PH3251- MATERIAL SCIENCE

REGULATION - 2021

DEPARTMENT OF PHYSICS

PH3251 **MATERIALS SCIENCE** **L T P C**
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COURSE OBJECTIVES:

- To make the students to understand the basics of crystallography and its importance in studying materials properties.
- To understand the electrical properties of materials including free electron theory, applications of quantum mechanics and magnetic materials.
- To instil knowledge on physics of semiconductors, determination of charge carriers and deviceapplications
- To establish a sound grasp of knowledge on different optical properties of materials, optical displays and applications
- To inculcate an idea of significance of nano structures, quantum confinement and ensuing nano device applications.

UNIT I CRYSTALLOGRAPHY 9

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.

UNIT II ELECTRICAL AND MAGNETIC PROPERTIES OF MATERIALS 9

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 bands in solids – tight binding approximation - Electron effective mass – concept of hole. Magnetic materials: Dia, para and ferromagnetic effects – paramagnetism in the conduction electrons in metals – exchange interaction and ferromagnetism – quantum interference devices – GMR devices.

UNIT III SEMICONDUCTORS AND TRANSPORT PHYSICS 9

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.

UNIT IV OPTICAL PROPERTIES OF MATERIALS 9

Classification of optical materials – Optical processes in semiconductors: 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 –excitonic state – Electro-optics and nonlinear optics: Modulators and switching devices – plasmonics.

UNIT V NANOELECTRONIC DEVICES 9

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.

TOTAL: 45 PERIODS

COURSE OUTCOMES:

At the end of the course, the students should be able to

- know basics of crystallography and its importance for varied materials properties
- gain knowledge on the electrical and magnetic properties of materials and their applications
- understand clearly of semiconductor physics and functioning of semiconductor devices
- understand the optical properties of materials and working principles of various optical devices
- appreciate the importance of functional nanoelectronic devices
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TEXT BOOKS:

1. V.Raghavan. Materials Science and Engineering: A First Course, Prentice Hall India Learning Private Limited, 2015.
2. S.O. Kasap, Principles of Electronic Materials and Devices, Mc-Graw Hill, 2018.
3. Jasprit Singh, Semiconductor Devices: Basic Principles, Wiley (India), 2007.
4. Jasprit Singh, Semiconductor Optoelectronics: Physics and Technology, Mc-Graw Hill India (2019)
5. G.W.Hanson. Fundamentals of Nanoelectronics. Pearson Education (Indian Edition), 2009.

REFERENCES:

1. R.Balasubramaniam, Callister's Materials Science and Engineering. Wiley (Indian Edition), 2014.
2. Wendelin Wright and Donald Askeland, Essentials of Materials Science and Engineering, CL Engineering, 2013.
3. Robert F.Pierret, Semiconductor Device Fundamentals, Pearson, 2006
4. Pallab Bhattacharya, Semiconductor Optoelectronic Devices, Pearson, 2017
5. Ben Rogers, Jesse Adams and Sumita Pennathur, Nanotechnology: Understanding Small Systems, CRC Press, 2017.

UNIT I - CRYSTALLOGRAPHY

Crystal structures: BCC, FCC and HCP - directions and planes - linear and planar densities –- crystal imperfections: edge and screw dislocations- grain and twin boundaries – Burger vectors and elastic strain energy – Slip systems – plastic deformation of materials – polymorphism – phase changes – nucleation and growth – homogenous and heterogeneous nucleation.

INTRODUCTION

The matters in this world are classified as solids, liquids and gases. These materials are made up of atoms and molecules. Materials differ from one another on their properties. These differences in properties of the solids are due to their structures. The behavior of a solid material is closely related to its structure.

CLASSIFICATION OF SOLIDS

On the basis of crystal structure materials are broadly classified as

1. Crystalline solids 2. Non-Crystalline or Amorphous solids

CRYSTALLINE SOLIDS OR CRYSTALS: Materials in which the atoms are arranged in systematic pattern are known as crystalline solids. They have well defined geometrical form. *Examples:* Diamond, copper, platinum, silver, polonium, etc.

The crystals are of two forms

1. Single crystal 2. Poly crystal

Single crystal contains only one crystal. Poly crystal is an aggregate of many small crystals separated by well-defined grain boundaries.

AMORPHOUS SOLIDS: Materials in which the atoms are arranged in an irregular fashion are known as non-crystalline solids. *Examples:* Plastics, Rubber and Glass

CRYSTALLOGRAPHY

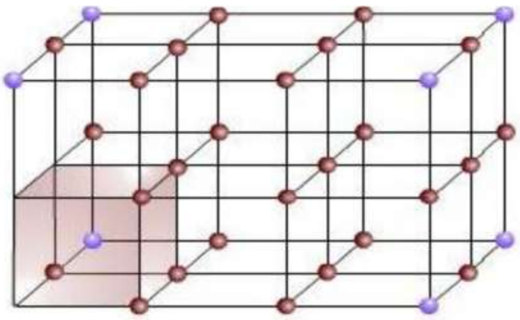
The branch of physics that deals with the structure, properties and external or internal symmetries in crystals are known as crystal physics or crystallography.

FUNDAMENTALS OF CRYSTALLOGRAPHIC TERMS

1. LATTICE: It is defined as an array of points which represents the position of atoms in the crystals in three dimensions. It is an imaginary concept.

2. SPACE LATTICE: The geometrical representation of the crystal structure in terms of lattice points is called space lattice, provided the environment about every point is identical to that of every other point.

2 dimensional form of space lattice



3 D form

3. LATTICE POINTS: The points in the space lattice are called lattice points

4. LATTICE LINE: The lines joining the lattice points are called as lattice line.

5. LATTICE PLANE: The place containing the lattice points are called as lattice plane.

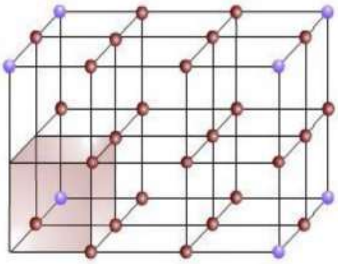
6. BASIS: The crystal structure is formed by associating unit assembly of atoms or molecules with every lattice point. This unit assembly of atoms or molecules is called basis or motif.

7. CRYSTAL STRUCTURE: Crystal structure is formed by combining space lattice with a basis.

Space lattice + Basis → Crystal Structure

8. UNIT CELL:

A unit cell is defined as the smallest geometric figure which on repetition in three dimension gives the actual crystal structure. It is also defined as fundamental elementary pattern with minimum number of atoms or molecules which represents the total characteristics of the crystal.



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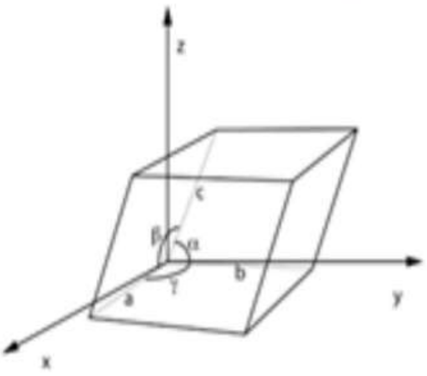
9. LATTICE PARAMETERS:

Fig shows the unit cell of a three-dimensional crystal lattice. The intercepts a, b and c are nothing but the edges of the unit cell which defines the dimensions of a unit cell. These are known as primitives or characteristic intercepts on the axes. The distance between two lattice points is known as axial length. The angles between (a, b), (b, c) and (c, a) are denoted by γ, α and βrespectively. These three angles (γ, α and β)



are called interfacial angles. Both intercepts and interfacial angles form the lattice parameters of unit cell.

