer.
- One ferromagnetic layer is pinned of magnetization is fixed.
- Adding a fourth layer.
- Other layer called free layer.
- Permalloy (Ni and Fe) is usually chosen for both ferromagnetic layers. This structure is called the Spin valve.
- As the bit travels under the head, the resistance goes down, the electrons do not scatter very much and the current flow increases.
- As the bit moves on, the resistance increases, electrons are scattered, current decreases.
- As the bit travels further from the head, the resistance peaks and the current decreases to its lowest point.
- As the resistance change large, small data bits can generate quite large resistance changes, increasing the capacity to store data bits in the hard disc.

### Q Explain about Exchange interaction and Ferromagnetism.

- Ferromagnetic Property exhibited by transition elements such as iron, cobalt and nickel at room temperature and earth elements like gadolinium and dysprosium.
- Alignment of dipoles
- Parallel alignment of dipoles not due to the magnetic force existing between any two dipoles.
- Reason, Magnetic potential energy is very small and smaller than thermal energy.

Under the Pauli's exclusion principle and electrostatic interaction energy are combined together and constitute a new kind of interaction known as exchange interaction.

• The exchange interaction is a quantum mechanical concept.

• The exchange interaction between any two atoms

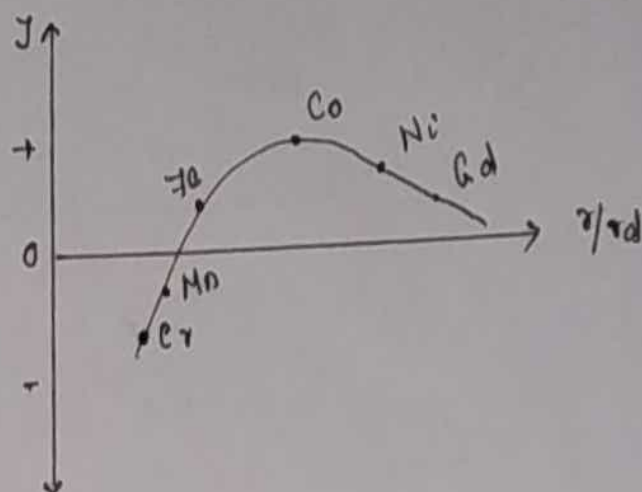
$$E_{ex} = -J_e g_1 g_2$$

where

$J_e$  - Numerical value of exchange integral

$g_1, g_2$  - Spin angular momenta

• The exchange energy value is negative



• Iron, Cobalt, nickel the exchange integral value is positive.

A plot between the exchange integral and the ratio of the interatomic separation to the radius of 3d orbital ( $r/r_d$ )



SEMICONDUCTORS AND TRANSPORT PHYSICS

Intrinsic Semiconductors - Energy band diagram - direct and indirect band gap semiconductors - Carrier concentration in intrinsic Semiconductors - extrinsic Semiconductors - Carrier Concentration in N-type & P-type Semiconductors - Variation of carrier Concentration with temperature - Carrier transport in Semiconductors : Drift, mobility and diffusion - Hall effect and devices - ohmic Contacts - Schottky diode.

- ① Derive an expression for the density of electrons in an intrinsic semiconductor.

Density of Electrons in conduction Band (Derivation)

The number of electrons per unit volume in conduction band for energy between  $E$  and  $E+dE$  is given by

$$dn = Z(E) F(E) dE \quad \rightarrow (1)$$

where

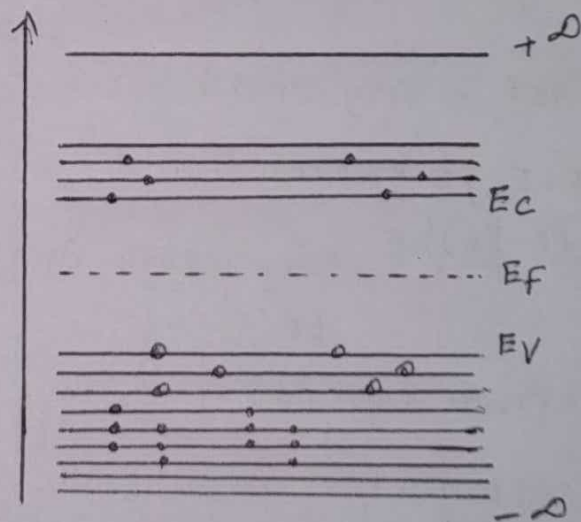
$Z(E)$  - Density of states in energy between  $E$  and  $E+dE$ .

$F(E)$  - Probability of electron occupancy.

Integrating eqn(1) between energy  $E_c$  and  $+\infty$ .

$$\int dn = n = \int_{E_c}^{+\infty} Z(E) F(E) dE \quad \rightarrow (2)$$

$E_c$  - bottom most level  
 $+\infty$  - upper most level in conduction band



Density of states in conduction band between the energy range  $E$  and  $E+dE$  is given by

$$Z(E) dE = \frac{4\pi}{h^3} (2m_e^*)^{3/2} E^{1/2} dE \quad \rightarrow (3)$$

Eqn (3) is replaced as  $(E - E_c)$

$$Z(E) dE = \frac{4\pi}{h^3} (2m_e^*)^{3/2} (E - E_c)^{1/2} dE \rightarrow (4)$$

The probability of electron occupation is given by Fermi distribution function

$$F(E) = \frac{1}{1 + e^{(E - E_f)/kT}} \rightarrow (5)$$

Substituting eqns (4) and (5) in

$$n = \int_{E_c}^{+\infty} \frac{4\pi}{h^3} (2m_e^*)^{3/2} (E - E_c)^{1/2} \times \frac{1}{1 + e^{(E - E_f)/kT}} dE$$

$$n = \frac{4\pi}{h^3} (2m_e^*)^{3/2} \int_{E_c}^{+\infty} \frac{(E - E_c)^{1/2}}{1 + e^{(E - E_f)/kT}} dE \rightarrow (6)$$

$kT$  - very small

$(E - E_f)$  is greater than  $kT$

$e^{(E - E_f)/kT}$  - very large compared to '1'.

From eqn (6) 1 from

denominator neglected.

$$1 + e^{(E - E_f)/kT} \approx e^{(E - E_f)/kT}$$

Now eqn (6) becomes

$$n = \frac{4\pi}{h^3} (2m_e^*)^{3/2} \int_{E_c}^{+\infty} \frac{(E - E_c)^{1/2}}{e^{(E - E_f)/kT}} dE$$

$$n = \frac{4\pi}{h^3} (2m_e^*)^{3/2} \int_{E_c}^{+\infty} (E - E_c)^{1/2} e^{-(E - E_f)/kT} dE$$

$$e^{-(E - E_f)/kT} dE$$

$$n = \frac{4\pi}{h^3} (2m_e^*)^{3/2} \int_{E_c}^{+\infty} (E - E_c)^{1/2} e^{-(E - E_f)/kT} dE$$

$$e^{(E_f - E)/kT} dE$$

$$n = \frac{4\pi}{h^3} (2m_e^*)^{3/2} e^{E_f/kT} \int_{E_c}^{+\infty} (E - E_c)^{1/2} e^{-E/kT} dE$$

$$\int_{E_c}^{+\infty} (E - E_c)^{1/2} e^{-E/kT} dE \rightarrow (7)$$

eqn (7) be changes as

$$n = \frac{4\pi}{h^3} (2m_e^*)^{3/2} e^{E_f/kT} \int_{E_c}^{+\infty} (E - E_c)^{1/2} e^{-(E - E_c)/kT} dE$$

$$n = \frac{4\pi}{h^3} (2m_e^*)^{3/2} e^{(E_f - E_c)/kT} \int_{E_c}^{+\infty} (E - E_c)^{1/2} e^{-x/kT} dx$$

$$\int_0^{\infty} x^{1/2} e^{-x/kT} dx \rightarrow (8)$$

using gamma function

$$\int_0^{\infty} x^{1/2} e^{-x/kT} dx = \frac{(kT)^{3/2} \pi^{1/2}}{2} \rightarrow (9)$$

Substituting eqn (9) in eqn (8)

$$n = \frac{4\pi}{h^3} (2m_e^*)^{3/2} e^{(E_f - E_c)/kT}$$

$$\left[ \frac{(kT)^{3/2} \pi^{1/2}}{2} \right]$$

$$n = \frac{2\pi}{h^3} (2m_e^*)^{3/2} (kT)^{3/2} \pi^{1/2} e^{(E_f - E_c)/kT}$$

$$n = \frac{2\pi \pi^{1/2} (2m_e^*)^{3/2} (kT)^{3/2}}{(h^3)^{3/2}} e^{(E_f - E_c)/kT}$$

$$n = 2 \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2} e^{(E_f - E_c)/kT}$$

② Derive an expression for the density of holes in an intrinsic semiconductor

• Electron is transferred from valence band to conduction band, a hole is created in valence band.

• Let  $dp$  be the number of holes per unit volume in valence band between the energy  $E$  and  $E + dE$

$$dp = Z(E) (1 - F(E)) dE$$

→ (1)

$Z(E) dE$  - Density of states in the energy range  $E$  and  $E + dE$ .

$F(E)$  - Probability of electron occupation

$1 - F(E)$  - Probability of an unoccupied electron state.

$$1 - F(E) = 1 - \frac{1}{1 + e^{(E - E_f)/kT}}$$

$$= \frac{1 + e^{(E - E_f)/kT} - 1}{1 + e^{(E - E_f)/kT}}$$

$$1 - F(E) = \frac{e^{(E - E_f)/kT}}{1 + e^{(E - E_f)/kT}}$$

→ (2)

$E$  - very small compared to  $E_f$

$(E - E_f)$  - negative quantity

$e^{(E - E_f)/kT}$  - very small and

it is neglected in the denominator term of eqn (2)

$$1 + e^{(E - E_f)/kT} \approx 1$$

$$\therefore 1 - F(E) = e^{(E - E_f)/kT}$$

③

→ (3)



Density of states in valence band

$$Z(E)dE = \frac{4\pi}{h^3} (2m_h^*)^{3/2} E^{1/2} dE \quad \rightarrow (4)$$

$m_h^*$  - effective mass of the hole in valence band.

$E_v$  = top energy level in valence band

$E_v - E$  = kinetic energy of the hole at level below  $E_v$

So  $E$  is replaced by the above eqn (4) as  $(E_v - E)$

$$Z(E)dE = \frac{4\pi}{h^3} (2m_h^*)^{3/2} (E_v - E)^{1/2} dE \quad \rightarrow (5)$$

Substituting eqn (5) and (6) in (1)

$$dp = \frac{4\pi}{h^3} (2m_h^*)^{3/2} (E_v - E)^{1/2} e^{(E - E_F)/kT} \cdot dE \quad \rightarrow (6)$$

By integrating eqn (6) between the limits  $-\infty$  to  $E_v$

$$\int dp = p = \int_{-\infty}^{E_v} \frac{4\pi}{h^3} (2m_h^*)^{3/2} (E_v - E)^{1/2} e^{(E - E_F)/kT} \cdot dE$$

$$p = \frac{4\pi}{h^3} (2m_h^*)^{3/2} e^{(E_F/kT)} \int_{-\infty}^{E_v} (E_v - E)^{1/2} e^{E/kT} \cdot dE$$

on eqn (7)

$$p = \frac{4\pi}{h^3} (2m_h^*)^{3/2} e^{(-E_F/kT)} \int_{-\infty}^0 x^{1/2} e^{(E_v - x)/kT} (-dx) \quad \rightarrow (8)$$

$$p = \frac{4\pi}{h^3} (2m_h^*)^{3/2} e^{(E_v - E_F)/kT} \int_0^{\infty} x^{1/2} e^{-x/kT} dx \quad \rightarrow (9)$$

(-ve sign is omitted by interchanging the limits)

using the gamma function

$$\int_0^{\infty} x^{1/2} e^{-x/kT} dx = \frac{(kT)^{3/2} \pi^{1/2}}{2} \quad \rightarrow (10)$$

Substituting eqn (10) in eqn (9)

$$p = \frac{4\pi}{h^3} (2m_h^*)^{3/2} e^{(E_v - E_F)/kT} \left[ \frac{(kT)^{3/2} \pi^{1/2}}{2} \right]$$

$$p = \frac{2\pi}{h^3} (2m_h^*)^{3/2} (kT)^{3/2} \pi^{1/2} e^{(E_v - E_F)/kT}$$

$$p = 2\pi \pi^{1/2} (2m_h^*)^{3/2} (kT)^{3/2} e^{(E_v - E_F)/kT}$$

$$(h^2)^{3/2}$$

$$p = 2 \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2} e^{(E_v - E_F)/kT}$$

3) Deduce the expression for intrinsic carrier concentration and write its limitations.

• Number of electrons in conduction band is equal to the number of holes in valence band.

• Intrinsic carrier concentration  $n_i$  is equal to electrons concentration in conduction band ( $n$ ) or holes concentration in valence band ( $p$ ).

$$n_i = n = p \rightarrow (1)$$

$$n_i \times n_i = n_i^2 = np \rightarrow (2)$$

Substituting the expressions of  $n$  and  $p$  in eqn (2)

$$n_i^2 = 2 \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2} e^{(E_F - E_C)/kT} \times$$

$$2 \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2} e^{(E_V - E_F)/kT}$$

$$n_i^2 = 4 \left( \frac{2\pi kT}{h^2} \right)^3 (m_e^* m_h^*)^{3/2} e^{(E_V - E_C)/kT}$$

$$n_i^2 = 4 \left( \frac{2\pi kT}{h^2} \right)^3 (m_e^* m_h^*)^{3/2} e^{-E_g/kT}$$

$\rightarrow (3)$

$E_C - E_V = E_g$  = forbidden energy gap

Taking square root on both sides eqn (3)

$$(n_i^2)^{1/2} = \left( 4 \left( \frac{2\pi kT}{h^2} \right)^3 (m_e^* m_h^*)^{3/2} e^{-E_g/kT} \right)^{1/2}$$

$$n_i = 4^{1/2} \left[ \left( \frac{2\pi kT}{h^2} \right)^{3/2} (m_e^* m_h^*)^{3/4} e^{-E_g/2kT} \right]$$

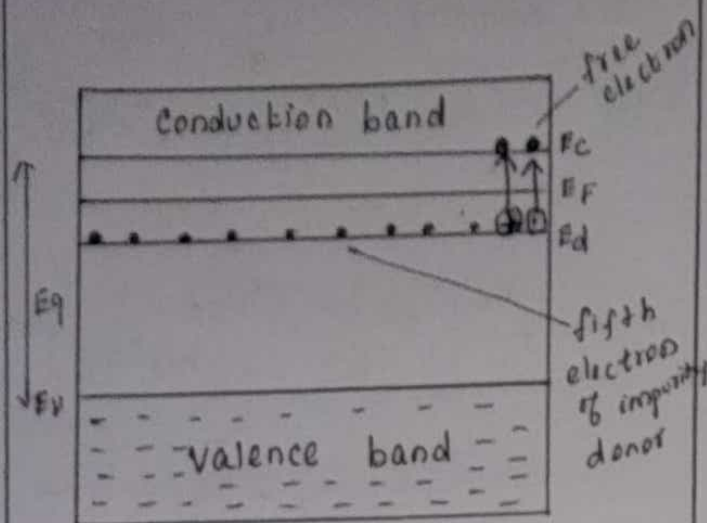
$$n_i = 2 \left( \frac{2\pi kT}{h^2} \right)^{3/2} (m_e^* m_h^*)^{3/4} e^{-E_g/2kT}$$

The above eqn is the intrinsic carrier concentration.

Limitations.

- Electrical conductivity is low.
- Germanium has a conductivity of  $1.67 \Omega^{-1}m^{-1}$  which is nearly  $10^7$  times smaller than that of copper.
- Electrical conductivity is a function of temperatures and increases exponentially as temperature increases.

④ obtain an expression for carrier concentration in n-type Semiconductors [Derivation]



• In n-type Semiconductor, the donor level is just below conduction band.

Density of electrons per unit volume in conduction band is given by

$$n = 2 \left[ \frac{2\pi m_e^* kT}{h^2} \right]^{3/2} e^{(E_F - E_c)/kT} \quad \rightarrow (1)$$

$E_c$  - Energy corresponding to the bottom most level of conduction band.

Density of ionised donors =

$$N_d [1 - F(E_d)]$$

$F(E_d)$  - Probability for finding electron in donor energy level

$1 - F(E_d)$  - Probability for finding ionised donors.