10. PRIMITIVE CELL: The primitive cell is the simplest type of unit cell which contains only one lattice point (only one atom) per unit cell. *Example:* Simple cubic

11. NON – PRIMITIVE CELLS: If more than one lattice point (more than one atom) in a unit cell, it is called a non-primitive cell. *Example:* BCC and FCC

THE CRYSTAL SYSTEMS & BRAVAIS LATTICES

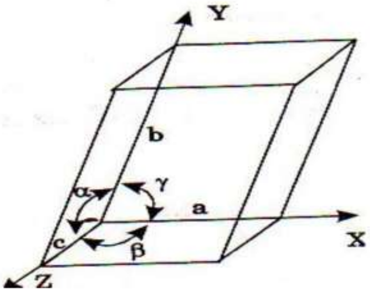
Crystals are classified into 7 crystal systems based on lattice parameters. The 7 basic crystal systems are

1. Triclinic 2. Monoclinic 3. Orthorhombic 4. Tetragonal 5. Hexagonal 6. Trigonal (or) Rhombohedral and 7. Cubic

BRAVAIS LATTICES: According to Bravais there are only 14 possible ways of arranging points in space lattice from the seven crystal systems such that all the lattice points have the same surroundings. These 14 space lattices are called the Bravais lattices.

Let us discuss seven crystal systems and each ***Bravais lattice*** now.

1. MONOCLINIC SYSTEM:



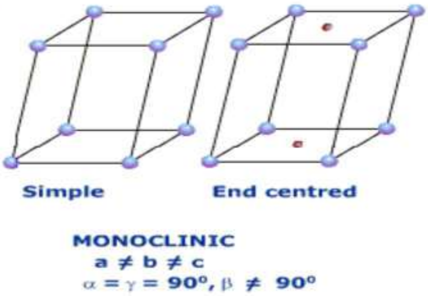
In this system three axes are of different lengths. Two axes are perpendicular to each other and third is obliquely inclined

i.e., $a \neq b \neq c$ and $\alpha = \gamma = 90^0$; $\beta \neq 90^0$

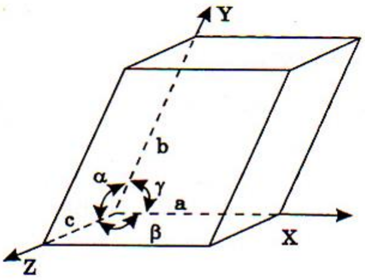
Example: Sodium Sulphite (Na_2SO_4), Ferrous Sulphate ($FeSO_4$)

Monoclinic latticehas two possible space lattices.

(a) Simple monoclinic lattice: It has lattice points at all 8 corners of the unit cell.



(b) Base centered monoclinic lattice: It has lattice points at all 8 corners of the unit cell and 2 lattice points each at the center of two faces opposite to each other.



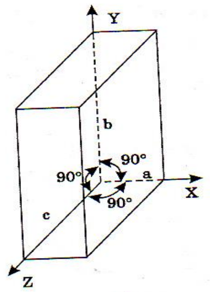
2. TRICLINIC SYSTEM:

In this all the crystal axes are of unequal lengths and all are oblique to each other. *i.e.,* $a \neq b \neq c$ *and* $\alpha \neq \beta \neq \gamma \neq 90^0$

Example: Copper sulphate ($CuSO_4$), Potassium dichromate ($K_2Cr_2O_7$)

Triclinic lattice has only one possible type of arrangement.

(a) Simple triclinic lattice: It has lattice points at all 8 corners of the unit cell.

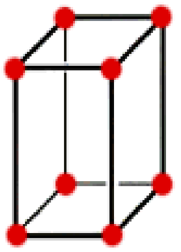


3. ORTHORHOMBIC SYSTEM: In this system three axes are of different lengths and are perpendicular to each other.

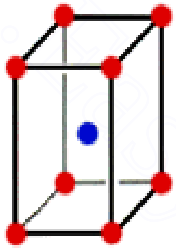
i.e., $a \neq b \neq c$ and $\alpha = \beta = \gamma = 90^0$

Example: Sulphur, Topaz

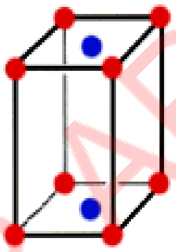
Orthorhombic systemhas four possible types of space lattices.



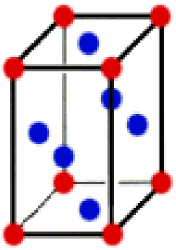
Simple orthorhombic



Body-centered orthorhombic



Base-centered orthorhombic



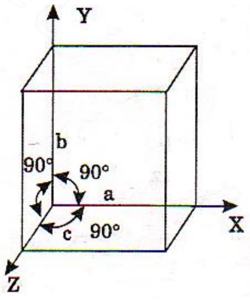
Face-centered orthorhombic

(a) **Simple Orthorhombic lattice:** It has lattice points at all 8 corners of the unit cell.

(b) **Body CenteredOrthorhombic lattice:** It has lattice points at all 8 corners of the unit cell and one lattice point at the centre of the body as shown in figure.

(c) **Face CenteredOrthorhombic lattice:** It has lattice points at all 8 corners of the unit cell and 6 lattice points at the centre of each of the 6 faces of the unit cell as shown in figure.

(d) **Base - CenteredOrthorhombic lattice:** It has lattice points at all 8 corners of the unit cell and 2 lattice points each at the centre of two faces (base) opposite to each other as shown in figure.



4. TETRAGONAL SYSTEM: In this the three axes are perpendicular to each other and two axes are equal in length and the third axis may be longer or shorter.

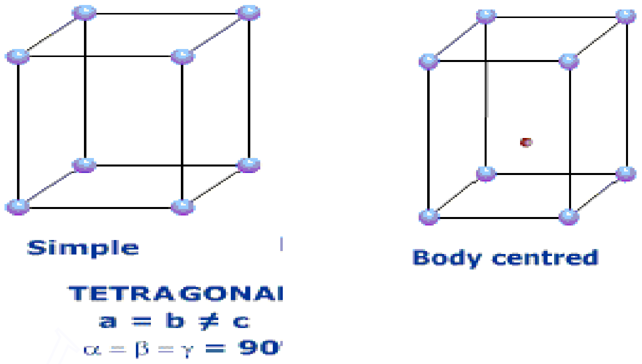
i.e., $a = b \neq c$ and $\alpha = \beta = \gamma = 90^0$

Example: Ordinary white tin, Indium, Tin oxide

Tetragonal lattice has two possible types of arrangement

(a) **Simple tetragonal lattice:** It has lattice points at all 8 corners of the unit cell.

(b) Body centered tetragonal lattice: It has lattice points at all eight corners of the unit cell and one lattice point at the centre of the body.



5. HEXAGONAL SYSTEM:

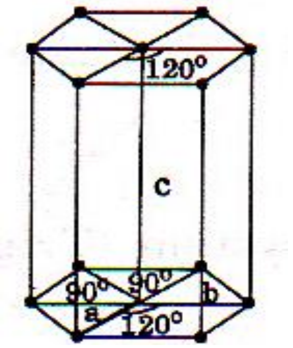
In this system, two axial lengths of unit cell (say horizontal) are equal and lying on one plane at an angle 120^0 with each other. The third axial length (say vertical) is either longer or shorter than other two and it is perpendicular to this plane.

i.e., $a = b \neq c$ *and* $\alpha = \beta = 90^0$; $\gamma = 120^0$

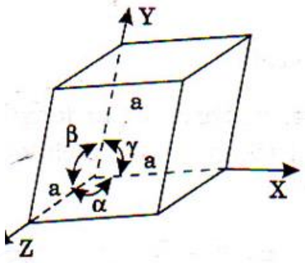
Example: Quartz, Tourmaline.

Hexagonal lattice has only one possible type of arrangement.

(a) Simple hexagonal lattice: It has lattice points at all 12 corners of the hexagonal prism and 2 lattice points each at the centre of two hexagonal faces of the unit cell.