$E_d$  - donor energy level

$N_d$  - donor concentration

The number of donor atoms per unit volume of the material

$$= N_d \left[ 1 - \frac{1}{1 + e^{(E_d - E_F)/kT}} \right]$$

$$= N_d \left[ \frac{1 + e^{(E_d - E_F)/kT} - 1}{1 + e^{(E_d - E_F)/kT}} \right] \quad \rightarrow (2)$$

$$= N_d \frac{e^{(E_d - E_F)/kT}}{1 + e^{(E_d - E_F)/kT}} \quad \rightarrow (3)$$

$e^{(E_d - E_F)/kT}$  is very small

in eqn (3) when compared to

Hence it is neglected

$$1 + e^{(E_d - E_F)/kT} \approx 1$$

Density of ionised donor =

$$N_d e^{(E_d - E_F)/kT} \quad \rightarrow (4)$$

Equating (1) & (4)

$$2 \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2} e^{(E_F - E_c)/kT} = N_d e^{(E_d - E_F)/kT}$$

$\rightarrow (5)$



rearranging the terms

$$\frac{e^{(E_F - E_C)/KT}}{e^{(E_D - E_F)/KT}} = \frac{N_d}{2 \left[ \frac{2\pi m_e^* KT}{h^2} \right]^{3/2}}$$

$$\frac{e^{(E_F - E_C)/KT}}{e^{-(E_D - E_F)/KT}} = \frac{N_d}{2 \left[ \frac{2\pi m_e^* KT}{h^2} \right]^{3/2}} \quad (6)$$

$$e^{(E_F - E_C - E_D + E_F)/KT} = \frac{N_d}{2 \left[ \frac{2\pi m_e^* KT}{h^2} \right]^{3/2}} \quad \rightarrow (6)$$

taking log on both sides

$$\log_e e^{(E_F - E_C - E_D + E_F)/KT} =$$

$$\log_e \left[ \frac{N_d}{2 \left[ \frac{2\pi m_e^* KT}{h^2} \right]^{3/2}} \right]$$

$$\frac{E_F - E_C - E_D + E_F}{KT} = \log_e \left[ \frac{N_d}{2 \left[ \frac{2\pi m_e^* KT}{h^2} \right]^{3/2}} \right] \quad (7)$$

$$(\because \log_e e^x = x)$$

$$2E_F - (E_C + E_D) = KT \log_e$$

$$\left[ \frac{N_d}{2 \left[ \frac{2\pi m_e^* KT}{h^2} \right]^{3/2}} \right]$$

(or)

$$2E_F = E_D + E_C + KT \log_e$$

$$\left[ \frac{N_d}{2 \left[ \frac{2\pi m_e^* KT}{h^2} \right]^{3/2}} \right]$$

$$E_F = \frac{E_D + E_C}{2} + \frac{KT}{2} \log_e$$

$$\left[ \frac{N_d}{2 \left[ \frac{2\pi m_e^* KT}{h^2} \right]^{3/2}} \right]$$

$\rightarrow (7)$

substituting the expression of  $E_F$  from (7) in (1)

$$n = 2 \left[ \frac{2\pi m_e^* KT}{h^2} \right]^{3/2} \exp$$

$$\left[ \frac{E_D + E_C}{2} + \frac{KT}{2} \log_e \left[ \frac{N_d}{2 \left[ \frac{2\pi m_e^* KT}{h^2} \right]^{3/2}} \right] \right]$$

$$n = 2 \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2} \exp \left[ \frac{E_d + E_c - 2E_c}{2kT} + \frac{1}{2} \log_e \left\{ \frac{N_d}{2 \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2}} \right\} \right]$$

$$n = 2 \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2} \exp \left[ \frac{E_d - E_c}{2kT} + \log_e \left\{ \frac{N_d^{1/2}}{2 \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2}} \right\}^{1/2} \right]$$

$$n = 2 \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2} e^{E_d - E_c / 2kT} e \log_e \left\{ \frac{N_d^{1/2}}{2 \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2}} \right\}^{1/2}$$

$$n = 2 \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2} e^{(E_d - E_c) / 2kT}$$

$$\left( \frac{N_d^{1/2}}{2^{1/2} \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/4}} \right)^{1/2}$$

Rearranging the eqn (9)

$$n = 2 \frac{N_d^{1/2}}{2^{1/2}} \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2} e^{(E_d - E_c) / 2kT}$$

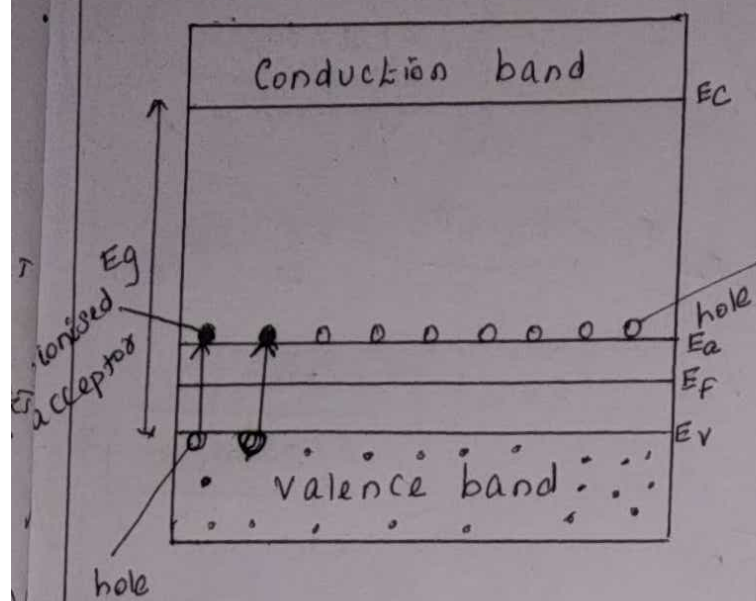
$$n = 2^{1/2} \times 2^{1/2} \frac{N_d^{1/2}}{2^{1/2}} \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2} \left( \frac{2\pi m_e^* kT}{h^2} \right)^{-3/4} e^{(E_d - E_c) / 2kT}$$

$$n = 2^{1/2} N_d^{1/2} \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/4} e^{(E_d - E_c) / 2kT}$$

$$n = (2 N_d)^{1/2} \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/4} e^{(E_d - E_c) / 2kT}$$

$\Delta E = E_c - E_d$ , ionisation energy of the donor

3/2) obtain an expression for concentration of Holes in valence band of p-type semiconductors (Derivation)



In p-type semiconductor, acceptor energy level is just above valence band.

Density of holes per unit Volume in valence band is given by

$$P = 2 \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2} e^{(E_v - E_f)/kT} \quad \rightarrow (1)$$

$E_v \rightarrow$  Energy corresponding to top most level of valence band.

Density of ionised acceptors  
 $= N_a F(E_a)$   $\rightarrow (2)$

$N_a$  - number of acceptor atoms per unit volume

$$F(E_a) = \frac{1}{1 + e^{(E_a - E_f)/kT}}$$

$E_a$  - acceptor energy level  
 $F(E_a)$  - Probability for finding electron in acceptor energy level.

The eqn (1) becomes, density of ionised acceptors =  $\frac{N_a}{1 + e^{(E_a - E_f)/kT}}$   $\rightarrow (2)$

$e^{(E_a - E_f)/kT}$  is a large quantity and thus '1' from the denominator of R.H.S of eqn (2) is neglected.

the eqn (2) is modified as

$$N_a F(E_a) = \frac{N_a}{e^{(E_a - E_f)/kT}}$$

$$N_a F(E_a) = N_a e^{-(E_a - E_f)/kT} \quad \rightarrow (3)$$

Density of ionised acceptors  
 $= N_a e^{(E_f - E_a)/kT}$

At equilibrium,

$$\left( \text{Density of holes in valence band} \right) = \left( \text{Density of ionised acceptors} \right)$$

$$2 \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2} e^{(E_v - E_f)/kT} = N_a e^{(E_f - E_a)/kT} \quad \rightarrow (4)$$



rearranging eqn (4)

$$\frac{e^{(E_V - E_F)/KT}}{e^{(E_F - E_A)/KT}} = \frac{N_A}{2 \left( \frac{2\pi m_h^* KT}{h^2} \right)^{3/2}}$$

$$\frac{e^{(E_V - E_F)/KT}}{e^{-(E_F - E_A)/KT}} = \frac{N_A}{2 \left( \frac{2\pi m_h^* KT}{h^2} \right)^{3/2}}$$

$$e^{(E_V - E_F - E_F + E_A)/KT} = \frac{N_A}{2 \left( \frac{2\pi m_h^* KT}{h^2} \right)^{3/2}} \quad \rightarrow (5)$$

Taking log on both sides in eqn (5)

$$\log_e e^{(E_V - E_F - E_F + E_A)/KT} = \frac{N_A}{2 \left( \frac{2\pi m_h^* KT}{h^2} \right)^{3/2}}$$

$$\frac{E_V - 2E_F + E_A}{KT} = \log_e \left[ \frac{N_A}{2 \left( \frac{2\pi m_h^* KT}{h^2} \right)^{3/2}} \right]$$

$$E_A + E_V - 2E_F = KT \log_e \left[ \frac{N_A}{2 \left( \frac{2\pi m_h^* KT}{h^2} \right)^{3/2}} \right]$$

Rearranging

$$2E_F = E_A + E_V - KT \log_e$$

$$\left[ \frac{N_A}{2 \left( \frac{2\pi m_h^* KT}{h^2} \right)^{3/2}} \right]$$

$$E_F = \frac{E_A + E_V}{2} - \frac{KT}{2} \log_e$$

$$\left[ \frac{N_A}{2 \left( \frac{2\pi m_h^* KT}{h^2} \right)^{3/2}} \right]$$

Substituting eqn of  $E_F$  from (7) in (1)

$$p = 2 \left( \frac{2\pi m_h^* KT}{h^2} \right)^{3/2} \exp$$

$$\left[ \frac{E_V - \left( \frac{E_A + E_V}{2} \right) - \frac{KT}{2} \log_e \left[ \frac{N_A}{2 \left( \frac{2\pi m_h^* KT}{h^2} \right)^{3/2}} \right]}{KT} \right]$$

$$p = 2 \left( \frac{2\pi m_h^* KT}{h^2} \right)^{3/2} \exp \left[ \frac{2E_V - E_A}{2KT} \right] + \frac{1}{2} \log_e \left( \frac{N_A}{2 \left( \frac{2\pi m_h^* KT}{h^2} \right)^{3/2}} \right)$$

$$P = 2 \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2} \exp \left[ \frac{E_v - E_a}{2kT} + \log_e \left[ \frac{\left( \frac{N_a}{2} \right)^{1/2}}{\left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2}} \right] \right]$$

$$P = 2 \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2} \exp \left[ \frac{E_v - E_a}{2kT} + \log_e \left( \frac{\left( \frac{N_a}{2} \right)^{1/2}}{\left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2}} \right) \right]$$

$$\log_e \left( \frac{\left( \frac{N_a}{2} \right)^{1/2}}{\left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2}} \right)$$

$$P = 2 \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2} e^{(E_v - E_a)/2kT}$$

$$e^{\log_e \left[ \frac{\left( \frac{N_a}{2} \right)^{1/2}}{\left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/4}} \right]}$$

$$P = 2 \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2} e^{(E_v - E_a)/2kT}$$

$$\frac{\left( \frac{N_a}{2} \right)^{1/2}}{\left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/4}}$$

$$P = 2 \frac{N_a^{1/2}}{2^{1/2}} \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2} e^{(E_v - E_a)/2kT}$$

$$P = 2^{1/2} 2^{1/2} N_a^{1/2} \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2} \frac{1}{2^{1/2}}$$

$$\left( \frac{2\pi m_h^* kT}{h^2} \right)^{-3/4} e^{(E_v - E_a)/2kT}$$

$$P = (2N_a)^{1/2} \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/4} e^{(E_v - E_a)/2kT}$$

→ (3)

$$P = (2N_a)^{1/2} \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/4} e^{-\Delta E/2kT}$$

where

$\Delta E = E_a - E_v$  is the ionisation energy of acceptors.

⑥ Write down the expression for mobility drift current and diffusion

### ① Mobility

mobility  $\mu$  is defined as the velocity of charge carrier per unit electrical field strength.

$\mu_n$  - electron mobility

$\mu_p$  - hole mobility  $\mu = v_d$

Electrical conductivity

when an external field  $E$  is applied, the electrons move with a drift velocity  $v_{dn}$ .

$$v_{dn} = \mu_n E \rightarrow (1)$$

$\mu_n$  - mobility of electron

$$J_n = n e v_{dn} \rightarrow (2)$$

$\sigma_n$  - conductivity of a Semiconductor due to free electrons.

$J_n$  - current density

$$J_n = \sigma_n E \rightarrow (3)$$

$$\sigma_n = \frac{J_n}{E} = \frac{n e v_{dn}}{E} \rightarrow (4)$$

Substituting eqn (1) in (4)

$$\sigma_n = \frac{n e \mu_n E}{E}$$

$$\sigma_n = n e \mu_n \rightarrow (5)$$

If  $P$  is the number of holes per unit volume and  $\sigma_p$  is the conductivity due to the drift of holes

$$\sigma_p = P e \mu_p \rightarrow (6)$$

$\mu_p$  - mobility of holes in the material.

Total conductivity  $\sigma$  due to free electrons and holes

$$\sigma = \sigma_n + \sigma_p$$

$$\sigma = n e \mu_n + P e \mu_p$$

$$\sigma = e (n \mu_n + P \mu_p)$$

$\sigma$  is the total conductivity of the material

For intrinsic Semiconductor

$$n = p = n_i$$

from eqn (7)

$$\sigma_i = e (n_i \mu_n + n_i \mu_p)$$

$$\sigma_i = e n_i (\mu_n + \mu_p)$$



## (ii) Drift current

### Definition

The electric current produced due to the motion of charge carriers under the influence of an external electric field is known as drift current.

Drift current density in a semiconductor due to electrons

$$J_n(\text{drift}) = n \mu_n e E \rightarrow (1)$$

Drift current density due to hole

$$J_p(\text{drift}) = p \mu_p e E \rightarrow (2)$$

where

$n$  and  $p$  are number of electrons and holes per unit volume -

Total drift current density

$$J = J_n(\text{drift}) + J_p(\text{drift})$$

$$J = n e \mu_n E + p e \mu_p E \rightarrow (3)$$

For intrinsic semiconductor

$$J = n_i e (\mu_n + \mu_p) E$$

$$(\because n = p = n_i)$$

## (iii) Diffusion current

### Definition

The non-uniform distribution of charge carriers creates the regions of uneven concentrations in the semiconductor.

The charge carriers move from the regions of higher concentration to the regions of lower concentration. This process is known as diffusion. The current is known as diffusion current.

Rate of flow of electrons through unit area =  $-D_n \left( \frac{dn}{dx} \right)$

$D_n$  - Proportionality constant and known as diffusion coefficient of electrons.

Rate of flow of electrons through unit area

$$= -e \times -D_n \left( \frac{dn}{dx} \right)$$

Rate of flow electrons through unit area is the diffusion current density of electrons  $J_n(\text{diffusion})$

$$J_n(\text{diffusion}) = e D_n \left( \frac{dn}{dx} \right)$$

$$J_p(\text{diffusion}) = -e D_p \left( \frac{dp}{dx} \right)$$

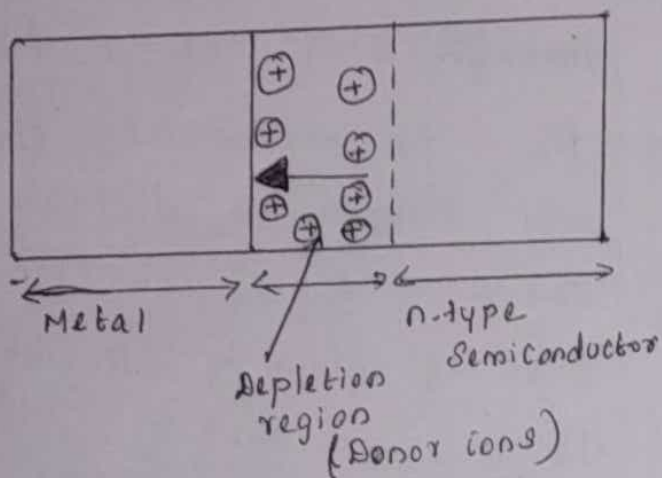
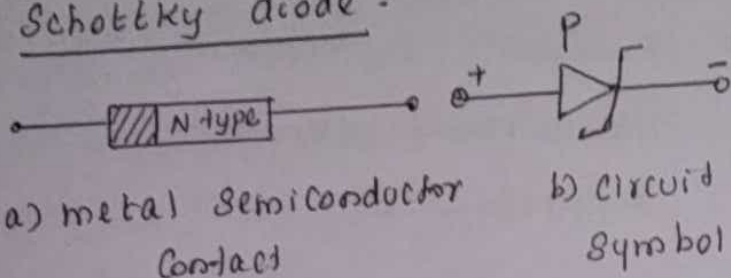
$D_p$  - diffusion constant of holes

# 7) Write notes on Schottky diode.

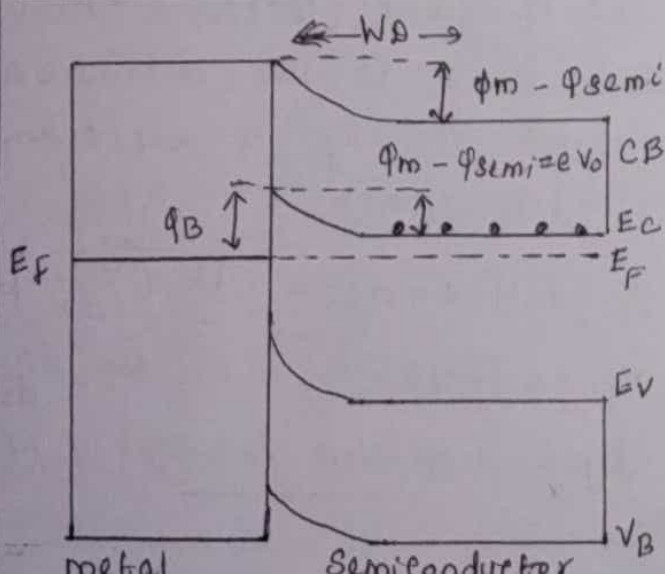
## Definition:

It is a junction formed between a metal and n-type semiconductor.

When the metal has a higher work function than that of n-type semiconductor then the junction formed is called Schottky diode.



## Energy band diagram



• when a Schottky junction is formed between metal and semiconductor, Fermi level lines up.

• Positive Potential is formed

• depletion region extends within a certain depth

• Bands bend up in the direction of the electric field produced in the depletion region.

$$eV_0 = \phi_m - \phi_{semi}$$

• Contact potential prevents further motion of the electrons between the metal and semiconductor. This is called the Schottky barrier.

## Working

• Voltage is applied in two ways

a) Forward bias

b) Reverse bias

## a) Forward bias

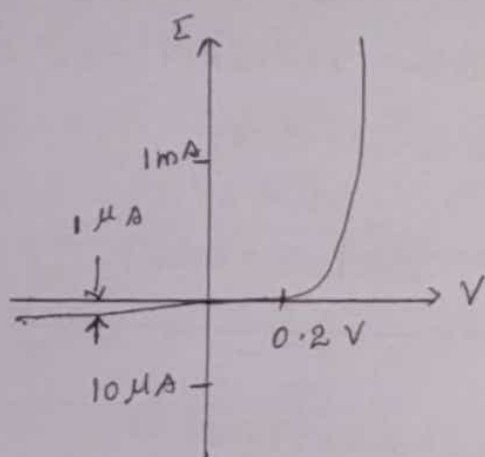
In this bias, metal is connected to positive terminal and n-type semiconductor is connected to negative terminal of the battery.

## b) Reverse bias :

In reverse bias, metal is connected to negative terminal and n-type semiconductor to positive terminal of the battery.