6. RHOMBOHEDRAL SYSTEM (TRIGONAL): In this system, three axial lengths of the unit cell are equal. They are equally inclined to each other at an angle other than 90^0



i.e., $a = b = c$ and $\alpha = \beta = \gamma \neq 90^0$

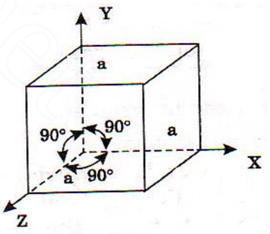
Example: Calcite, Bismuth, $CaSO_4$

Rhombohedral lattice has only one possible type of arrangement

(a) Simple Rhombohedral lattice: It has lattice Points at all 8 corners of the unit cell.

7. CUBIC SYSTEMS:

In this crystal system, all the three axial lengths of the unit cell are equal, and they are perpendicular to each other.



i.e., $a = b = c$ and $\alpha = \beta = \gamma = 90^0$

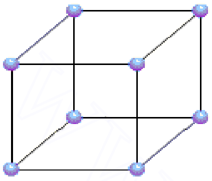
Example: Iron, Copper, Sodium Chloride (NaCl), Calcium Fluoride (CaF_2)

Cubic lattice has three possible types of arrangements.

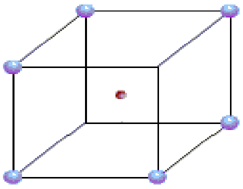
(a) Simple (or primitive) cubic lattice: It has lattice points at all 8 corners of the unit cell as shown in figure.

(b) Body centered cubic lattice: It has lattice points at all 8 corners of the unit cell and one lattice point at the centre of the body as shown in figure.

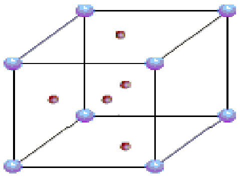
(c) Face centered cubic lattice: It has lattice points at all 8 corners of the unit cell and one lattice point at the centre of each of 6 faces of the cube as shown in the figure.



Simple cube



Body centred cube (fcc)



Face centred cube (fcc)

These 14 types of space lattices are called Bravais lattices. It is mathematically proved that there are only 14 independent ways of arranging points in three dimensional space such that each arrangement confirms to the definition of space lattice.

l. No.	Crystal System	Bravais lattice	
1.	Cubic	3	Simple Body centered Face centered
2.	Tetragonal	2	Simple Body centered
3.	Orthorhombic	4	Simple Body centered Base centered Face centered
4.	Monoclinic	2	Simple Base centered
5.	Triclinic	1	Simple
6.	Rhombohedral (Trigonal)	1	Simple
7.	Hexagonal	1	Simple
Total		**14**	

Sl. No	Crystal systems	Axial lengths (a, b, c)	Interfacial angles (α, β, γ)	Example
1.	Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^0; \beta \neq 90^0$	Na_2SO_4, $FeSO_4$
2.	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^0$	$CuSO_4$, $K_2Cr_2O_7$
3.	Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^0$	Sulphur, Topaz
4.	Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^0$	Ordinary white tin, Indium
5.	Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^0; \gamma = 120^0$	Quartz, Tourmaline
6.	Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^0$	Calcite, Bi, Sb, $CaSO_4$
7.	Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^0$	Iron, Copper, NaCl, CaF_2

CHARACTERISTICS OF THE UNIT CELL

A unit cell is characterized by the following properties.

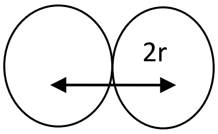
- *Number of atoms per unit cell*
- *Coordination number*
- *Nearest neighboring distance*
- *Atomic radius*
- *Packing factor*

1. Number of atoms per unit cell: The total number of atoms present in an unit cell is known as number of atoms per unit cell or effective number.

2. Coordination number: It is the number of nearest atoms directly surrounding a particular atom. If the coordination number is high, then the crystal is highly closely packed. If it is low, then the structure is loosely packed.

3. Nearest neighbouring distance (2r): It is the distance between the centers of two nearest neighbouring atoms. It is expressed in terms of the length of edge of the unit cell *'a'* and it is *'2r'*

$a = 2r$



4. Atomic radius (r): It is half of the distance between two nearest neighbouring atoms in a crystal. It is denoted by *'r'*

$r = \frac{a}{2}$, Where $a \rightarrow$ cube edge (edge distance)

5. Packing factor (PF): Packing factor is defined as the ratio of the total volume occupied by the atoms in a unit cell to the total volume of a unit cell. It is also known as density of packing.

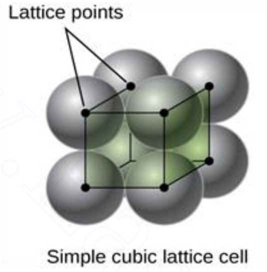
$$\text{Packing factor } (PF) = \frac{\text{Total volume occupied by the atoms in a unit cell } (v)}{\text{Total volume of the unit cell } (V)} = \frac{v}{V}$$

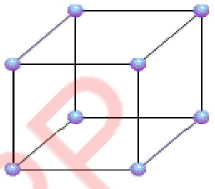
$$= \frac{Number\ of\ atoms\ present\ in\ a\ unit\ cell\ \times Volume\ of\ one\ atom}{Total\ volume\ of\ the\ unit\ cell}$$

CRYSTAL STRUCTURES (SC, BCC, FCC, HCP and DIAMOND CUBIC)

It is noted that a large number of metallic crystal structures have HCP, FCC and BCC structures. Simple Cubic (SC) structure is very rare in metals.

SIMPLE CUBIC STRUCTURE: Figure shows the unit cell of a simple cubic structure. In this structure, there is one atom at each of the 8 corners of the unit cell. Let us find the characteristics of the SC structure.





Simple cube

1. Number of atoms per unit cell:

Simple cube has 8 corners, each corner has 1 atom. But each corner atom is shared by 8 adjacent unit cells. So, each atom will give its $\frac{1}{8}^{th}$ part to one unit cell

$$Total\ number\ of\ atoms\ in\ one\ unit\ cell = \frac{1}{8} \times total\ no.of\ corner\ atoms$$

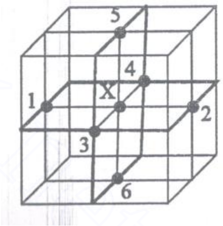
$$= \frac{1}{8} \times 8 = 1$$

$Total\ number\ of\ atoms\ in\ one\ unit\ cell = 1$

Thus, the simple cubic is a primitive cell.

2. Co-ordination number

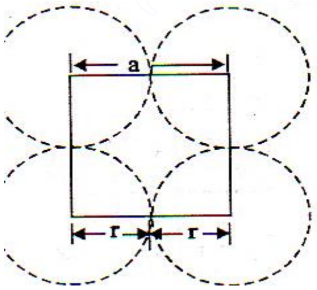
If we consider on corner atom as X, then it is directly surrounded by 6 other atoms. So, Coordination number is 6.



3. Atomic radius:

Consider a face of unit cell of simple cubic structure as shown in figure. The atoms touch each other along the edges of the cube.

The distance between the centre of the nearest atoms is equal to the cube edge *a*. If *'a'* is the side of the unit cell and *'r'* be the radius, then



$$2r = a\ ; \qquad \boxed{r = \frac{a}{2}}$$

4. Packing factor:

$No. of\ atoms\ per\ unit\ cell\ =\ 1$

$Volume\ of\ one\ atom = \frac{4}{3}\pi r^3$ $\qquad$ $Volume\ of\ atoms\ in\ the\ unit\ cell, v = 1 \times \frac{4}{3}\pi r^3$

$Volume\ of\ the\ unit\ cell, V = a^3$ $\qquad$ $\therefore Packing\ factor\ P.F = \frac{v}{V} = \frac{4/3\pi r^3}{a^3}$

$$P.F = \frac{\frac{4}{3\pi r^3}}{(2r)^3} \qquad (\because a = 2r)$$

$$P.F\ =\ \frac{4\pi r^3}{8\times3\times r^3} P.F\ = \frac{\pi}{6} \qquad P.F = 0.5236$$

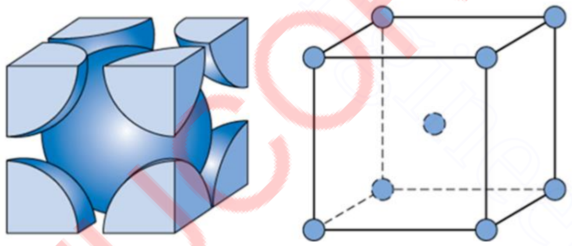
$$Packing\ factor\ =\ 0.5236 \times 100\ \% \qquad \boxed{P.F = 52\%}$$

Therefore 52% of the volume of unit cell is occupied by atoms and remaining 48% is vacant.