- External potential applied in the same direction as the junction potential.
- Increases the width of depletion region
- No flow of electron from semiconductor to metal.
- Schottky junction acts as a rectifier.

## V-I characteristics



- Exponential increase in current in the forward bias
- Small current in reverse bias-

## Advantages of Schottky diode

- High efficiency
- It operates at high frequency
- It produces less noise
- Depletion region is negligible in Schottky diode.

## Applications

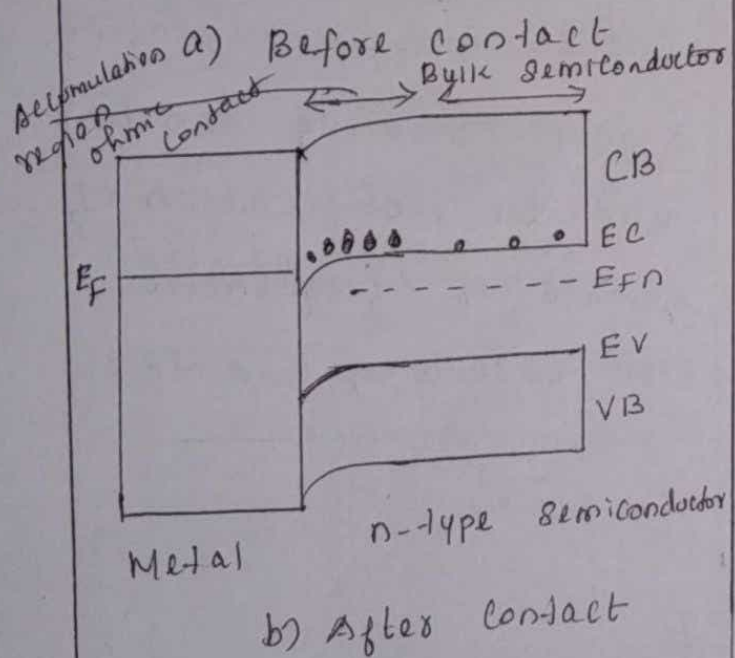
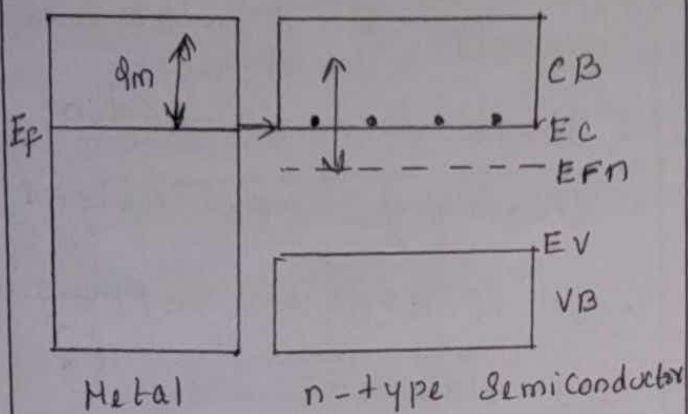
- It is used in logic circuits.
- It is used in power supplies.
- It is used to detect signals.
- It is used in radio frequency applications.
- It is used in clipping and clamping circuits and in computer gating.
- Schottky diode can be used for rectification of signals of frequencies even exceeding 300 MHz.



## 8) Write notes on ohmic contacts

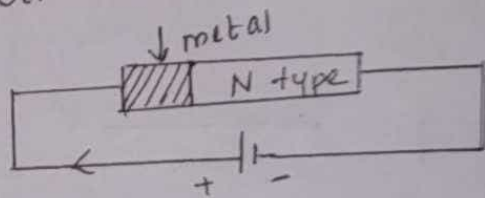
### Definition:

An ohmic contact is a type of a metal semiconductor junction. It is formed by a contact of a metal with a heavily doped semiconductor. When the semiconductor has a higher work function than that of metal, then the junction formed is called the ohmic junction.

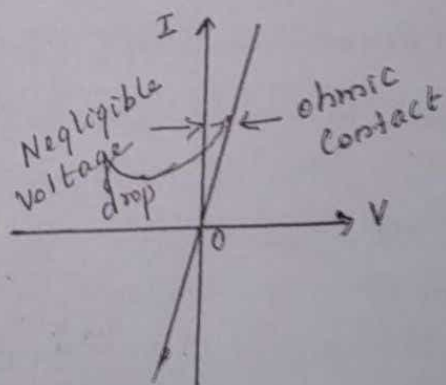


### Working

- At equilibrium, the electrons move from the metal to the empty states in the conduction band of semiconductor.
- Accumulation region near the interface.
- Accumulation region has a higher conductivity than the bulk semiconductor due to higher concentration of electrons.
- Ohmic contact behaves as a resistor conducting in both forward and reverse bias.
- Bulk resistivity of the semiconductor.



### V-I characteristics



The current is directly proportional to the potential across the junction

- ohmic contacts are non-rectifying
- Show negligible voltage drop

### Applications

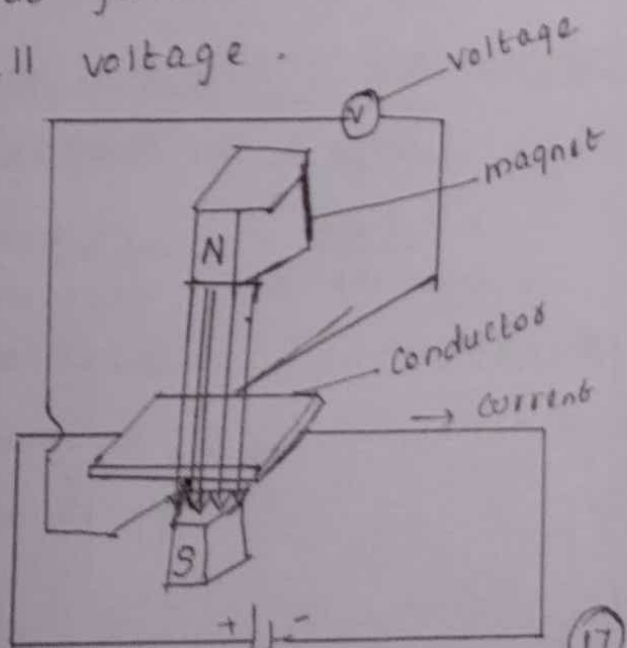
The use of ohmic contacts is to connect one semiconductor device to another, an IC, or to connect an IC to its external terminals.

### Discuss about Hall effect

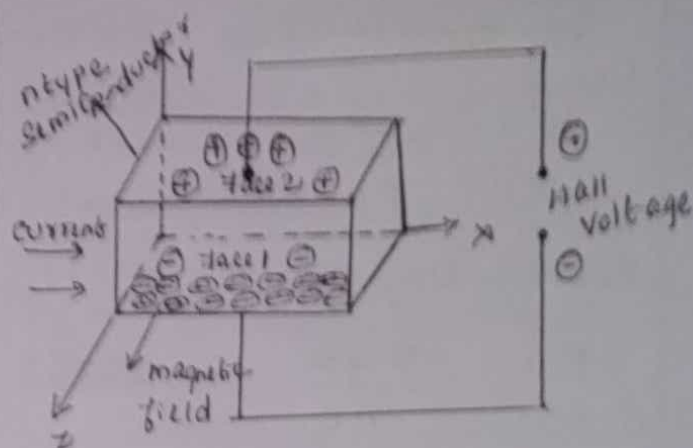
#### Statement

When a conductor carrying a current ( $I$ ) is placed perpendicular to a magnetic field ( $B$ ), a potential difference is produced inside the conductor in a direction perpendicular to both current and magnetic field.

This phenomenon is known as Hall effect. The voltage thus generated is called Hall voltage.



### Hall effect in n-type Semiconductor



- Consider n-type of semiconductor, in the form of rectangular slab.
- Current flows in x-direction
- Magnetic field  $B$  is applied in z-direction.
- Due to Hall effect, voltage is developed along y axis.
- Current flow right to left along x-direction.

Downward force experienced by the electron =  $Bev$

→ (1)

upward force acting on each electron  $= e E_H \rightarrow (2)$

At equilibrium downward force balances upward force

$$Bev = e E_H$$

$$E_H = Bv \rightarrow (3)$$

The current density  $J_x$  along  $x$  direction is related to velocity  $v$

$$J_x = -nev \rightarrow (4)$$

$n$  - concentration electrons

$$v = \frac{-J_x}{ne} \rightarrow (5)$$

Substituting eqn (5) in (3)

$$E_H = \frac{-B J_x}{ne} \rightarrow (6)$$

$$E_H = R_H J_x B \rightarrow (7)$$

$$R_H = -\frac{1}{ne} \text{ (for electrons)}$$

$$R_H = \frac{E_H}{J_x B}$$

$R_H$  - constant, known as Hall coefficient.

• negative sign indicates the electric field developed in negative  $y$ -direction

Hall effect in  $p$ -type Semiconductors

$$E_H = R_H J_x B$$

$$R_H = + \frac{1}{pe}$$

$p$  - concentration of holes

The positive sign indicates the electrical field develops in positive  $y$ -direction.

Hall coefficient in terms of Voltage

$t$  - thickness of the sample

$V_H$  - Voltage

$$V_H = E_H t \rightarrow (1)$$

$E_H$  - Hall field

$$V_H = R_H J_x B t \rightarrow (2)$$

If  $b$  - breadth of the sample

Cross sectional area of the sample  
(A) = Breadth ( $b$ )  $\times$  thickness ( $t$ )  
 $= bt$

$$J_x = \frac{I_x}{\text{Area of the sample (A)}} = \frac{I_x}{bt} \rightarrow (3)$$

Substituting eqn (3) in (2)

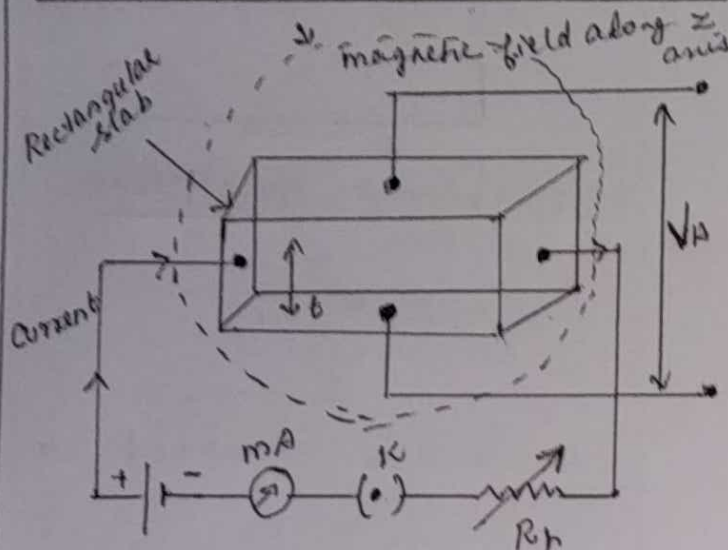
$$V_H = \frac{R_H I_x B t}{bt}$$



$$V_H = \frac{R_H I_x B}{b}$$

Hall coefficient  $R_H = \frac{V_H b}{I_x B}$

### Determination of Hall Coefficient



- A semiconductor is taken in the form of a rectangular slab
- $t$  - thickness,  $b$  - breadth
- Current  $I_x$  ampere is passed into this sample along  $x$ -axis by connecting it to a battery.
- It is placed in between north and south poles of an electro-magnet.
- Magnetic field is applied along  $z$ -axis
- Due to Hall effect, Hall voltage is developed.

- Voltage is measured by fixing two probes at the centres of the bottom and top faces of the sample.
- By measuring Hall voltage, Hall Coefficient is determined

$$R_H = \frac{V_H b}{I_x B}$$

From Hall Coefficient, Carrier concentration and mobility can be determined.

### Applications of Hall effect

#### i) Determination of Semiconductor type

- used to find whether a given semiconductor is  $n$ -type or  $p$ -type.

#### ii) Calculation of carrier concentration

$$n = \frac{1}{e R_H}$$

#### iii) Determination of mobility

$$\sigma_c = n e \mu_c$$

$$\mu_c = \frac{\sigma_c}{n e}$$

$$\mu_c = \sigma_c R_H$$

By measuring electrical conductivity and Hall coefficient of a sample, mobility of charge carriers can be calculated.

## Q-1 Explain about Hall devices

The device which uses the Hall effect for its application is known as Hall device.

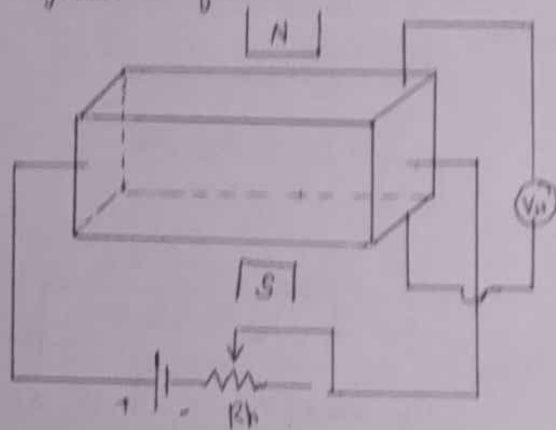
Three types of Hall devices

They are

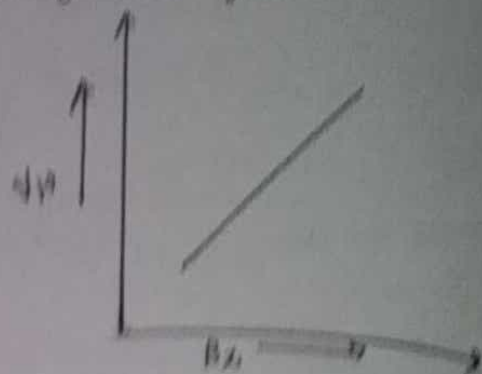
- Gauss Meter
- Electronic Multiplier
- Electronic Wattmeter

### a) Gauss Meter

- Hall voltage  $V_H = \frac{R_H B_z I_x}{b}$
- $V_H \propto B_z$
- $R_H$  and  $b$  constant
- Current  $I$  through Hall element is kept constant.
- This principle is used in Gauss meter.
- It is used for measuring magnetic field.



The graph can be also used to measure any unknown magnetic fields.



### b) Electronic Multiplier

$$V_H = \frac{R_H B_z I_1}{b}$$

$R_H$  and  $b$  constant

$$V_H \propto B_z I_1$$

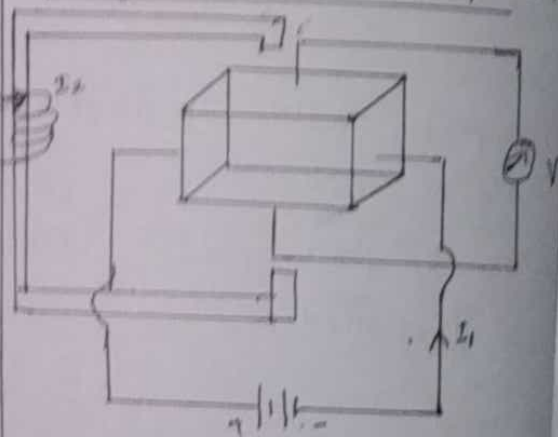
Magnetic field  $B_z$  is proportional to current ( $I_2$ )

$$B_z \propto I_2$$

$$V_H \propto I_1 I_2$$

$V_H$  is a measure of the product of two currents.

Basic principle used in analog electronic multipliers.

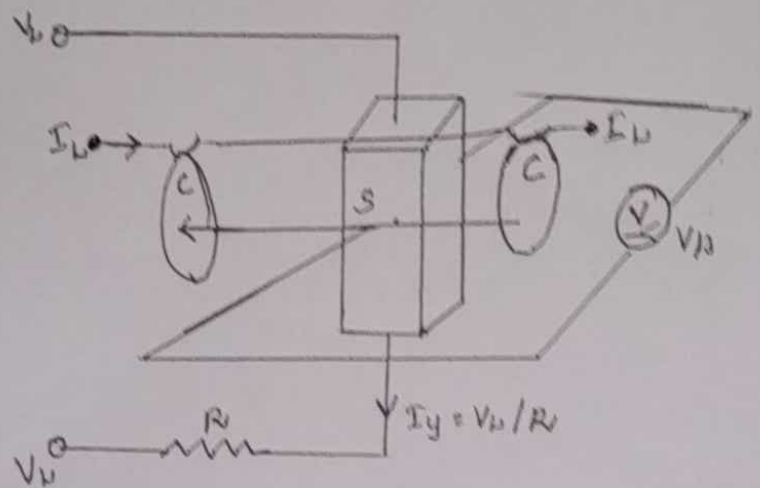
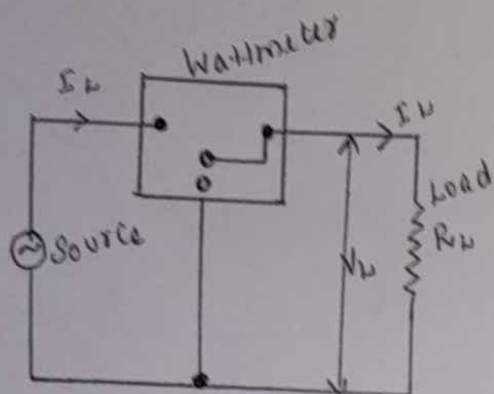


## c) Electronic WATTMETER

- Hall effect is used to measure electrical power dissipated in a load.
- Principle known as Hall effect - Watt meter
- S - Hall effect sample.
- $B_z$  - magnetic field
- $I_L$  - Load current
- CC - coils

The voltage across the load  $V_L$  drives the current

$$I_y = \frac{V_L}{R} \text{ through the sample.}$$



$V_L$  - Load voltage,

$I_L$  - Load current, C - coils to set

96 "t" thickness of the sample,

magnetic field B

$$V_H = \frac{R_{12} B_z I_y}{t}$$

$$V_H \propto B_z \cdot I_y \quad (R_{12} \text{ \& t are constants})$$

$$\text{Since } B_z \propto I_L$$

$$I_y \propto V_L$$

$$\boxed{V_H \propto I_L V_L}$$

- electric power dissipated by the load.
- $V_H$  can be calibrated to read power directly.



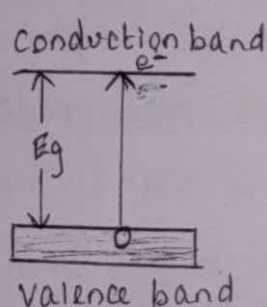
## Optical Properties of Materials

classification of optical materials - optical processes in semi conductors: optical absorption and emission, charge injection and recombination, optical absorption, loss and gain. Optical Processes in quantum wells - optoelectronic devices: light detectors and solar cells - light emitting diode - laser diode - optical processes in organic semiconductor devices - electronic state - Electro-optics and nonlinear optics: Modulators and switching devices - plasmonics.

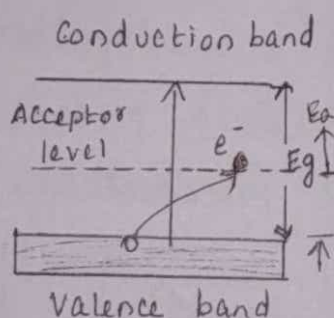
### ① Explain absorption and emission of light in semiconductors

• In intrinsic semiconductors Si, Ge and GaAs, light photons is absorbed to create electron hole pairs.

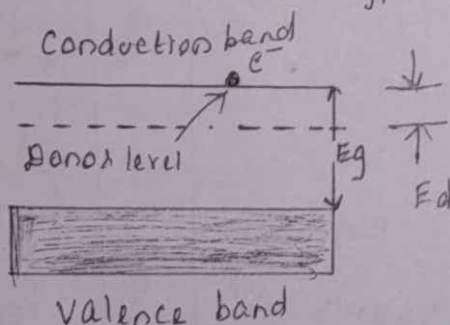
• Absorption causes electrons to jump across the energy band gap from the valence band to the conduction band.



a) Intrinsic



b) P-type



c) n-type

• Transition occurs

$$h\nu > E_g \rightarrow (1)$$

$h$  - Planck's constant

$\nu$  - Frequency of the light photon

$$\frac{hc}{\lambda} > E_g \rightarrow (2) \quad (\because \nu = c/\lambda)$$

• Maximum wavelength is about  $0.7 \mu\text{m}$ .

$$E_g(\text{meV}) = \frac{hc}{\lambda_{\text{max}}} \rightarrow (3)$$

Substituting the values

$$E_g(\text{meV}) = \frac{(6.62 \times 10^{-34}) (3 \times 10^8)}{0.7 \times 10^{-6}} = 2.84 \times 10^{-19} \text{ J}$$

$$= \frac{2.84 \times 10^{-19}}{1.6 \times 10^{-19}}$$

$$(1 \text{ eV} = 1.6 \times 10^{-19} \text{ J})$$

$$E_g(\text{min}) = 1.8 \text{ eV}$$

- Semiconductors are opaque.

In extrinsic semiconductors the presence of acceptor and donor impurities creates new energy levels namely

acceptor level ( $E_a$ ) and donor level ( $E_d$ ).

- Lie within the band gap of the material.

## ② Write notes on charge injection and Radiative Recombination

- Electrons and holes can be injected into the conduction band and valence band.

- Absorption of photons creates electron hole - pairs.

- Use an external battery bias.

- Electrons and holes recombine with each other.

- Electrons in the conduction band will return to the valence band.

- Two processes

- i) Radiative Processes
- ii) non-radiative Processes -

- In radiative process the electron hole pair recombines and a photon is emitted.

- Inverse of the photon absorption process -

- Electron hole pairs can also recombine without emitting light.

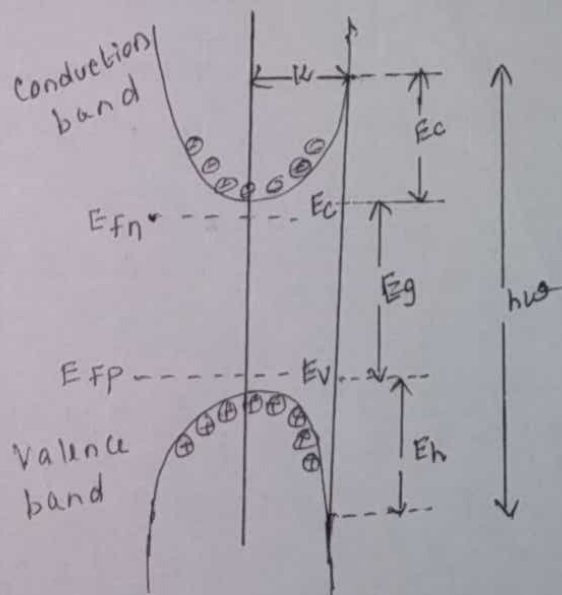
- They may emit

i) heat

ii) photon

iii) long wavelength photon together with a phonon.

Such processes are non-radiative processes.



- Electrons and holes are pumped into the semiconductor
- Recombine through the process of spontaneous emission.

### Types of carrier injections

i) Minority carrier injection

ii) Strong injection

iii) Weak injection

iv) At low injection

### i) Minority Carrier Injection

If  $n \gg p$ , sample is heavily doped n-type, recombination rate is proportional to the

minority carrier density.

### ii) Strong injection

• High density of both electron and holes is injected.

• Rate of recombination proportional to the majority charge carrier.

### iii) Weak injection

Rate of recombination is very low

### iv) At low injection

The electrons have a low probability to find a hole with which to recombine.

Write short notes in Carrier Generation and Recombination Processes.

### Carrier generation

The carrier generation is the process where by electrons and holes are created.

Three types of carrier generation.

i) Photogeneration

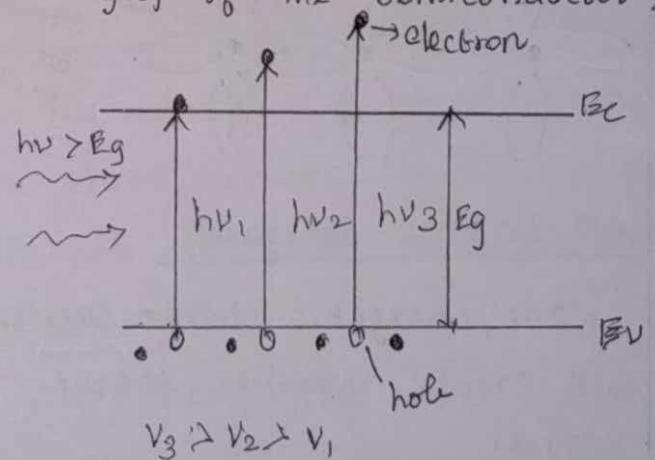
ii) Phonon generation

iii) Impact ionization

### i) Photogeneration

• Light of frequency  $\nu$  falls on a semiconductor.

•  $h\nu$  be the energy of light photon greater than the band gap of the semiconductor,



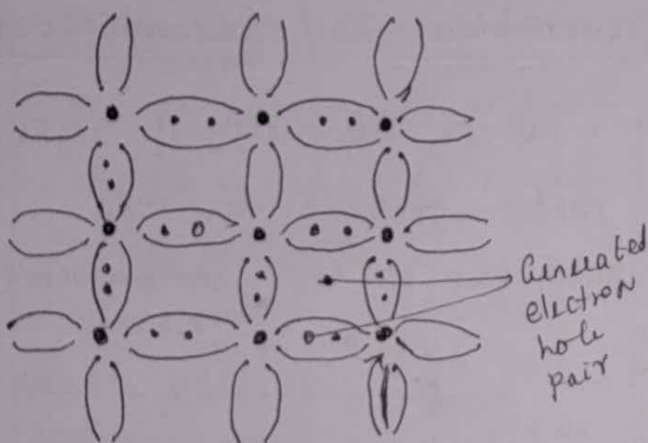
• By absorption of light photon, generating an electron hole pair.



- For different wavelengths of light with different energies, it can take an electron in higher conduction band state.

### (i) Phonon Generation

- occurs when a semiconductor is under thermal excitation
- With increase in temperature of the semiconductor, lattice vibrations increase which give rise to more phonons.
- Due to more lattice vibrations, covalent bonds in the semiconductor break down and electron-hole pairs are generated.

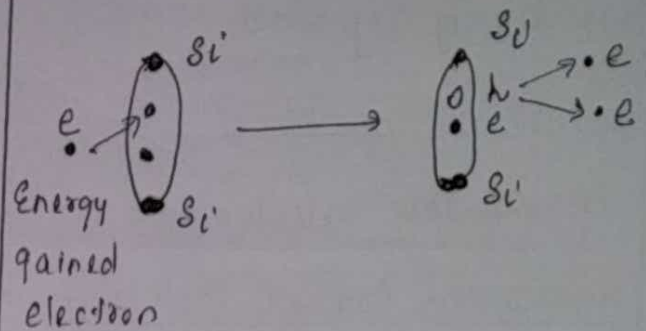


### (ii) Impact Ionization

- One energetic charge carrier will create another charge carrier.
- When a semiconductor is under an electric field, electrons gain energy from the applied electric field and hit other Si-atoms.

- In this process a bond breaks out generating more carriers.

- For a very high electric field it results in avalanche break down.



### Recombination Process

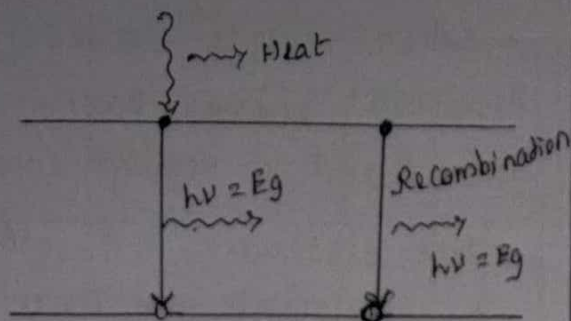
The recombination is the process where by electrons and holes are annihilated.

Recombination occurs in three ways

- i) Radiative Recombination
- ii) Shockley Read Hall Recombination
- iii) Auger Recombination

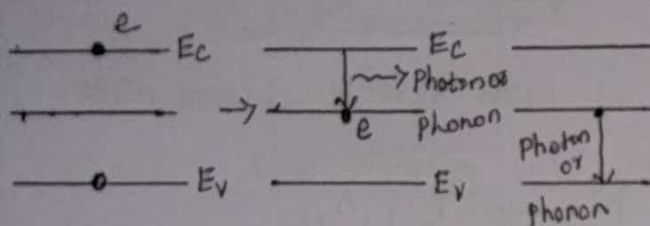
#### i) Radiative Recombination

- occurs direct band gap semiconductors.
- Electrons from conduction band minimum falls to valence band maximum without changing the momentum.
- One photon of energy  $h\nu$  is emitted.



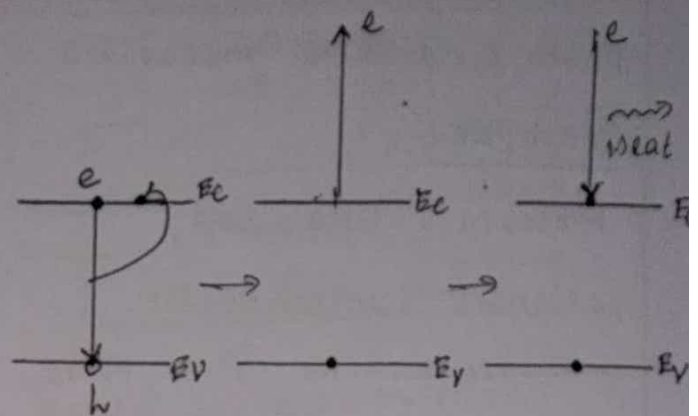
- Direct recombination.

## ii) Shockley-Read-Hall Recombination



- Intermediate between  $E_c$  and  $E_v$  by radiating energy as photons or phonons.
- Electron jumps from that intermediate level to the valence band.

## iii) Auger Recombination



- Three carriers are involved.
- Electron and a hole recombine.
- Energy is given to the third free electron in the conduction band.
- Auger recombination occurs heavily doped material.

## h) Explain about light detectors

### Definition :

It is a device which converts light signal into electrical wave forms.

### Types of photo detectors

3 types

- i) Photo emissive
- ii) Photo conductive
- iii) Photo voltaic

### 1) Photo emissive photo detector

The emission of electrons from a photo cathode by the incident photon is called photo emission.

### Examples

- a) photo tubes
  - b) Photo multiplier tubes
- Size very large
  - Not suitable for use as fibre optic detectors.

## ii) Photo conductive devices

- Variation of resistance due to incident light on the photo conductive materials.

### Examples:

Materials like  $\text{CdS}$ ,

Intrinsic semiconductor materials like  $\text{PbS}$ ,  $\text{PbTe}$

Extrinsic semiconductor like doped  $\text{Ge}$  and  $\text{Si}$ .

- Not suitable for use in fibre optic Communication Purposes

- Low frequency response.

## iii) Photovoltaic devices

Semiconductor junction photo diodes are called as photo Voltare devices.

- Ideal for fibre systems.

Three forms of devices

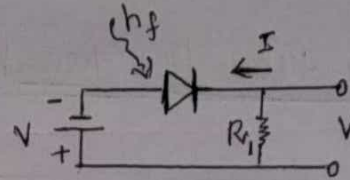
1. PN junction photo detector
2. PIN photo diode
3. Avalanche photo diode (APD)

### 1) PN junction Photo detector

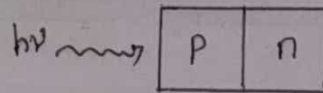
- It explains the basic detection mechanism of a junction detector.

- When reverse biased, the potential energy barrier between the P and n regions increases.

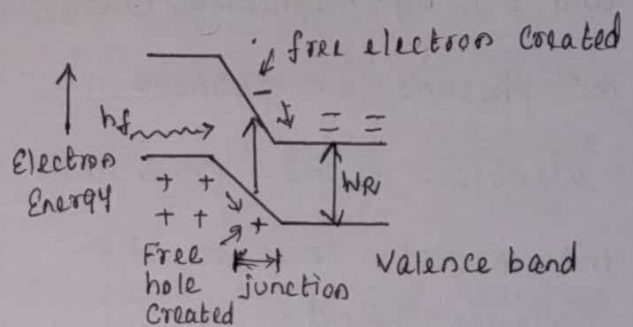
- Free electrons and free holes cannot climb the barrier, so no current flows



a) Reverse - biased diode



b) Pn junction



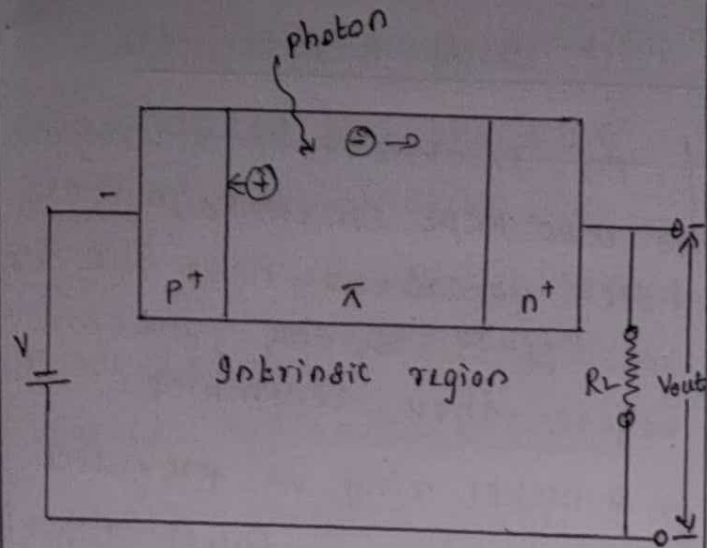
c) Energy level diagram

- Barrier exists.
- No free charges in the junction is called depletion region
- Absorbed energy raises a bound electron across the band gap.

## ii) PIN photo diode

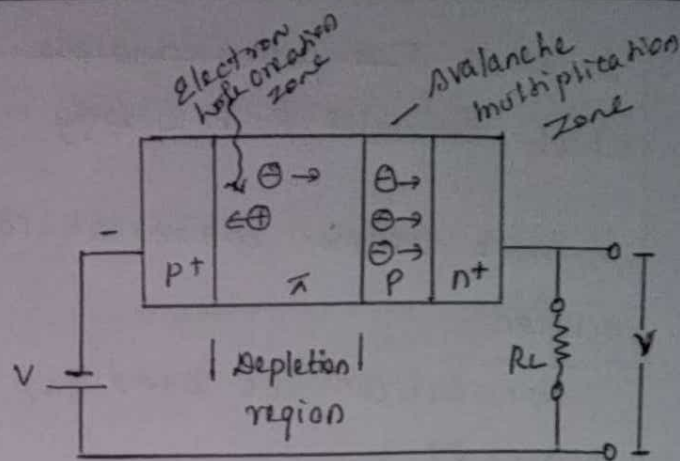
- Intrinsic region decreases the junction capacitance called Positive Intrinsic Negative (PIN) Photo diode.





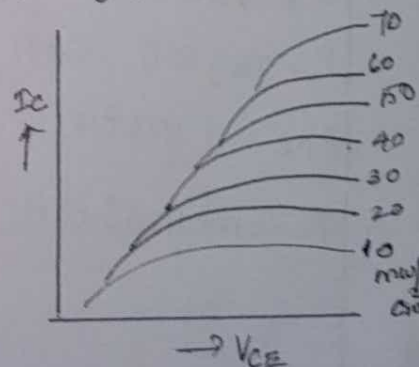
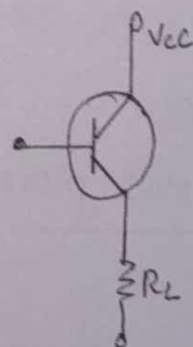
- Reverse biased
- Reverse biasing is used to attract the charge carriers from the intrinsic regions.
- When light is incident on the PIN diode, the intrinsic region receives more amount of light because of its large size.
- Photons produce electron hole pairs.
- Electrons are raised from the valence band to the conduction band, leaving the hole.
- Electrons are attracted by the reverse biasing.
- Conduction band creates the flow of charge.
- Light energy gets converted into electrical energy.