Example: Only one element Polonium (Po) at certain temperature range exhibits this structure.

BODY CENTERED CUBIC STRUCTURE (BCC)

This type of unit cell has 8 corners, and each corner has one atom and one more atom present at the centre of the body. Let us find the characteristics of a BCC unit cell.



1. Number of atoms per unit cell:

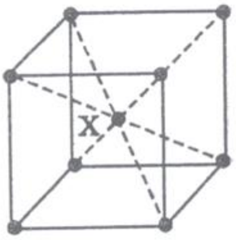
Body centered cube has 8 corners, each corner has 1 atom. But each corner atom is shared by 8 adjacent unit cells. So, each atom will give its $\frac{1}{8}^{th}$ part to one unit cell

$$Total\ number\ of\ corner\ atoms\ in\ one\ unit\ cell = \frac{1}{8} \times total\ no. of\ corner\ atoms$$

$$Total\ number\ of\ corner\ atoms\ in\ one\ unit\ cell = \frac{1}{8} \times total\ no. of\ corner\ atoms = \frac{1}{8} \times 8$$

$Number\ of\ body\ centerd\ atoms\ in\ one\ unit\ cell = 1$

$Total\ number\ of\ atoms\ in\ one\ cell\ is = \left(\frac{1}{8} \times 8\right) + 1 = 1 + 1 = 2\ atoms$

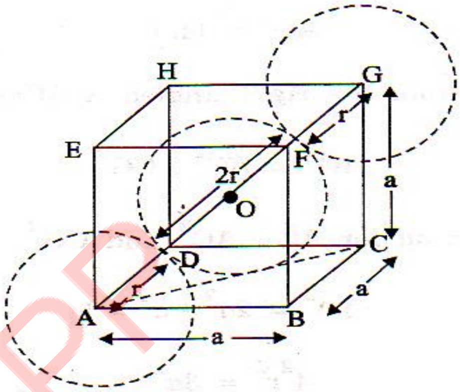


2. Co-ordination number:

If we consider the body centered atom, it is directly surrounded by 8 corner atoms. So, the coordination number is 8.

3. Atomic radius:

Here the corner atoms do not touch each other. But each corner atom touches the central atom. The side of a unit cell is 'a'. Consider the atoms at A, G and O at the centre of the cell. These atoms lie in one straight line along the body diagonal AG.



From fig., $AG^2 = AC^2 + CG^2 \quad ----(1)$

$AC^2 = AB^2 + BC^2 \quad ----(2)$

Substitute (2) in (1), we get

$$AG^2 = AB^2 + BC^2 + CG^2$$

$AG = 4r; \quad AB = a; \quad BC = a; \quad CG = a$

$(4r)^2 = a^2 + a^2 + a^2$

$16r^2 = 3a^2 \qquad r^2 = \frac{3a^2}{16} \qquad \boxed{r = \frac{\sqrt{3}a}{4}}$

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

4. Packing factor

$No.of\ atoms\ per\ unit\ cell\ =\ 2 \qquad \therefore Volume\ of\ two\ atoms, v = 2 \times \frac{4}{3}\pi r^3$

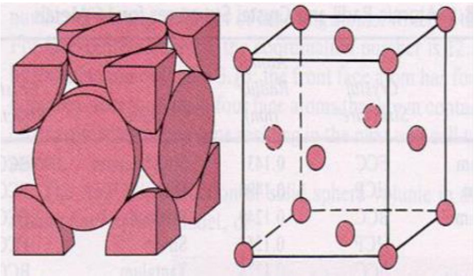
$Volume\ of\ unit\ cell, V = a^3 \qquad Packing\ Factor = \frac{v}{V} = \frac{2\times 4/3\pi r^3}{a^3}$

$$P.F\ = \frac{2 \times 4 \times \pi r^3}{3 \times \left(\frac{4r}{\sqrt{3}}\right)^3}$$

$$P.F\ = \frac{2 \times 4 \times \pi \times r^3 \times 3 \times \sqrt{3}}{3 \times 4 \times 4 \times 4 \times r^3}$$

$P.F\ = \frac{\sqrt{3}\pi}{8} \qquad P.F = \frac{1.732 \times 3.14}{8} \qquad P.F = 0.68 \qquad \boxed{P.F = 68\%}$

$\therefore$ 68% of the volume is occupied by atoms and 32% volume is vacant.



Example: Tungsten, Chromium and Molybdenum

FACE CENTERED CUBIC STRUCTURE (FCC)

This type of unit cell has 8 corners and each corner has 1 atom also each face (totally 6 faces) has 1 atom at its centre.

1. Number of atoms per unit cell:

A unit cell of FCC structure has 8 corner atoms; each corner atom is shared by 8 adjoining cells.

$\therefore$ Number of atoms in unit cell due to the contribution of corner atoms$=\frac{1}{8}\times 8 = 1$ atom.

Also there are 6 face centered atoms and each face centered atom is shared by 2 adjacent unit cells.

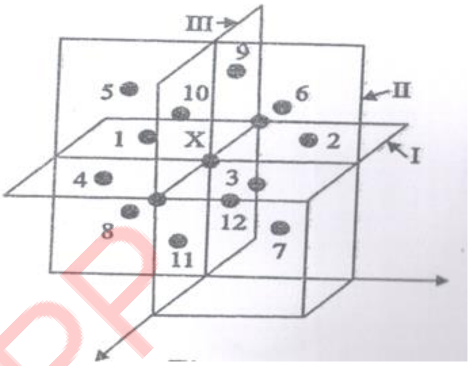
$\therefore$ $Number\ of\ face\ centered\ atoms\ in\ the\ unit\ cell\ = 1/2 \times 6 = 3\ atoms.$

$\therefore$ $Total\ number\ of\ atoms\ in\ a\ unit\ cell\ = 1 + 3 = 4$

2. Co-ordination number:

FCC structure has 8 atoms at the 8 corners and 6 atoms at the centers of six faces of a unit cell. If we consider corner atom as X, then it is directly surrounded by 12 other atoms (both corner and face centered atoms).

$\therefore$ The co-ordination number is = 12.



3. Atomic radius:

The atoms touch each other along the diagonal of any face of the cube. The length of diagonal of the face is $4r$

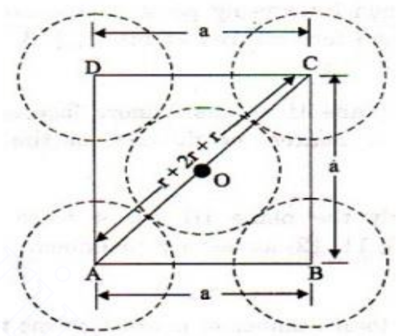
$in\ \triangle ABC,$ $AC^2 = AB^2 + BC^2$

From the figure, $AC = 4r;\ AB = a;\ BC = a$

$$(4r)^2 = a^2 + a^2$$

$$16r^2 = 2a^2$$

$$r^2 = \frac{2a^2}{16} \qquad \boxed{r = \frac{\sqrt{2}a}{4}} \qquad \boxed{a = \frac{4r}{\sqrt{2}}}$$



4. Packing factor:

Number of atoms per unit cell = 4 $\therefore$ Volume of 4 atoms, $v = 4 \times \frac{4}{3}\pi r^3$