### iii) Avalanche Photo diodes (APD)



- Based on the principle of avalanche multiplication of the current.
  - Heavily doped  $P^+$  and  $n^+$  regions.
  - Diode is reverse biased using 50-300V.
  - Incident on the depletion region.
  - The incident light produces electron and hole pairs.
  - Electrons move towards the P-region.
  - High reverse bias.
  - The holes move towards the  $P^+$  regions without producing further multiplication.
- Photo Transistor

• Another type of photo detector



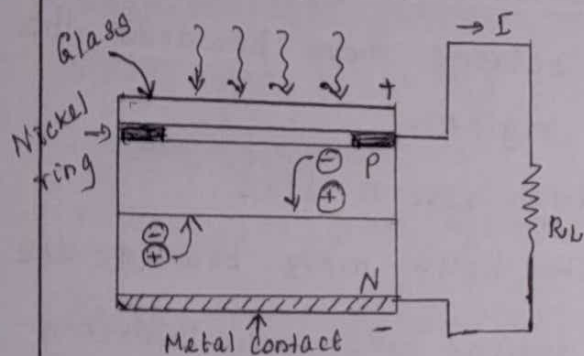
## ⑥ Explain the construction and working of a solar cell

It is a P-N junction diode which converts solar energy

- most common material is Silicon.
- For Silicon the band gap is  $1.12 \text{ eV}$

### Construction

- Consists of P-N junction diode made of Silicon.
- The P-N diode is packed in a can with glass window on top such that light may fall upon P and N type materials.
- The inward arrow indicates the incoming light.



- The thickness of the P-region is kept very small.
- Electrons generated in P-region can diffuse to the junction before recombination takes place.

• The thickness of N-region is also kept small to allow holes generated near the surface to diffuse to the junction before they recombine.

• A nickel ring is provided around the P-layer which acts as the positive output terminal.

• A metal contact at the bottom serves as the negative output terminal.

### Working

• Photon energy is sufficient to break the covalent bond and produce electron hole pairs.

• Electron hole pairs are generated in both P and N sides of the junction.

• Electrons and holes reach the depletion region by diffusion.

• Separated by the strong barrier electrical field existing there.

• Minority current which is directly proportional to the illumination of light and the

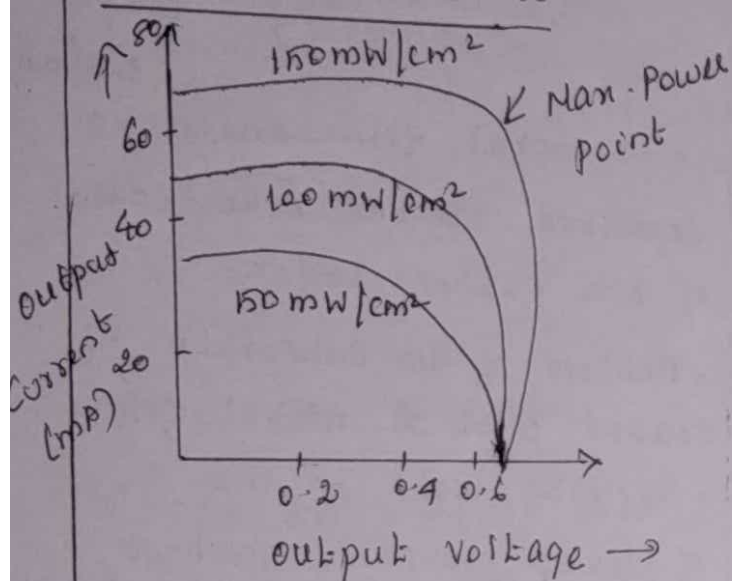
⑧ Surface are being exposed to light.

- Electrons and holes are accumulated on the two sides of the junction.

- The open circuit voltage produced for a Silicon solar cell is typically 0.6 V

- Short circuit current is about  $40 \text{ mA/cm}^2$

### V-I characteristics



The maximum power output is obtained when the solar cell is operated at the knee of the curve.

### Advantages

- Solar cell operates with fair efficiency
- unlimited life
- mass produced

- High Power Capacity per weight

- size is small and compact.

### Disadvantages

- Solar energy is not available round the clock.

- It cannot be obtained during night time.

### uses :

- used to give power to the calculators and watches
- used to provide commercial electricity.
- Solar cells are used on satellites and space vehicles to supply power to electronic and other equipments and to charge storage batteries.



## ⑥ Describe the construction and working of LED

It is a p-n junction diode which emits light when it is forward biased.

### Principle

The injection of electrons into the p-region from n-region makes a direct transition from the conduction band to valence band. Then, the electrons recombine with holes and emits photons of energy  $E_g$ . The forbidden energy gap is given by

$$E_g = h\nu \rightarrow (1)$$

$h$  - Planck's constant

$\nu$  - Frequency of the emitted radiation

$$\nu = c/\lambda \rightarrow (2)$$

$c$  - velocity of the light

$\lambda$  - wavelength of the light

$$E_g = \frac{hc}{\lambda} \rightarrow (3)$$

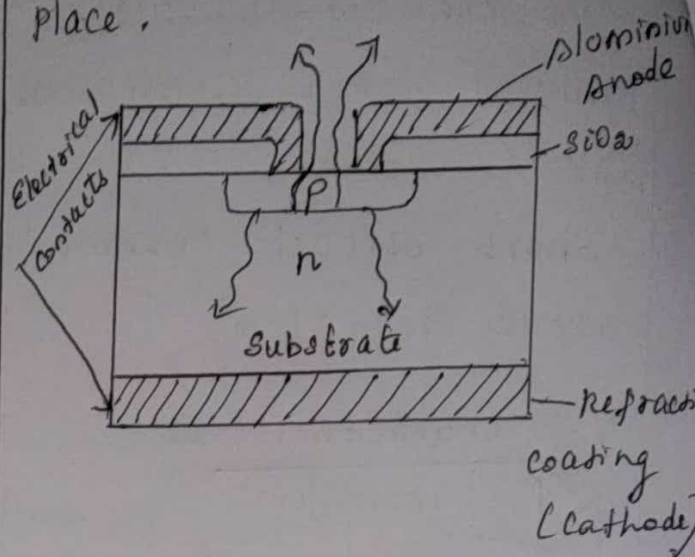
$$\lambda = \frac{hc}{E_g} \rightarrow (4)$$

### Construction

- n-type layer is grown on a substrate
- p-type layer is deposited

by diffusion.

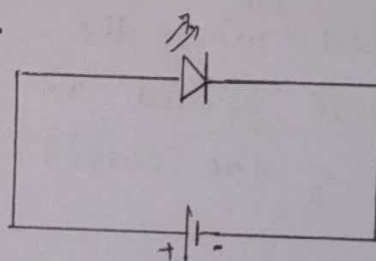
- Carrier recombination takes place.



- A metal film anode is deposited at the outer edges of the p-type layer

- Bottom of the substrate is coated with a metal film.

- reflects light to the surface of device provides cathode connection.



Circuit



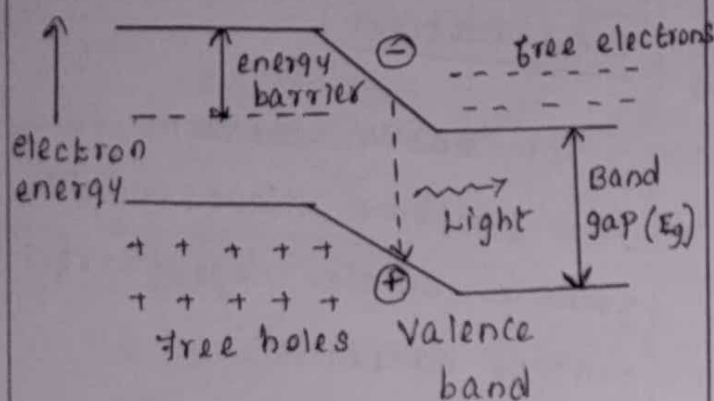
Symbol of LED

### Working

- when p-n junction is forward biased, barrier width is reduced.

- raising the potential energy on the n-side and lowering on p-side

- The free electrons and holes sufficient energy to move into the junction region.
- Light radiation from LED is caused by the recombination of holes and electrons that are injected into the junction by a forward bias voltage



### Advantages of LEDs

- LEDs are smaller in size. a small space to form numerical display.
- LED's can be turned ON and OFF in less than 1 nano second. So they are known as fast devices.
- Variety of LED's are available which emit light in different colours like, red, green, yellow etc.
- Long life time
- Low drive voltage and low noise

- Easily interfaced to digital logic circuits.
- Operated over a wide range of temperatures

### Disadvantages of LEDs

- Require high power
- Preparation cost is high when compared to LCD.

### Applications and uses of LEDs

- They are widely used in numeric and alphanumeric display devices.
- used as an indicator lamps
- used as light sources in fibre optic communication system.
- used in burglar alarms.
- used for picture phone.
- used as a pilot light
- used with photo diodes or photo transistors to enable short range wireless communication.

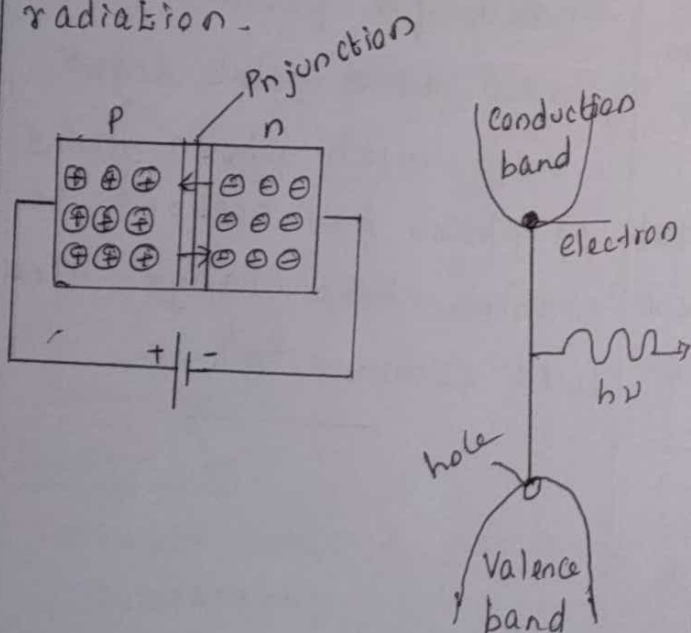
# ⑦ Explain the construction and working of Laser diode.

## Definition!

It is a specially fabricated P-n junction diode. This diode emits laser light when it is forward-biased.

## Principle

When the P-n junction diode is forward-biased, the electrons from n-region and holes from p-region cross the junction and recombine with each other. During the recombination process, the light radiation is released from a direct band gap semiconductors like GaAs. The light radiation is known as recombination radiation.



- Photon emitted during recombination stimulates other electrons and holes to recombine.

- Stimulated emission takes place, Laser light is produced.

## Construction

- The active medium is a P-n junction diode made from a single crystal of gallium arsenide.

- Crystal is cut in the form of platelet, thickness of 0.5mm

- This platelet consists of two regions n-type and p-type

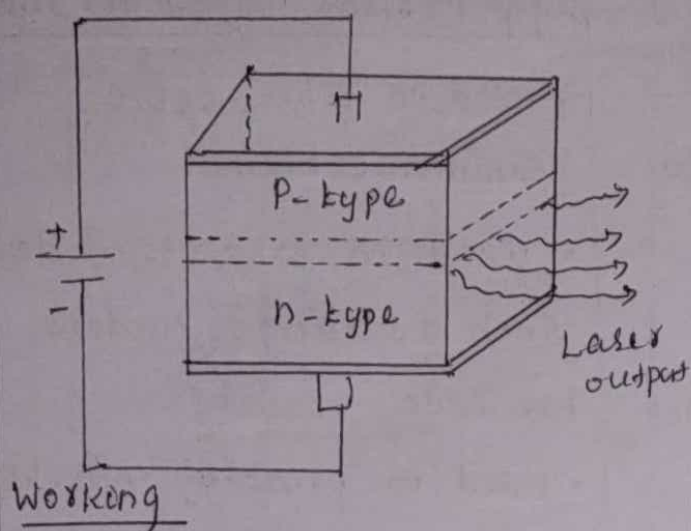
- The metal electrodes are connected to both upper and lower surfaces of the semiconductor diode.

- Forward bias voltage is applied.

- Photon emission is stimulated.



- The end faces of the Pn junction are well polished and parallel to each other.
- Act as optical resonator.
- Light comes out



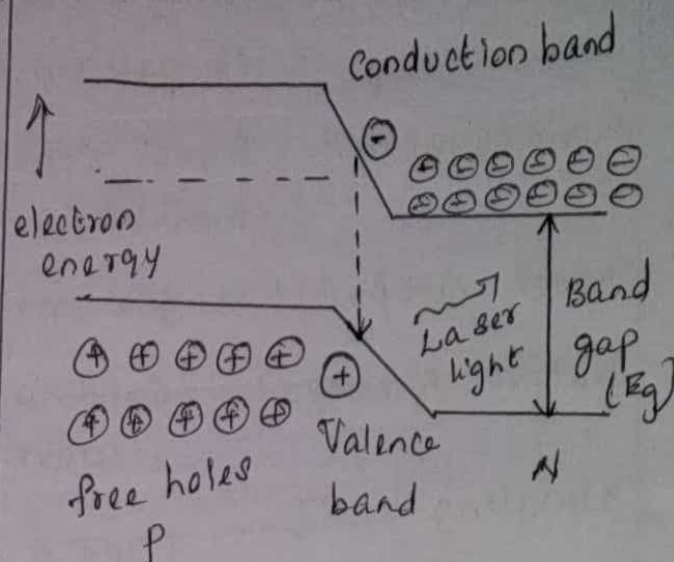
Working

- P-n junction is forward biased, electrons and holes are injected into junction region.

- Junction contains a large number of electrons in conduction band and holes in the valence band.

- Electrons and holes recombine with each other.

- Light photons are produced.



- When forward biased voltage is increased, more light photons are emitted.
- Photons trigger a chain of stimulated recombinations.
- Photons move the junction travel back and forth by reflection between two polished surfaces.

- After gaining, Laser beam of wavelength  $8400 \text{ \AA}$  is emitted from the junction

$$E_g = h\nu = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc}{E_g}$$

$$(\nu = c/\lambda)$$

### Characteristics

- Type : Solid state Semiconductor laser

Active medium : single crystal  
of gallium arsenide

Pumping method : Direct Conversion  
method

Power output : a few mW

Nature of output : Continuous  
wave

Wavelength of  
output :  $8300 \text{ \AA}$  to  
 $8500 \text{ \AA}$

### Advantages

- Small in size and compact
- High efficiency
- Operated with less power than ruby and  $\text{CO}_2$ .
- Continuous wave output

### Disadvantages :

- Large divergence
- Poor monochromaticity
- Poor coherence and stability.

### Applications of Laser Diode

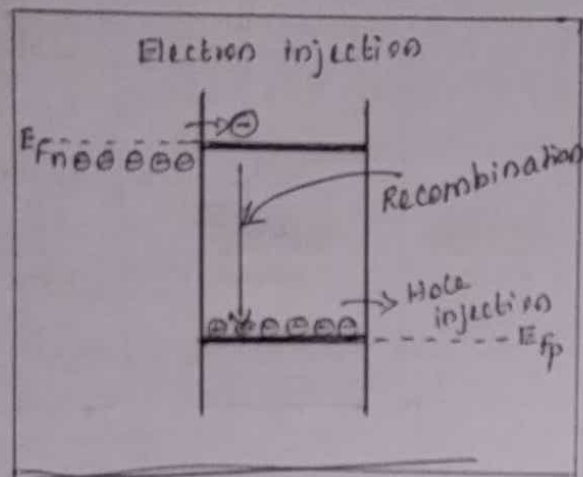
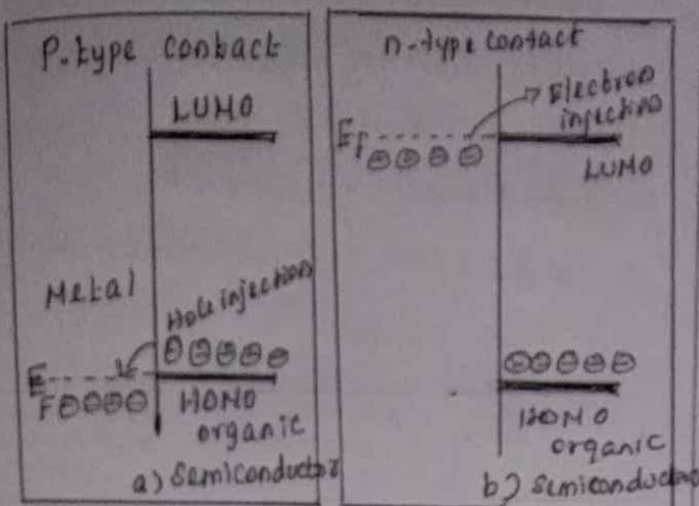
- Used in fibre optic communication
- Used in measuring devices such as range finders, bar code readers.
- Used in printing industry
- Used in laser medicine, dentistry.

## ⑧ Write short notes in optical Processes and devices and Excitonic State

### i) Optical Processes and devices

- Polymer based devices are now used for back lights of liquid crystal displays, displays of devices, such as cell phones or watches.
- It is used in the commercial technologies such as televisions, solar cells, etc.

- Polymer LEDs were first demonstrated in 1990.
- Very attractive because of potential large area applications and mechanical flexibility.
- In organic semiconductors the nature of atomic bonding, results in very narrow range energy levels.

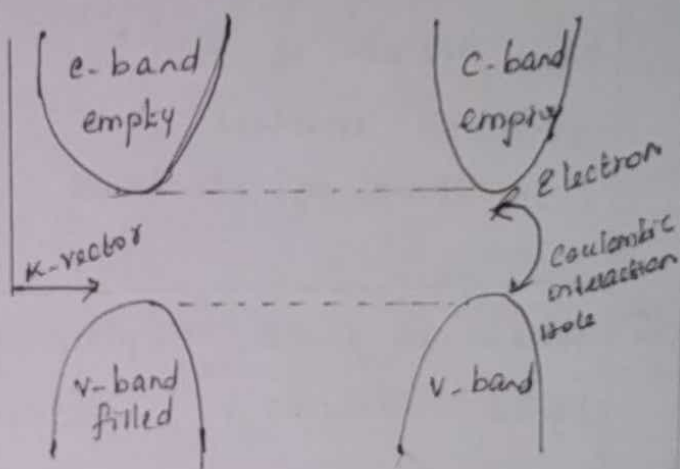


- When Fermi energy of the metal is close to the HOMO level, electrons from this level can move into the metal.
- Metal acts as a p-type contact.
- Metal work functions are close to the LUMO state.
- The n-contacts injects an electron while diffuses into the semiconductor.
- Recombining with a hole in the HOMO level.
- Electron finally leaves the HOMO state.

- The difference is due to the formation of exciton state.
- Bound state of electrons.
- e-h interacting through Coulombic interaction.

## (ii) Excitonic State

- Two bands are separated by band gap.
- Single electron energy momentum.



- Consider an electron being removed from the valence band and excited to a higher energy state.
- The lowest energy needed to excite the system is the band gap energy  $E_g$ .
- Electron and hole interact with each other.



- The bound state of electron hole system is called exciton.
- The exciton energy is slightly lower than the band gap energy of the semiconductor.

• Excitonic states observed in optical absorption spectra and used for many optoelectronic devices.

• The exciton binding energy is quite large

• Exciton creates photons.

The process of light

emission involves

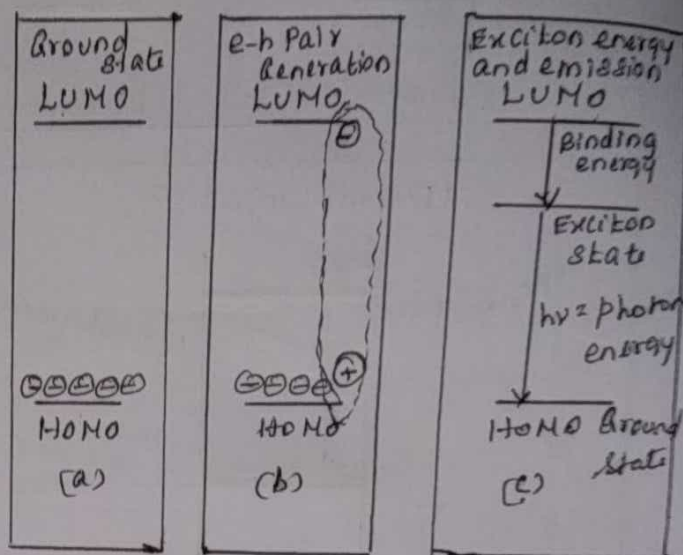
i) Injection of electrons

(holes) from the contacts

ii) diffusion of the carrier in LUMO or HOMO states.

iii) exciton formation

iv) exciton recombination to emit a photon



⑨ What is OLED? Explain the basic concept of OLED, types, advantages, disadvantages and applications

organic light emitting diodes are solid state devices made up of thin films of organic molecules that produce light with the application of electricity.

• Consists of a film of organic compounds.

### Principle

An electron moves from cathode to the emissive layer and the hole moves from the anode to the conductive layer and they recombine to produce photons. This is the principle used in OLED.

~~Introduction~~ Wabli

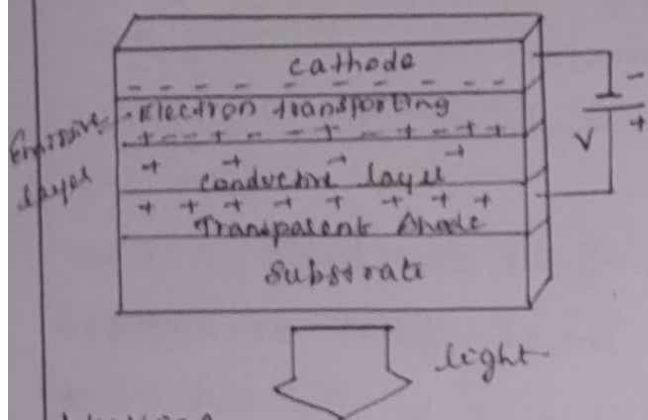
## Construction

• Two organic layers

1) Emissive layer

2) Conductive layer

All the layers are grown over a transparent substrate through which the light has to be emitted.



## Working

• Forward bias voltage is applied across the OLED

• By applied voltage, the Cathode gives electrons to the emissive layer.

• Emissive layer becomes rich in negatively charged particles

• Conductive layer becomes rich in positively charged particles.

• Due to electrostatic force, they come closer and recombine with each other.

• The recombination of electrons and holes occurs closer to the emissive layer.

• Holes move faster than electrons.

• Recombination produces light.

## Advantages

• Robust design : use in portable devices such as Cellular phones, digital video, Cameras, DVD players etc

• Viewing angle : upto 160 degrees

• High Resolution :

Videos and graphics

• Electronic paper :  
paper-thin

• Production Advantages :

Upto 20% to 50% cheaper than LCD processes.

• Video Capabilities :

Display and Cellular Phone market

• Power usage :

Takes less power

## Drawbacks

- The biggest technical problem for OLEDs is the limited life time of the organic materials.
- The intrusion of water into displays can damage or destroy the organic materials.
- Color - The reliability of the OLED is still not upto the mark. After a month

of use, the screen becomes uniform.

## Applications

- used in television screens, computer displays, advertising, information and indication
- OLED technology is used in commercial applications such as small screens for mobile phones and portable digital audio players, car radios, digital cameras.

## ⑩ Describe about plasmonics

- Plasmonics or nanoplasmonics refers to the generation, detection and manipulation of signals at optical frequencies along metal dielectric interfaces in the nanometer scale.

### Principle

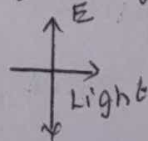
- Plasmonics typically called surface plasmon polaritons (SPPs).
- Coherent
- electromagnetic wave interface between a dielectric
- Strong light matter interactions.
- Metal oscillates with the electromagnetic wave.

- Signals are large
- Limits signal transfer distances to the sub-centimeter range

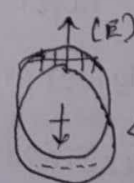
## Surface Plasmon Resonance (SPR)

The collective oscillation of the free electrons with respect to the fixed positions of the positively charged nuclei is called plasmon.

Electric field



Time



t



$t + T/2$

$T$  = Life time of dipolar oscillation



• The free surface electrons can collectively oscillate to produce the surface plasmon.

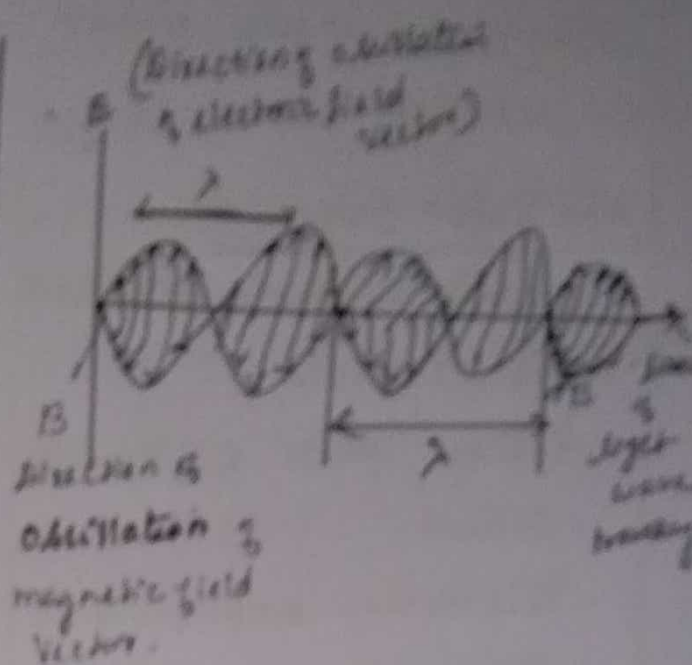
• Due to quantum confinement, the surface plasmon is localized and it is called the localized surface plasmon (LSP).

• Incident light cause a oscillating dipole moment.

• Explained for a spherical nano particle.

• Collective oscillation of free surface electrons reaches maximum at a specific frequency of the incident light.

• It produces the surface plasmon resonance (SPR) and the light is absorbed (called plasmon absorption).



### uses of plasmonics

• Plasmonic gold and silver nano particles have unique optical, electrical and thermal properties and hence are used in applications such as antimicrobial coatings and molecular diagnostics.

• Useful in color engineering

ii) Write Short notes on i) Non linear optics, ii) Modulation of light

### i) Non linear optics

The field of study in which the matter responds in a non-linear manner to the incident light radiation is known as non-linear optics.

• Material which exhibit non-linear effect are called non linear materials.

• The dependence of optical properties such as refractive index on the electric and magnetic fields associated

with light is also known as non-linear effect.

### Non linear properties

- Second harmonic generation
- optical mixing
- optical phase conjugation
- Soliton
- Parametric amplification
- Self focussing

### Second Harmonic Generation

In linear medium, Polarization  $P$  is directly proportional to the electric field  $E$

$$P \propto E$$

$$P = \epsilon_0 \chi E$$

$\epsilon_0$  - Permittivity of free space

$\chi$  - electrical susceptibility.

$$P = \epsilon_0 \left( \chi_1 E + \chi_2 E^2 + \chi_3 E^3 + \dots \right)$$

$\chi_1$  - linear susceptibility

$\chi_2, \chi_3$  - higher order non linear susceptibilities.

### ii) Modulation of light

Modulation is the process of varying one of the parameters such as amplitude, intensity, frequency, phase and polarization of a carrier wave in accordance with signal to carry the signal information.

• Demodulation means the reverse process of modulation.

• Two schemes used to modulate the optical signals in LED or LASER diodes.

i) Direct modulation

ii) External modulation.

#### i) Direct Modulation

• Electronic circuit is designed to simply modulate the current injected into the device.

• Optical output is controlled by the injected current.

• The driver for direct modulation may be a FET or an HBT hetero bipolar transistor.

• Direct modulations has several problems.

• Limit in upper modulation frequencies.

• Shift in emission frequency

### ii) External Modulation

• The electro-optic effect is most widely used for high speed applications.

• most comparable with modern electronics.

• Electro optic effect involves the change in the refractive index.

• Electro optic effect is quite small.

• High fields are needed to cause optical modulation.

• Lithium-niobate is the most widely available electro optic material.

• Quantum well modulators plays a role in optical modulation.

### Modulators

The different electro optic modulators are

a) Electro optic modulators based on Kerr effect.

b) Electro optic modulators based on Pockels effect

c) Electro absorption modulators by Franz Keldysh and Stark effect

d) Quantum well electro absorption modulator

### i) Kerr effect

Optical anisotropy induced in an isotropic liquid under the influence of the electric field is known as the Kerr effect.

• Studying the effect.

• Two plane electrodes of length  $L$  are arranged parallel to each other.

• When a voltage is applied to the electrodes a uniform electric field is produced in the cell.

• The Kerr cell is placed between a crossed polarizer system.

• Align along the electric field direction



• Molecules are asymmetric, the alignment causes anisotropy and becomes double refracting

The induced birefringence is proportional to the square of the applied electric field ( $E$ ) and to the wavelength of incident light ( $\lambda$ ).

$$\Delta \mu \propto \lambda$$

$$\Delta \mu \propto E^2$$

$$\Delta \mu = K \lambda E^2$$

where

$K$  - Kerr constant.

• The vibration direction of plane polarized light passing between crossed polarizer is rotated.

uses :

- i) an electro optic shutter in high-speed photography
- ii) light chopper in the measurement of the speed of light.

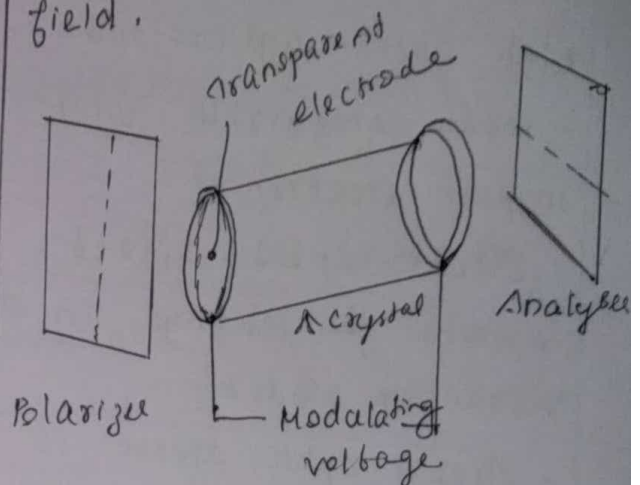
Pockels Effect

F. Pockels discovered in 1893 that the application of an electric field to piezoelectric

crystals makes them birefringent.

• transparent electrodes are deposited on opposite sides of the crystal.

• crystal is oriented with its optic axis along the direction of the electric field.



The birefringence induced in the crystal is proportional to the strength of the applied field

$$\Delta \mu \propto E$$

$$\Delta \mu = K E$$

• Total birefringence is equal to  $\lambda/2$ .

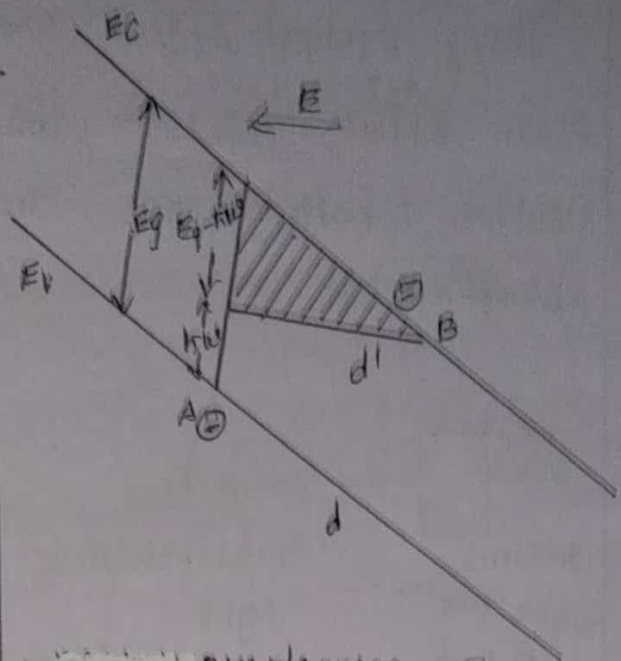
• The device switches on and off periodically.

• Pockels cells are used in fast switching applications and in fibre optics.

used to obtain amplitude, frequency or phase modulation.

• The piezoelectric crystals of ammonium dihydrophosphate and potassium dihydrophosphate are widely used in Pockels cell.

• Kerr and Pockels cells are widely used as electro-optic shutters in Q-switching of lasers.



• ~~When~~ overlapping of wave functions within the energy gap increases.

• When there is no photon the valence electron has to tunnel through a triangular barrier of height  $E_g$  and thickness  $d = E_g/qE$ .

• The absorption of photon by the electron depends on the strength of applied field.

iii) Franz-Keldysh and Stark effect electro absorption

Modulators

i) Franz-Keldysh effect

The absorption of light photons having energies less than the band gap energy of the semiconductor by applying a strong electric field is called as Franz-Keldysh effect.

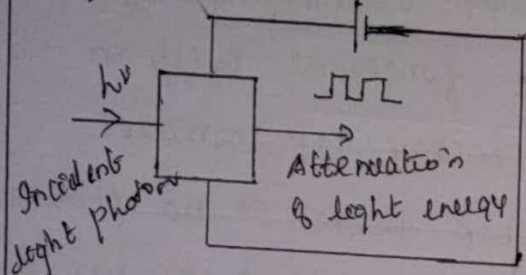
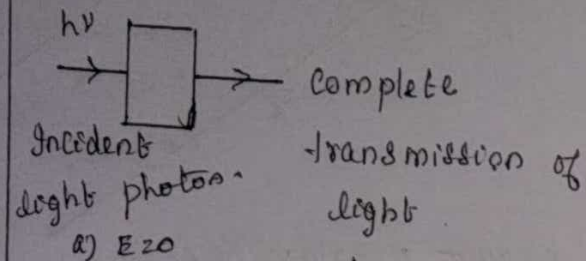
• When there is no photon and the electric field, the wave functions of electron at A and B are decaying without overlapping in the band gap.

ii) Stark effect

The energy level splitting of the outer 2s or 2p states and hence absorption of photon whose energy is less than the band gap by an applied electric field is called Linear Stark effect.



• Franz-Keldysh effect and Stark effect refer to the electron tunneling via electro absorption.



• Applying Sequence of electric pulses. These type of modulators are called electroabsorption modulators.

• No applied field the light photon is completely transmitted without any absorption.

When the bias pulses are applied which correspond to the signal to be transmitted there is attenuation of transmitted light depending upon the value of magnitude of applied bias pulses.

## Drawbacks

- Electro absorption effects are very weak.
- To increase the electro absorption effect, very large electric fields are needed.

## iv) quantum well electro absorption modulators

- The electron is confined in the region defined by the well width.
- When there is an applied transverse electric field the bending of quantum well takes place.
- Electron and hole wave functions are pushed toward the opposite sides of the well.

$$E_{ph} = E_e + E_h + E_{g(well)} - E_{ex}$$

$E_e, E_h$  - electron and hole, Subband energies

$E_{ex}$  - binding energy of exciton

$E_{g(well)}$  - band gap energy between conduction band and valence band.



$E_{ex}$  - Little change

$E_{gl(well)}$  - Very small change due to Stark effect

- reduction in  $E_e$  and  $E_h$

Subband energies.