Volume of unit cell $V = a^3$

Packing factor $PF = \frac{v}{V}$

$$P.F = \frac{4 \times 4\pi r^3}{3 \times a^3}$$

$$But\ a = \frac{4r}{\sqrt{2}} \qquad \therefore PF = \frac{4 \times 4\pi r^3 \times 2\sqrt{2}}{3 \times 4 \times 4 \times 4 \times r^3} \qquad P.F = \frac{\sqrt{2}\pi}{6}$$

$$P.F = \frac{1.414 \times 3.14}{6} \qquad P.F = 0.74$$

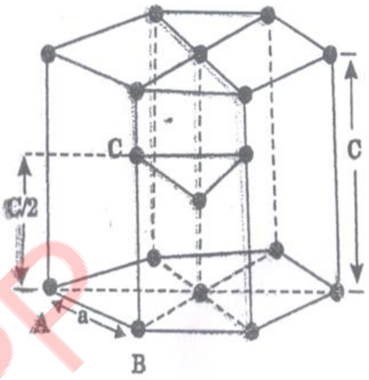
$$Packing\ factor = 0.74 \times 100\ \% \qquad \boxed{P.F = 74\%}$$

In FCC unit cell, 74% of the volume is occupied by atoms and 26% volume is vacant.

Example: Copper, Aluminium, Nickel, Gold, Lead and Platinum.

HEXAGONAL CLOSE-PACKED STRUCTURE

It has three layers. At the bottom layer, it has 6 corners and each corner has 1 atom and one more atom present at the centre of the bottom face. Also at the top layer, it has 6 corners and each corner has 1 atom and one more atom present at the centre of the top face. Then the middle layer has 3 atoms at a distance $\frac{c}{2}$ from bottom or top layer. These 3 atoms are present totally inside the unit cell.



Height of the hexagon is *'c'* (distance between bottom and top layer is *'c'*)

1. Number of atoms per unit cell:

Each corner atom is shared by 6 other unit cells.

$$\therefore\ Number\ of\ corner\ atoms\ in\ the\ upper\ hexagonal\ plane\ is = \frac{1}{6} \times 6 = 1$$

$$Number\ of\ corner\ atoms\ in\ the\ lower\ hexagonal\ plane\ is = \frac{1}{6} \times 6 = 1$$

Each face centered atom is shared by 2 adjacent unit cells.

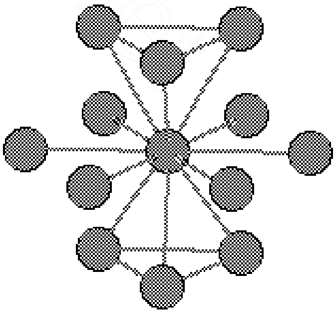
$$Total\ number\ of\ face\ centered\ atoms\ in\ the\ lower\ and\ upper\ planes = \frac{1}{2} \times 2 = 1$$

There are 3 atoms present inside the unit cell (at the middle layer) which are not shared.

$$\therefore\ Total\ number\ of\ atoms\ in\ the\ HCP\ crystal\ is\ 1 + 1 + 1 + 3 = 6$$

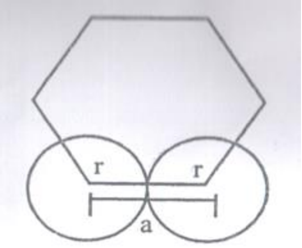
2. Co-ordination number:

In the bottom layer the face centered atom has 6 nearest neighbour in the same plane. Then at a distance of $\frac{c}{2}$ there will be 3 atoms above and below the layer. In total there are 12 nearest neighbors.



Coordination number = 12.

3. Atomic radius:



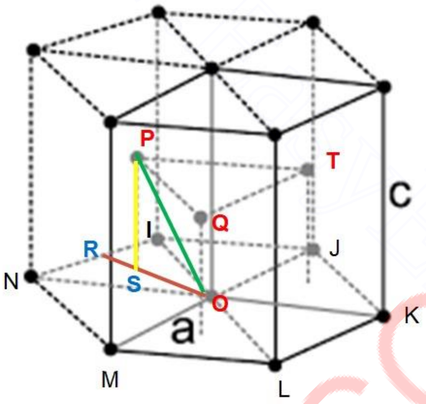
Atoms touch each other along the diagonal of the hexagon. ∴ The nearest neighbouring distance

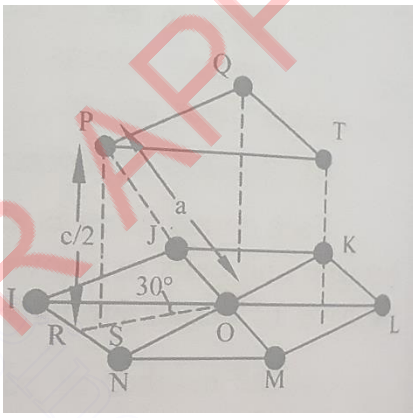
is $a = 2r$ $\therefore r = \frac{a}{2}$

4. Calculation of c/a ratio:

Let *'c'* be the height of the unit cell and *'a'* is the distance between the neighboring atoms. Let I,J,K,L,M,N and N are the corner atoms and O be the base atom in the bottom layer of the HCP structure ad P,Q,T are the middle layer atoms.

Here I, N and O represents the bottom layer atoms. Now, let us draw the normal line OR from O to the line IN, which bisects the line IN at a point R.





From figure in △IRO $\cos 30° = \frac{OR}{OI}$

$$OR = OI\cos 30°$$

$$OR = \frac{a\sqrt{3}}{2} \text{----------(1)}$$

But, from fig, $OS = \frac{2}{3}OR$ -----------(2)

Substituting for OR, we get $OS = \frac{2}{3}\frac{a\sqrt{3}}{2}OS = \frac{a}{\sqrt{3}}$ -----------(3)

In the ΔSOP, $OP^2 = OS^2 + SP^2$ --------------(4)

Substituting the values for OP = a, $OS = \frac{a}{\sqrt{3}}$ and $SP = \frac{c}{2}$ in equation (4), we get

$$a^2 = \frac{a}{\sqrt{3}}^2 + \frac{c^2}{2} \text{ ----------(5)}$$

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

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

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

$$\frac{c^2}{4} = \frac{2a^2}{3} \qquad \frac{c^2}{a^2} = \frac{8}{3}$$

$$\frac{c}{a} = \sqrt{\frac{8}{3}} \qquad \frac{c}{a} = \frac{\sqrt[2]{2}}{\sqrt{3}} = \frac{2 \times 1.414}{1.732} \qquad \frac{c}{a} = 1.633$$

5. Packing factor:

(i)To find volume of all the atoms in a unit cell, v:

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

$$v = \frac{6 \times 4}{3} \times \pi \left[\frac{a}{2}\right]^3$$

$$v = \frac{6 \times 4 \times \pi \times a^3}{3 \times 8}$$

$$v = \pi a^3 \qquad -------(1)$$

(ii)To find the volume of the unit cell, V:

$$Volume\ of\ the\ hexagon = Area\ of\ the\ base \times Height \qquad -----(2)$$

Base of the hexagon has 6 similar triangles so,

$$Area\ of\ the\ base = 6 \times Area\ of\ \Delta ABO \qquad -----(3)$$

$$Area\ of\ the\ triangle = \frac{1}{2} \times Base \times height$$

$$Area\ of\ the\ \Delta ABO = \frac{1}{2}(BO)(AY)$$

$$= \frac{1}{2} a . \frac{a\sqrt{3}}{2}$$

$$Area\ of\ the\ \Delta ABO = \frac{a^2\sqrt{3}}{4} \qquad -----(4)$$

Substitute (4) in (3) we get, $\therefore Area\ of\ the\ base = 6 \times \frac{a^2\sqrt{3}}{4}$

$$Area\ of\ the\ base = \frac{3\sqrt{3}a^2}{2} \qquad -----(5)$$

Substitute (5) in (2) we get,

$$Volume\ of\ the\ unit\ cell\ (hexagon), V = \frac{3\sqrt{3}a^2c}{2} \qquad ----(6)$$

$Height\ of\ the\ hexagon = c$

$$\therefore Packing\ factor = \frac{v}{V} \qquad ------(7)$$

Substitute (1) and (6) in (7) we get,

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

$$\frac{c}{a} = \frac{\sqrt{8}}{\sqrt{3}} \qquad \because \frac{a}{c} = \frac{\sqrt{3}}{\sqrt{8}}$$

$$P.F = \frac{2\pi}{3\sqrt{3}}\left[\frac{a}{c}\right]$$

$$P.F = \frac{2\pi}{3\sqrt{3}}\left(\frac{\sqrt{3}}{\sqrt{8}}\right) \qquad \because \sqrt{8} = \sqrt{2\times2\times2}$$

$$= 2\sqrt{2}$$

$$P.F = \frac{2\pi}{3\times2\sqrt{2}}$$

$$P.F = \frac{\pi}{3\sqrt{2}} = \frac{3.14}{3\times1.414}$$

$$P.F = 0.74$$

$$Packing\ factor = 0.74\times100\ \%$$

$$\boxed{\therefore PF = 74\%}$$

∴ 74% of the volume is occupied by the atoms and the remaining 26% is free or vacant

Example: Magnesium, Zinc, Titanium, Zirconium, Beryllium and Cadmium.

DIRECTIONS AND PLANES

MILLER INDICES

Miller introduced a set of three numbers to designate a plane in a crystal. This set of three numbers are said to be miller indices of the plane. The orientations of planes in a crystal may be described in terms of their intercepts.

In figure OA has 2 units of axial length and OB has 2 units of axial length and OC has only one unit of axial length. ∴ The numerical parameters are [2,2,1]. Miller described the orientation of a plane by the reciprocal of its numerical parameters rather than by its linear parameters. These reciprocals are converted into whole numbers. They are called Miller indices. ∴ The miller indices of the above plane is [1/2, 1/2, 1/1]

∴ i.e., [1, 1, 2] The general expression for indices is (h, k, l). The symbol for a family of plane is <h, k, l>

Definition:*Miller indices are the three possible integers which have the same ratios as the reciprocals of the intercepts of the plane concerned on the three axes.*

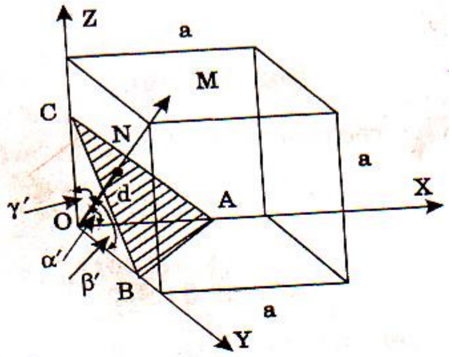
PROCEDURE FOR FINDING MILLER INDICES:

- Find the intercepts of a plane along the three axes.
- Take reciprocal of these intercepts.
- Reduce the reciprocals into whole numbers.
- Enclose these integers in parenthesis to get Miller indices.

The following points are important for getting the Miller indices.

- When a plane is parallel to one of the co-ordinate axes, then it will meet the axis at infinity$[\frac{1}{\infty} = 0]$, the Miller indices for that axis is zero.
- When the intercept of a plane is on the negative part of any axis, then a minus sign is included in the miller indices.

d – SPACING IN CUBIC LATTICE



Consider a cube crystal. Let *'a'* bethe length of cube edge. Consider a plane ABC as shown in figure. Draw a perpendicular ON from origin to the plane ABC, which represents the interplanar distance.

OA, *OB* and *OC* are the intercepts on the *X*, *Y*, *Z* axes due to the plane α', β', γ' are the angles between the reference axes *OX*, *OY*, *OZ* and *ON* respectively.

Miller indices of a plane are the smallest integers of the reciprocals of its intercepts. They can be expressed in reciprocals of miller indices. $OA: OB: OC = \frac{1}{h}:\frac{1}{k}:\frac{1}{l}$

$$OA: OB: OC = \frac{a}{h}:\frac{a}{k}:\frac{a}{l}$$

$$\therefore OA = \frac{a}{h}; \qquad OB = \frac{a}{k}; \qquad OC = \frac{a}{l}$$

From the figure, $cos\alpha' = \frac{ON}{OA} = \frac{d}{a/h} = \frac{dh}{a}$

$$cos\beta' = \frac{ON}{OB} = \frac{d}{a/k} = \frac{dk}{a}$$

$$\cos\gamma' = \frac{ON}{OC} = \frac{d}{\frac{a}{l}} = \frac{dl}{a}$$

By the law of direction cosine is $\cos^2\alpha' + \cos^2\beta' + \cos^2\gamma' = 1$

Substituting the values $\left(\frac{dh}{a}\right)^2 + \left(\frac{dk}{a}\right)^2 + \left(\frac{dl}{a}\right)^2 = 1$

$$\frac{d^2}{a^2}(h^2 + k^2 + l^2) = 1$$

$$d^2 = \frac{a}{h^2 + k^2 + l^2}$$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

This is the relation between *d* and *hkl.*

DENSITY OF CRYSTAL

This is defined as: $Density\ of\ the\ crystal\ (\rho) = \frac{Mass\ of\ unit\ cell}{Volume\ of\ unit\ cell}$

$$Mass\ of\ unit\ cell\ = \frac{Atomic\ mass}{Avogadronumber} \times Number\ of\ atoms\ per\ unit\ cell$$

$$Mass\ of\ unit\ cell\ = \frac{M}{N_A} \times n$$

n → number of atoms per unit cell and

N_A → Avogadro's number,

M → the atomic weight and

a → side of a cubic unit cell

$$p\ = \frac{nM}{a^3 N_A}$$

LINEAR DENSITY

Linear Density (L.D.): It is defined as number of atoms per unit length whose centres on the direction vector for specific crystallographic direction. This is defined as the number of atoms per unit length along a specific crystal direction. i.e.,

$$Linear\ Density = \frac{Number\ of\ atoms\ centred\ on\ direction\ vector}{Length\ of\ direction\ vector}$$