• The ground state inter-subband energy separation is very small. This results in a shift of the absorption spectrum to lower energies. This shift is the dominant effect which results a pronounced red shift of the absorption edge. This shift is called quantum confined Stark effect (QCSE)

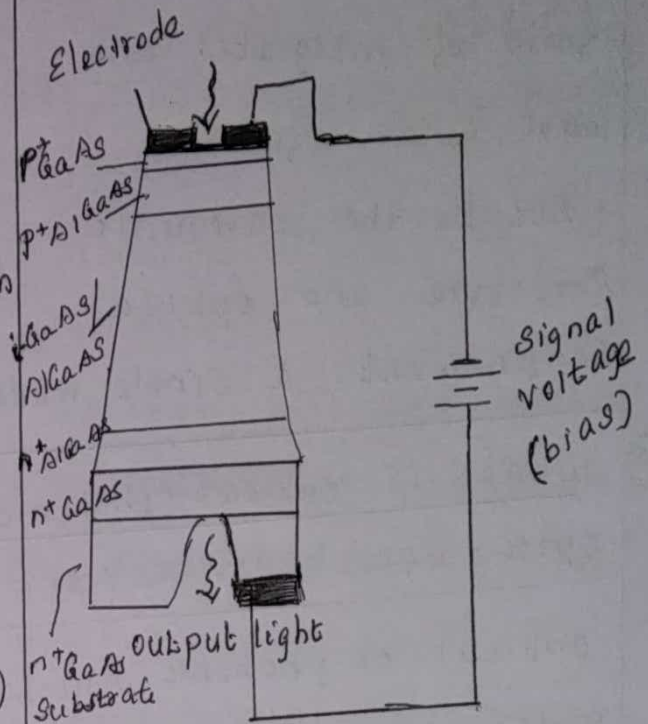
• Shift is proportional to square of the electric field and to fourth power of the quantum well width.

• Input light is completely transmitted through the quantum well material.

• Efficient intensity modulation of light

P-i (MQW) - n diode quantum well electroabsorption modulator

Construction working



• The optical window is situated at the top of the p-i-n diode is about half of the diode area.

• The p-i-n diode is made by Photo lithography, Selective etching and ohmic contact formation.

• GaAs substrate is not transparent to light, it is selectively etched under the active region of the diode.

The light is transmitted through the diode or normal to the plane of the quantum well layers.

- It is available in the form of integrated and wave guide form.
- Due to the waveguide structure and optical confinement, a single mode

transmission.

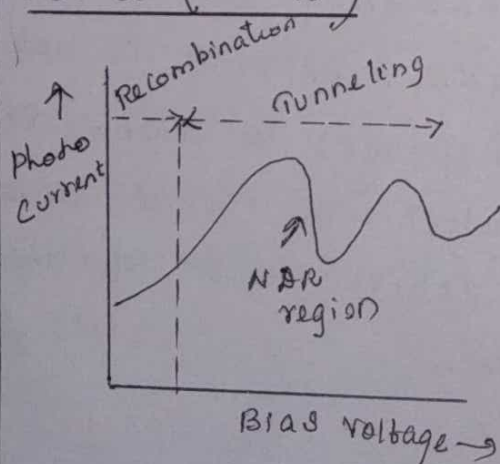
- there is no applied transverse electric field, there is no flow of current in the external circuit.

The modulation of light takes place which is proportional to the applied transverse electric field or bias signal.

(12) What is optical (photonics) switching? Explain Electro optic effect device (SEED)

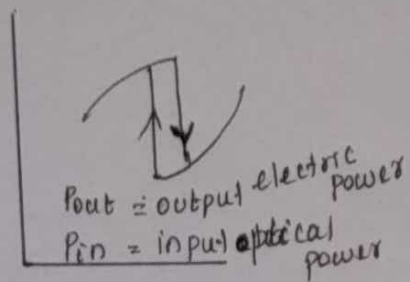
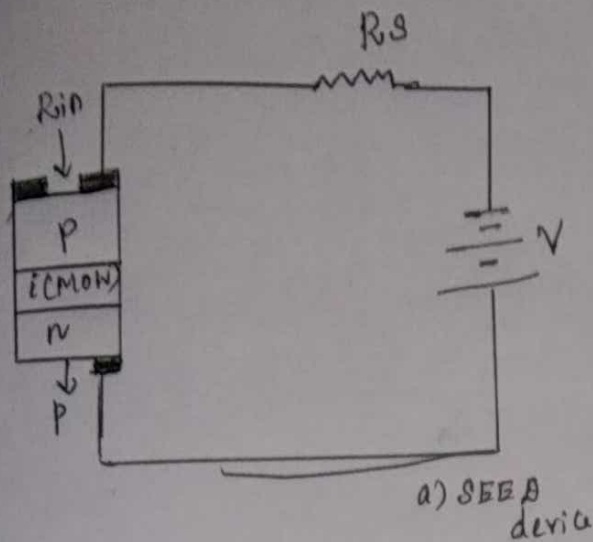
Optical or photonic switching refers to a phenomenon in which transmission of an optical field through a device is switched among two or more possible states by optical means.

Self Electro optic Effect Device (SEED)



- In P-i(MQW)-n diode, when the reverse bias voltage increases to a large value,
- The photocurrent bias voltage characteristic curve, exhibits negative differential resistance region.
- NDR occurs the heavy-hole and light-hole absorption peaks cross the photon energy of the input light.
- NDR Effect is exploited in SEED.
- SEED device exhibits Photonic switching, bistability and optically induced oscillations.





b) Photonic Switching

$P_{in}$  - incident optical power

$P_{out} = I^2 R_s$  - electric output power

$I$  - photo current flowing through resistance  $R_s$

### Working

- At low bias voltages and low optical power most of the incident light is transmitted.
- Photo current increases due to recombination of electrons and holes.
- The voltage drop  $I^2 R_s$  across the series resistor increases.

- Supply voltage remains constant
- The negative bias across the diode decreases.
- The heavy hole absorption peak is shifted to higher energies.
- Transmission of light is decreased.
- The heavy hole and light hole absorption peaks cross the photon energy of the input light.
- photo current decreases
- output electric power also decreased.
- state of the device is altered by optical power.
- The photonic or optical switching is obtained by light beams with two different powers one for complete transmission and other one for control.
- Due to the asymmetric shapes of the heavy hole and light hole absorption curve.
- Feedback due to the series resistor is optoelectronic type.



## Unit : V

### Nanoelectronic Devices

Quantum confinement - Quantum structures = quantum wells, wires and dots - Zener - Bloch oscillations - Resonant tunneling - quantum interference effects - mesoscopic structures - single electron phenomena - single electron transistor - Semiconductor photonic structures - 1D, 2D and 3D photonic crystal. Active and passive optoelectronic devices - photo processes - Spintronics - Carbon nanotubes ; Properties and applications.

① Write short notes on <sup>i)</sup> Quantum Confinement and <sup>ii)</sup> Quantum Structures, <sup>iii)</sup> Density of States

#### ① Quantum Confinement

##### Definition

It is a process of reduction of the size of the solid that the energy levels inside become discrete.

• In this case, small "droplets" of isolated electrons are created.

• The energy of a small volume of such materials are quantized just like an atom.

• Size of the particle is too small to be comparable to the wavelength of the electron.

• Small percentage of electrons move during confinement and majority of electrons tightly bound within inner orbitals.

• To reduce dimensions of a given volume, either bottom up approach or top down approach is followed.

• Bottom up approach - Low volume structures are built atom by atom.

• Top down approach - material is removed from one or more of three dimensions.

## 2) quantum structure

### Definition:

When a bulk material is reduced in its size, at least one of its dimension in the order of few nanometres, then the structure is known as quantum structure.

- Three dimensions to confine the bulk material.

A structure in which the motion of the electrons or holes are confined in one or more directions by potential barriers is called quantum confined structure.

#### • 3 types

- i) quantum well
- ii) quantum wire
- iii) quantum dot

### i) quantum well (2-dimension)

#### Definition:

When the electrons are confined inside a region of minimal width in one dimension 'quantum well' is created.

If one dimension is reduced to the nanometre range while the other two dimensions

remain large, then get a structure as quantum well.

### Explanation

- 2 D structure
- Larger structure
- Free to move in two directions.
- Particles are confined in one dimension to be quantum confinement.
- quantum well structure has important applications

### use

- used to make semiconductor lasers and other important devices.

### ii) quantum wire (1 dimension)

#### Definition:

When the electrons are confined in two mutually perpendicular directions, then the structure is known as quantum wire.

If two dimensions are reduced and one remains large, the resulting structure is quantum wire.

### Explanation :

- Considered to be in 1-D quantum confinement.
- Carrier is only free to move its trajectory along the wire.

Example : nanowires, nanorod and nanotube

### iii) Quantum Dots (0-dimension)

#### Definition :

When all the three dimensions are minimized the resulting structure is known as quantum dot.

#### Explanation

- Only confined states
- has many thousands of atoms

#### use :

used in quantum computer and quantum dot lasers.

### iii) Density of states in Quantum well, Quantum wire and Quantum dot structure

#### Bulk structure :

The density of state of a bulk material is given by

$$Z(E) = \frac{8\pi\sqrt{2} m^{3/2}}{h^3} (E - E_c)^{1/2}$$

$E_c$  = bottom of conduction band energy.

$m^*$  = effective mass of electron

### Quantum well structure

- Electrons move freely in two directions (2D) in one direction.

The density of state of the quantum well structure

$$Z(E) = \frac{4\pi m^*}{h^2} E_0 > E_c, \quad i=1, 2, 3$$

### Quantum wire structure

- Provides only one non confinement direction.
- Carrier can move freely along one direction (1D)
- remaining two directions are confined for charge carrier.
- The density of states of quantum wire is proportional to  $\frac{1}{\sqrt{E}}$ .

$$Z(E) = \frac{2\sqrt{2} m^*}{h} (E - E_1)^{-1/2} \quad i=1, 2, 3$$



## Quantum dots

- all directions are confined
- no direction in which electron movement is free.

$$\chi(E) = \delta(E - E_c), \quad i = 1, 2, 3$$

- form discrete bunches of varying densities.

## 2) Write short note on Zener - Bloch oscillations

### Definition:

The oscillation of a particle confined in a periodic potential when a constant force is acting on it.

- First pointed by Bloch and Zener.

- Studying the electrical properties of crystals.

### Derivation

Zener Bloch oscillation of the particle is derived by considering the one dimensional equation of motion for an electron in constant electric field 'E'

$$F = \frac{dp}{dt} = -eE \quad \rightarrow (1)$$

p - momentum of electron

From de Broglie's concept

$$\text{momentum } p = h/\lambda$$

h - Planck's constant

$\lambda$  - de Broglie wavelength

(or)

$$p = \frac{h}{2\pi} \times \frac{2\pi}{\lambda}$$

$$= \hbar k \quad \rightarrow (2)$$

$$k = 2\pi/\lambda, \quad \hbar = h/2\pi$$

Substituting (2) in (1)

$$\frac{d}{dt}(\hbar k) = -eE$$

$$\hbar \frac{dk}{dt} = -eE$$

$$\frac{dk}{dt} = -\frac{eE}{\hbar} \quad \rightarrow (3)$$

on integration eqn (3)

$$k(t) = k(0) - \frac{eE}{\hbar} t$$

The velocity  $v$  of the electron

is given by

$$v(k) = \frac{1}{\hbar} \frac{dE}{dk}$$

$E(k)$  - energy band

Suppose energy band has the (tight binding) form

$$E(k) = A \cos ak$$

$a$  - lattice parameter

$A$  - constant

$v(k)$  is given by

$$v(k) = \frac{1}{\hbar} \frac{dE}{dk} = -\frac{Aa}{\hbar} \sin ak$$

The electron position  $x$  is

given by

$$x(t) = \int_0^t v(k(t')) dt'$$

$$x(t) = \int_0^t -\frac{Aa}{\hbar} \sin ak dt' = \int_0^t -\frac{Aa}{\hbar} \sin a \left( k(0) - \frac{eE}{\hbar} t' \right) dt'$$

$$\left( \frac{eE}{\hbar} t' \right) dt'$$

$$x(t) = x(0) - \frac{A}{eE} \cos \left( \frac{aeEt}{\hbar} \right)$$

The angular frequency of the oscillation

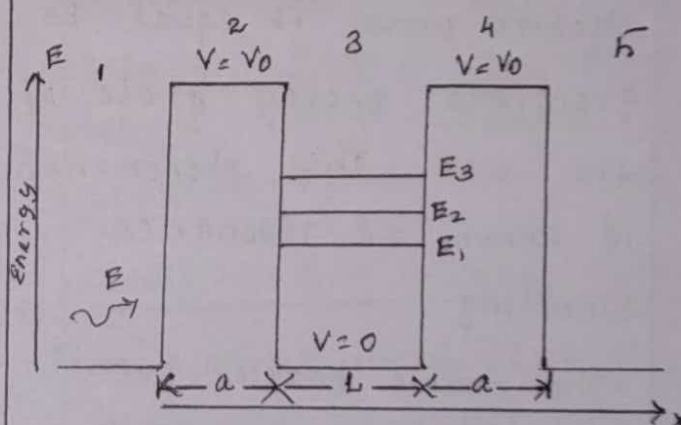
$$\omega_B = \frac{aeEt}{\hbar}$$

## Write notes on Resonant Tunneling

### Definition

The phenomenon in which the tunneling current reaches peak (maximum) value, when the energy of incident electron wave is equal to quantized energy state of the quantum well formed by the double symmetric barriers is known as resonant tunneling.

### Explanation



- Two barriers of width  $a$  separated by a potential well of small distance  $L$ .
- Leads to the concept of resonant tunneling

- Thin to allow tunneling
- Well region between two barriers is also sufficiently narrow to form discrete energy levels.
- Analysis of the double barrier structure is essentially the same as considered for single barrier tunneling.

$$E = E_n = \frac{n^2 h^2}{8 m_e L^2}$$

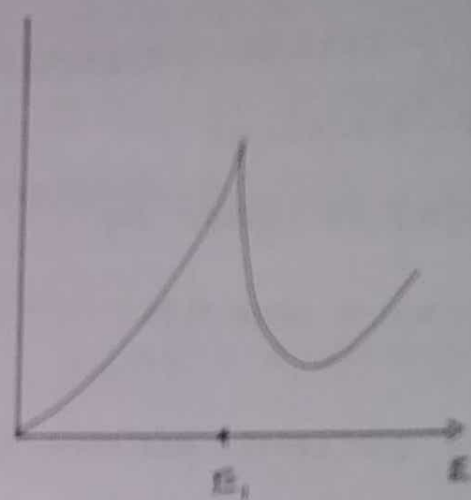
$$n = 1, 2, 3, \dots$$

Transmission probability of the double symmetric barrier is maximum and hence, the tunneling current reaches peak value when energy of electron wave is equal to quantised energy state of the well. This phenomenon is known as resonance tunneling.

The double barrier tunnel junction has important applications to a device known as a resonant tunneling diode.

•  $E$  is very different from the energy of a discrete state  $E_n$ , transmission is low.

•  $E$  tends to  $E_n$ , transmission will increase, becoming a maximum when  $E = E_n$



As  $E$  increases, tunneling will increase, reaching a peak when  $E = E_1$ .

• After that point, a further increase in  $E$  will result in a decreasing current.

• This decrease of current with an increase of bias is called negative resistance.



## Write short notes on 1) Single Electron Phenomena

### ii) Coulomb - Blockade effect.

#### 1) Single electron phenomena

- In electronics, transistor is the most important device.
- Use to compute - binary switches turning ON and OFF making logic decisions.
- Today microchips have over a billion transistors, each one turning ON and OFF of a billion times every second.
- Technology resolution drops enabling even smaller transistors.
- More transistors are squeezed into the same amount of semiconductor space.
- When each transistor is reducing to a few atoms or a single molecule, quantum effects will play a significant role.
- Present day, transistors require closer to 10,000 electrons.
- Very well be practical and necessary to move electrons one at a time.
- Single electron devices are sensitive to the transfer of even

#### Single electron charge.

- Provide a single electron devices potential application of ultra large scale integrated circuits with device size in the order of nanometres.

### ii) Coulomb - Blockade Effects

- As the size of the quantum dot decreases, the charging energy  $W_c$  of a single excess charge on the dot increases.

#### Definition

The charging effect which blocks the injection or rejection of a single charge into or from a quantum dot is called coulomb blockade effect.

#### Condition for Coulomb blockade

If two or more charges near one another, they exert coulomb forces upon each other.

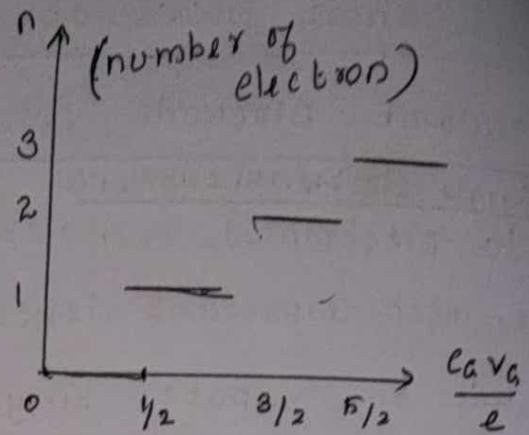
$$W_c = \frac{e^2}{2C} \gg kT$$

C - Capacitance of the quantum dot

T - Temperature of the system

$W_c$  - charging energy and this is the energy to add one negatively charged electron to the dot.

- By applying a positive bias to the gate electrode, an electron can be attracted to the quantum dot.



- In the single electron box, the electron number of the quantum dot is controlled one by one by utilizing the gate electrode.

⑤ Write notes on i) Single Electron Tunneling ii) SET

Tunneling is the way the electrons cross both the physical barriers and the energy barriers separating a quantum dot from the bulk material that surrounds it.

- Control the addition
- removal of electrons in a quantum dot.
- When the size gets reduced the capacitance also reduces to a small value.

- $W = \frac{Q^2}{2C}$ , become larger than the thermal energy  $kT$ .
- The quantization of charge can dominate and tunneling of single electrons across leaky capacitors carries the current. This is called single electron tunneling.

ii) SET

Single switching devices are essential elements in ultra large scale integrated circuits.

## Definition :

SET is three terminal switching device which can transfer electrons from source to drain one by one.

## Construction and working

- Tunneling junctions in place of PN-junctions
- quantum dot in place of the channel region of the FET.
- To control tunneling a voltage bias to the gate electrode is applied.
- A separate voltage bias is applied between source and drain electrodes for the current direction.

For current to flow gate bias voltage must be large enough to overcome the Coulomb blockade energy.

Energy -  $E$ , charge -  $Q$

Potential difference -  $V$

$$E = VQ$$

Charge of an electron  $Q = e$

$$V = \frac{E}{e} = \frac{W_c}{e}$$

Since  $E = W_c$

$W_c$  - charging energy

$$V = \frac{\frac{e^2}{2C}}{e} = \frac{e}{2C} \rightarrow (1)$$

• voltage applied  $\left( \because W_c = \frac{e^2}{2C} \right)$

to the quantum dot, an electron can tunnel through Coulomb blockade of the quantum dot.

• once the quantum dot gets an electron, its potential energy rises.

• Dot is empty and potential is lower again the process repeats.

• When gate voltage  $V_g$  is zero, no current flows

• The first gate voltage which is large enough to move an electron through the Coulomb blockade is called  $V_{\text{Coulomb}}$ .

• For single electron tunneling  $V_g = V_{\text{Coulomb}}$  if the gate voltage equals



$$V_{\text{Coulomb}} + \frac{e}{2e} + \frac{e}{2e} = V_{\text{Coulomb}} + \frac{e}{e}$$

- Number of electrons in the quantum dot is controlled using the gate voltage.
- ON and OFF states can be utilized to make an effective switch out of a SET.
- The gate voltages for a SET are a few millivolts and source-to-drain currents are in the pico ampere range.

#### Advantages

- No wire is needed between arrays. The size of each cell can be as small as 2.5 nm.

• used for the next generation quantum number.

#### Limitations:

- It is very hard to fabricate by traditional optical lithography and semiconductor process.
- Circuits must be arranged into larger 2D patterns.

#### Applications:

- used for mass data storage.
- used in highly sensitive electrometer.
- used in sensor technology, and digital electronic circuits.

### ② Discuss on Spintronics

- Spin of the electron can be used rather than its charge to create a remarkable new generation of spintronic devices.
- Spintronics is the abbreviation of spin transport also known as spin electronics.

#### Principle

- Information is stored into spins as a particular spin orientation.
- The spins being associated to mobile electrons carry the information along a wire.
- The information is read at a terminal.

## Spintronic Devices

### Spin Valve

- A Spin valve is a device which provides the Giant Magnetoresistive effect.

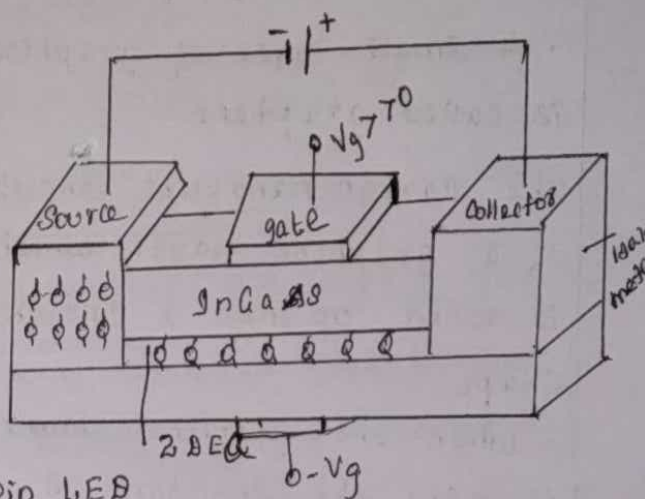
- highly resistive or highly conductive.
- very fast switching speeds and reduced power consumption.

### Spin FET

- A Spin based Field Effect Transistor.
- Spins have to be injected from Source into the non-magnetic layer, then transmitted to the Collector.
- Reach the Collector due to the spin-orbit coupling effect.
- The net spin polarization is reduced.
- Electrical field is applied Perpendicularly to the plane.
- When  $V_g$  is zero the injected spins which are transmitted through the 2DEG (2-Dimensional Electron Gas), reducing the net spin polarization.

When  $V_g \gg 0$  the precession of the electrons is controlled with electrical field thereby allowing the spins to reach at the collector with the same polarization.

- By controlling the gate voltage and polarity the current in the collector can be modulated just like the MOSFET of the conventional electronics.



Spin LED

Due to this spin dependent polarization a device such as a Spin LED can be used to produce light of a specific polarization.

- Spin LEDs can be used in the study and development of other spintronic devices.

## Advantages of Spintronic devices over Conventional electronic devices

- Spintronic devices are new logic devices which enhances functionality, high speed and reduced power consumption.
- Less power dissipation.

### ⑦ Write short notes on Carbon Nanotubes (CNT)

• A group of nanostructures with large potential applications are Carbon nanotubes.

• The hexagonal lattice of carbon is simply graphite.

• A single layer of graphite is called graphene.

The carbon nanotube consists of a graphene layer which is rolled up into a cylindrical shape.

• When the graphene layer is rolled, the structure is tube like and it is a single molecule.

#### Structures of CNT :

CNTs have many structures on the basis of their length, type of spiral and number of layers.

- Act as both a metal or a semiconductor.

#### Types of CNT structure

• 3 types

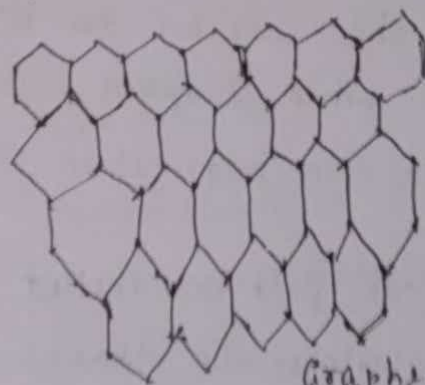
i) Arm-chair structure

ii) zig-zag structure

iii) chiral structure.

#### Arm chair structure

• axis of the tube parallel to C-C bonds of the carbon hexagons.



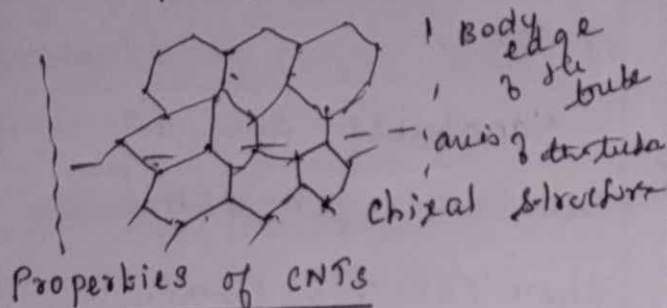
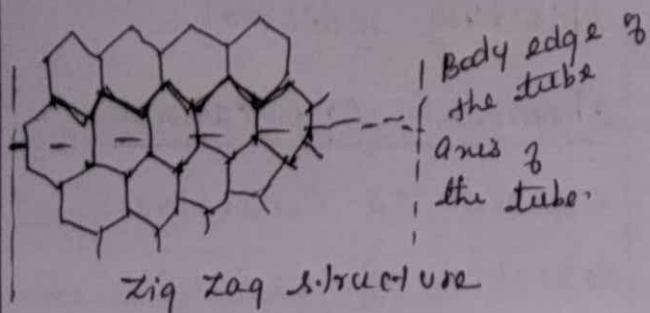
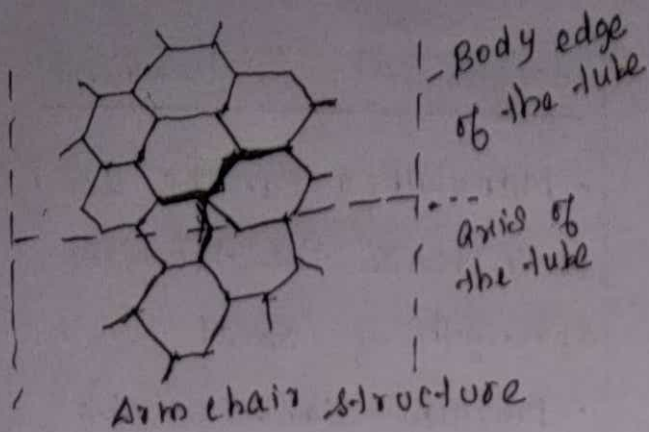
Graphene sheet

#### ii) Zig zag and chiral

• Zig zag structure consists of tube axis perpendicular to C-C bonds.

• In chiral structure C-C bond inclined towards the axis of the tube.





### Properties of CNTs

#### a) Electrical Properties

- i) Depending on the diameter and chirality.
- ii) Energy gap of semiconducting chiral carbon nanotubes is inversely proportional to the diameter of the tube.
- iii) Reaches a minimum value
- iv) Discrete electronic states that are coherent between the electrical contacts.

#### b) Mechanical Properties

- i) Strength of the carbon-carbon bond is very high

ii) Young's modulus of CNT is about 1.8 TPa

iii) High ultimate tensile strength.

iv) Ability to withstand extreme strain.

#### c) Physical Properties

i) High strength-to-weight ratio.

ii) Light weight applications.

iii) Surface area of nanotubes is the order of 10-20 m<sup>2</sup>/g higher than graphite.

#### d) Chemical Properties

- i) Nanotubes are highly resistant to any chemical reaction.
- ii) Temperature is not a limitation in practical application of nanotubes.

#### e) Thermal Properties

- High thermal conductivity
- Value increases with decrease in diameter.

## Applications of Carbon Nano tubes

### Electrical and Electronics applications

- used in development of flat Panel displays.
- Vacuum tube lamps that are bright as conventional light bulbs with long life time and more efficient can be produced using CNT.
- Switching time of the devices is very fast.
- Carbon nanotubes with diameters of 2nm have low resistance.

### Computer applications

Carbon nanotubes can be used to make a computer switching device.

### Battery technology

- Carbon nanotubes have many applications in battery technology.
- Lithium is a charge carrier in some batteries, stored inside nanotube.

## Mechanical Applications

- Nanotubes can be used to increase the tensile strength of steel.
- Provides light weight shielding material.

### Chemical Applications

- used as sensitive detector of various gases.
- Nanotubes act as catalysts for some chemical reactions.

# write notes on Semiconductor for photonic structures

## Photonic Crystals

- It is a medium in which refractive index varies periodically on the order of wavelength of light.
- Guide the motion of photons using the photonic band gap.
- Made from periodic patterns of materials with different permittivities.
- Interface between two materials of different permittivity, the photon may be reflected.
- Arrangement of atoms in a material's crystal lattice.
- Photonic band gap is a range of photon wavelengths are forbidden.
- Cannot pass through the photonic crystal.
- A photonic crystal can organize photons based on their energy.

## Types of photonic crystals

• 3 types

- i) 1D photonic crystal
- ii) 2D photonic crystal
- iii) 3D photonic crystal

### 1D photonic crystal

- 1D photonic crystal is a one-dimensional virtual medium.
- Different dielectric constant are periodically deposited.
- A Bragg grating is an example of this type of photonic crystal.

### Applications

- A graphene-based Bragg grating supports excitation of surface electromagnetic waves in the periodic structure by using He-Ne laser 633 nm as the light source.
- 1D graphene dielectric photonic crystal can act as a far IR filter.



## 2D photonic crystals

- Periodically modulated in two dimensions.

The permittivity of the periodic medium is given by

$$\epsilon(r + a_j) = \epsilon(r)$$

## 3D photonic crystals

- Dielectric constant is made to vary periodically in three dimensions.
- Prohibits electromagnetic propagation.
- The large 3D periodic nanostructures can be produced by
  - Layer by layer photolithography
  - Colloidal self assembly
  - Direct laser writing
  - Holographic lithography.

## Q) Write short notes on photo process

There are important processes. They are

- i) photon absorption
- ii) photon emission
- iii) photon scattering.

- An electron across the band gap separating the unfilled conduction band of silicon from the filled valence band. This is known as "interband absorption".

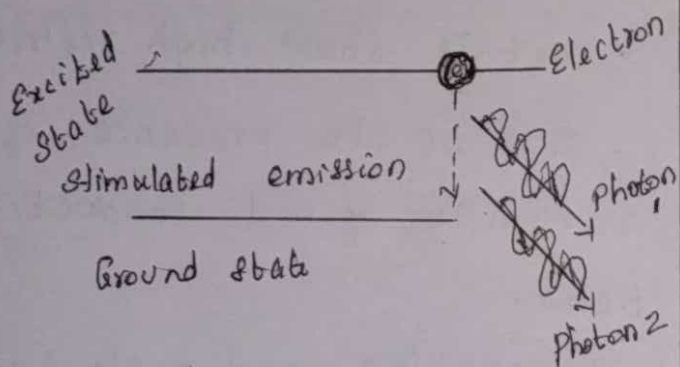
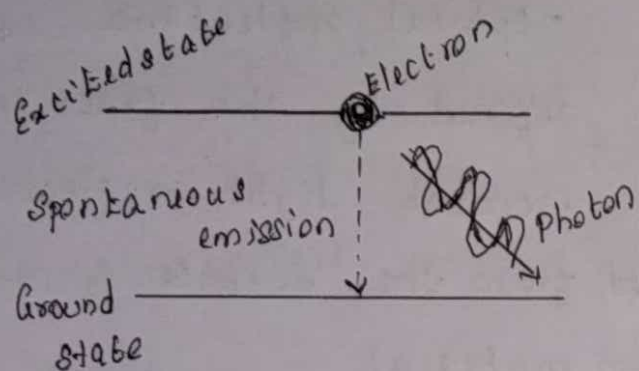
- In conductors, numerous available energy states within the partially filled valence band and valence electrons can also absorb lower energy photons. This is known as "intraband absorption".

## Spontaneous and Stimulated emission

An excited electron can emit a photon on its own or when prompted by an incoming photon.

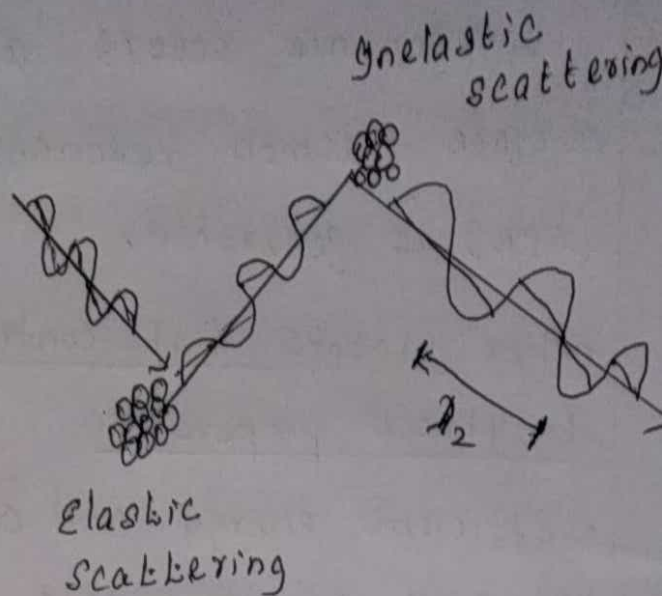
• Electron drops back to its ground state.

• In stimulated emission, the incoming photon is not absorbed by the electron but continues on, in phase and in the same direction as the newly emitted photon 2.



### Photon Scattering

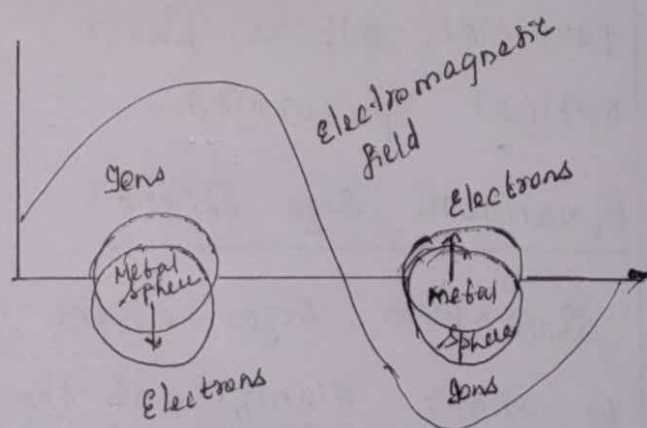
A kind interaction between photons and matter is scattering. Scattering occurs when a photon changes direction after it strikes a bit of matter. This is usually a type of scattering called elastic scattering.



### Photo process in nano structures

change in optical properties is due to the quantum confinement of electrons in nanomaterials and surface plasma resonance.

### Surface Plasmon



Surface Plasmon is the natural oscillation of electron gas inside the nanosphere.



• resonance occurs and surface plasmon resonance (SPR) is generated.

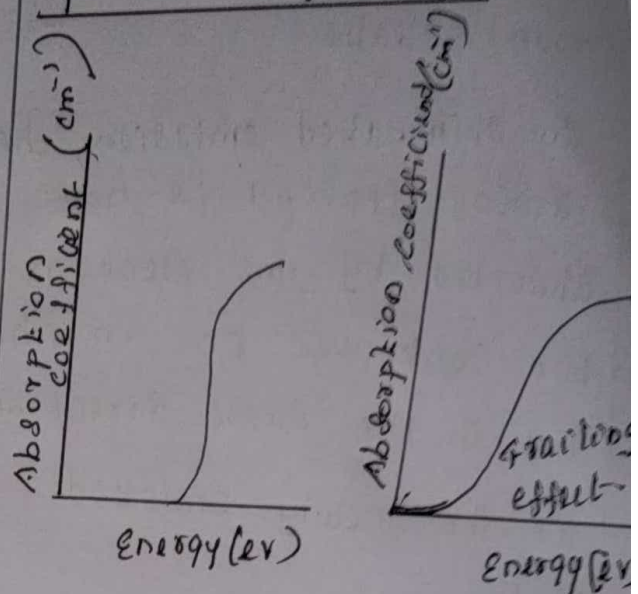
### Other factors that contribute to photon properties

- Efficient energy and charge transfer in nanoscale dimension further contribute to the novel properties.
- Linear and nonlinear optical properties of the material can be finely tuned by controlling their dimension and surface chemistry.
- A change in size of the edge semiconductor nanoparticles alters their optical properties.

### Quantum Size Effect

Quantum size effect is most significant in semiconductor nanoparticles.

### Optical Reflectance



- Optical reflectance is defined by the fraction of incident light reflected from the surface of a material.
- Metals show high reflectance.
- Due to the presence of a partially filled conduction band.
- Absorption and reflection of photons take a continuum of energies from the infra red to visible region.

### Applications based on photo process.

Optical properties of nano materials in the areas of optical detectors, lasers, sensors, imaging, photoelectrochemistry.



1. Suitable for optoelectronic materials such as switches, amplifiers, gratings, splitters and detectors.
  2. widely used in polymers to increase their refractive index, which makes them suitable as optical components.
  3. Nanoparticles in coatings improve shielding against electromagnetic fields in computers.
  4. LEDs and organic LEDs developed using nanomaterials show better resolution of images.
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