The unit of linear density is m^{-1}, nm^{-1}

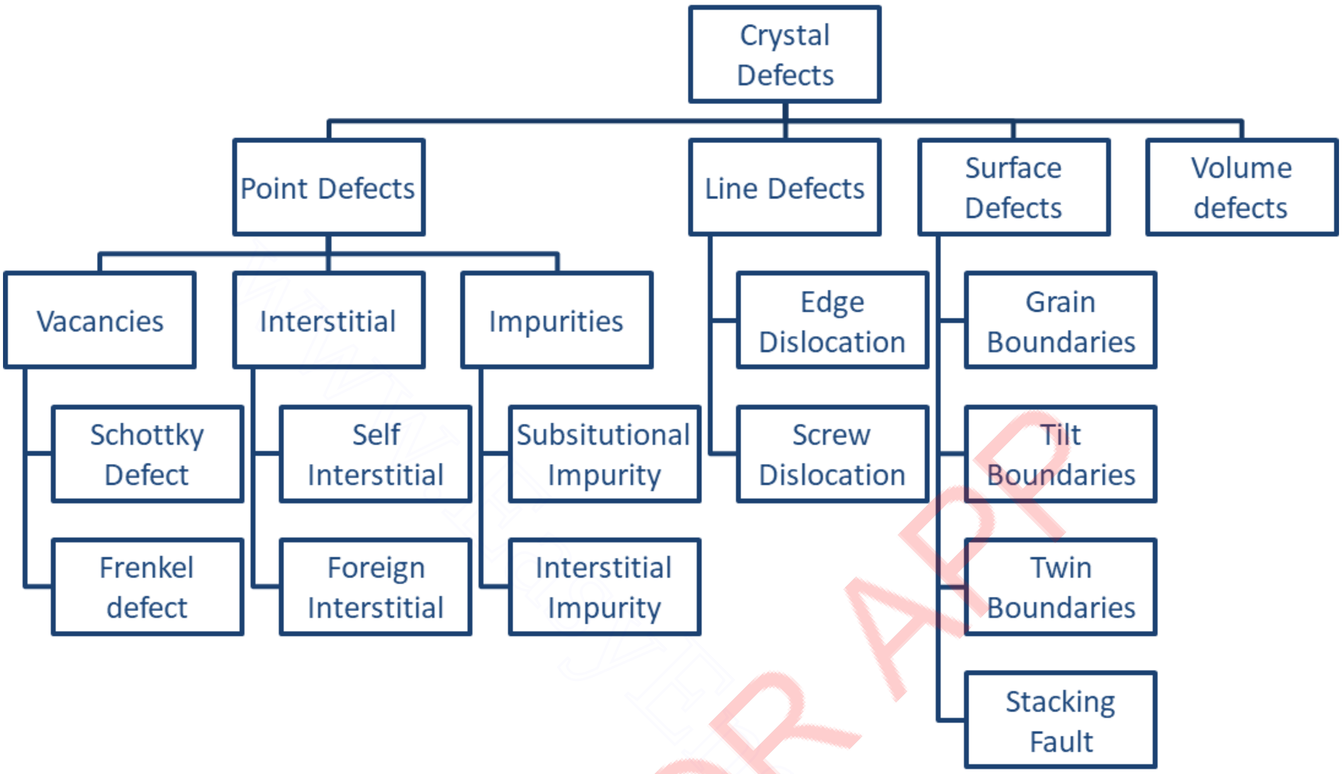
PLANAR DENSITY

The planar density of a crystal is the density of atoms in a crystal plane. This is defined as the number of atoms per unit area on a crystal plane. This affect significantly the rate of plastic deformation. It is defined as the number of atoms per unit area

$$\text{Planar Density} = \frac{\text{Number of atoms in a plane}}{\text{The area of the plane}}$$

The unit of planar density is m^{-2}, nm^{-2}

CRYSTAL IMPERFECTIONS



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

1. POINT DEFECT

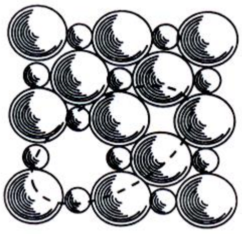
Point defects are crystalline irregularities of atomic dimensions. They are imperfect points like regions in the crystal. Point defects take place due to imperfect packing of atoms during crystallization. They produce distortion inside the crystal structure. They produce strain only in its surroundings but does not affect the regularity in other parts of the crystal.

The different types of point defects are **a. Vacancies b. Interstitial c. Impurities**

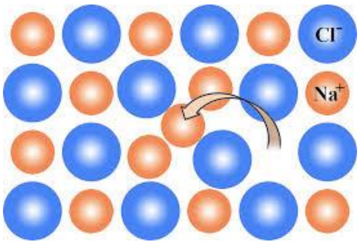
a. VACANCIES

A vacancy is the simplest point defect in a crystal. It refers to a missing atom or vacant atomic site. These defects may arise due to imperfect packing during crystallization.

Two kinds of vacancies – a) Schottky defect b) Frenkel defect



Schottky Defect



Frenkel Defect

a) Schottky defect refers to the missing of pair of positive or negative ions in an ionic crystal. Since pair is missing, the electrical neutrality is maintained.

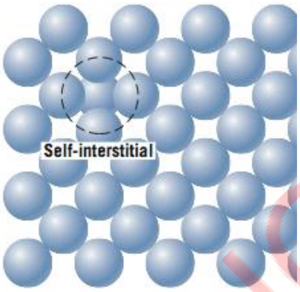
b) Frenkel defect is a combination of vacancy and interstitial defects.

(ii) **INTERSTITIAL DEFECT:** When an extra atom occupies interstitial space within the crystal structure without removing the parent atom, the defect is called interstitial defect.

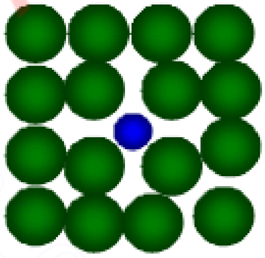
Two kinds of Interstitial defect – a) Self interstitial b) Foreign interstitial

a) Self interstitial: if the atom from the same crystal occupies the interstitial site.

b) Foreign interstitial: if an impurity atom occupies the interstitial site.



Self-interstitial



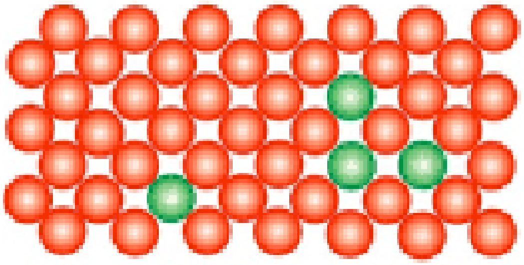
Foreign interstitial

C. IMPURITIES: When a foreign atom is added to the crystal lattices, they are known as impurities. The impurity defect may be of two types

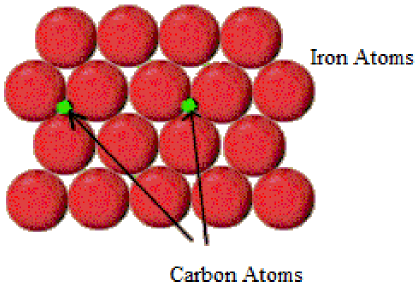
1. Substitutional impurity 2. Interstitial impurity

SUBSTITUTIONAL IMPURITY: It refers to a foreign atom that substitutes for or replaces a parent atom in the crystal. Pentavalent or trivalent impurity atoms doped in silicon or germanium are also substitutional impurities in the crystal.

INTERSTITIAL IMPURITY: An interstitial defect arises when an atom occupies a definite position in the lattice that is not normally occupied in the perfect crystal. If a small sized atom occupies the void space in the parent crystal without disturbing the parent atoms from their regular sites, then it is called as ‘interstitial impurity’.



Substitutional impurity

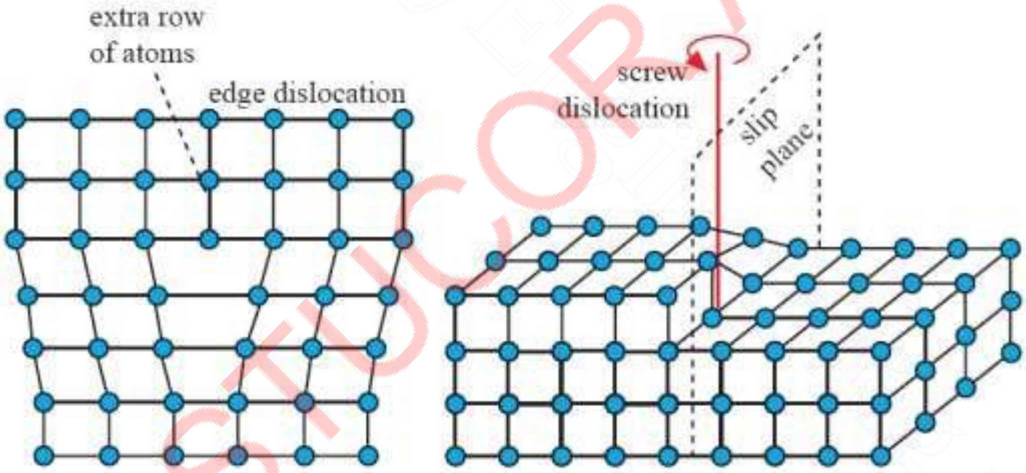


Interstitial impurity

2. LINE DEFECTS OR DISLOCATIONS

The defects due to dislocation or distortion of atoms in a line is known as line defects. Line defects are also called dislocations.

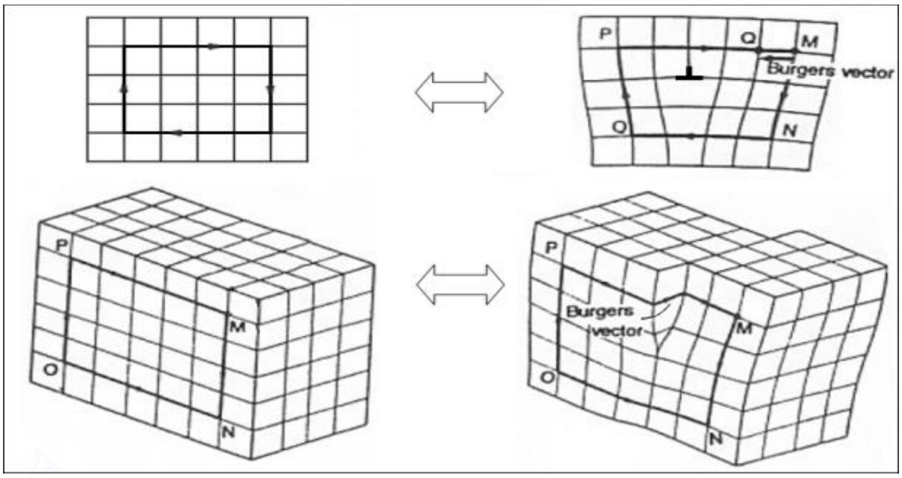
(i) EDGE DISLOCATION: An edge dislocation arises when one of the atomic planes forms partially and does not extend through the entire crystal. Edge dislocation may be of positive edge dislocation and negative edge dislocation.



ii) SCREW DISLOCATION: Screw dislocation is due to displacement of atoms in one part of a crystal relative to rest of the crystal. The displacement terminates within the crystal. The term screw is to represent that one part of the crystal is moving in spiral manner about the dislocation line.

BURGER VECTOR

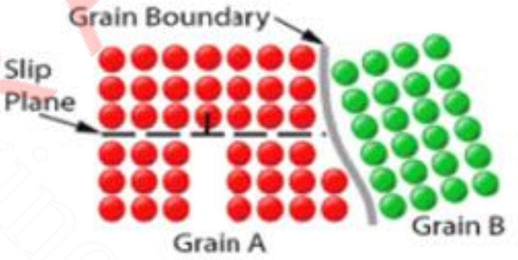
The vector which indicates the direction and magnitude of the shift of the lattice on the slip plane is called a burger vector. Burger vector can be found by burger’s loop by taking integral lattice translations in each pair of parallel sides in the region of interest.



3. SURFACE DEFECTS

The defects on the surface of a material are called surface defects or plane defects. They are also known as two dimensional imperfections. Some of the surface defects are

1. Grain boundaries
2. Tilt Boundaries
3. Twin boundaries
4. Stacking Faults

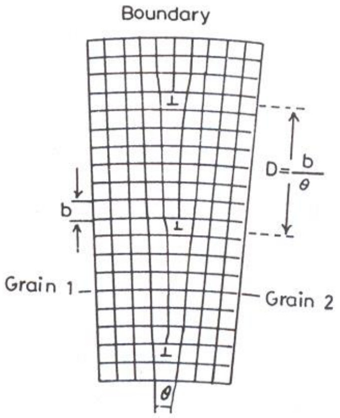


GRAIN BOUNDARIES: A polycrystalline material consists of several small sized regions known as grains. The line separating each grain is said to be grain boundary. Whenever the grains of different orientation separate the general pattern of atoms the defect caused is called grain boundary.

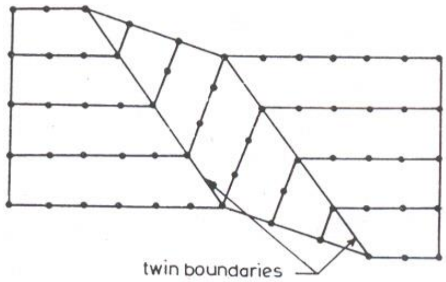
TILT BOUNDARIES

This is called low-angle boundary as the orientation difference between two neighbouring crystals is less than 10°. In general, low-angle boundaries can be described by suitable arrays of dislocation. Low-angle tilt boundary is composed of edge dislocation lying one above the other. The angle or tilt will be

$\theta = \frac{b}{D}$ where b = Burgers vector and D = the average vertical distance between dislocations.



Tilt Boundaries



Twin boundaries

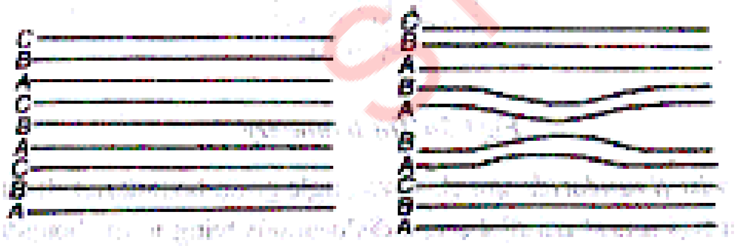
TWIN BOUNDARIES

If the atomic arrangement on one side of a boundary is a mirror reflection of the arrangement on the other side, then it is called as twin boundary. As they occur in pair, they are called twin boundaries. At one boundary, orientation of atomic arrangement changes. At another boundary, it is restored back. The region between the pair of boundaries is called the twinned region. These boundaries are easily identified under an optical microscope.

STACKING FAULT

Whenever the stacking of atomic planes is not in a proper sequence throughout the crystal, the fault caused is known as stacking fault. For example, the stacking sequence in an ideal FCC crystal may be described as A-B-C-A-B-C- A-B-C-……. But the stacking fault may change the sequence to A-B-C-A-B-A-B-A-B-C. The region in which the stacking fault occurs (A-B-A-B) forms a thin region and it becomes HCP.

This thin region is a surface imperfection and is called a stacking fault.



ELASTIC STRAIN ENERGY

- Up to the elastic limit of a sample, all the work done in stretching it is stored potential energy, or **Elastic Strain Energy**. This value can be determined by calculating the **area under the the force-extension graph**. If the sample obeys Hooke’s Law, and is below the elastic limit.

- When we apply force to the material, it will deform. The external force will do work on the material, which will be stored in the material as strain energy. Under the elastic limit, the work done by external force will be equal to the strain energy stored (Work-energy theorem). It can also be calculated by calculating the area under the curve of the Stress vs Strain graph up to the elastic limit. The strain energy up to the elastic limit is also known as Resilience. The unit of strain energy is N−m or Joules.
- Before going for the derivation of the strain energy formula, we will have to make certain assumptions for the ideal condition.

The assumption for Strain Energy Formula

1. The material should be elastic.
2. Stress developed should be within the proportional limit.
3. Load should be gradually applied.

Let at any instant, the material having original length LL and having area AA is elongated by xx unit.

From Hooke's law,

$$\text{Stress} = \text{E} \times \text{Strain}$$

$$\Rightarrow \frac{F}{A} = E\frac{x}{L}$$

$$\Rightarrow F = \frac{EAx}{L}$$

So, the force is variable and gradually increasing with deformation. Let for small deformation dx differential work done will be dW. We know that the work done by the variable force is given by,

$dW = \vec{F} \cdot d\vec{s} = F\,dx$ (Both force and displacement have the same direction)

$$W = \int_0^{\Delta L} F dx$$

$$W = \int_0^{\Delta L} \frac{EAx}{L} dx$$

$$W = \left[\frac{EAx^2}{2L}\right]_0^{\Delta L} = \frac{EA(\Delta L)^2}{2L}$$

Thus the total strain energy (U) for small deformation will be,

$$U = \frac{EA(\Delta L)^2}{2L}$$

$$= \frac{1}{2} \times \left(E \times \frac{\Delta L}{L}\right) \times AL \times \frac{\Delta L}{L}$$

$$== \frac{1}{2} \times (E \times \text{strain}) \times AL \times \text{strain}$$

$$= \frac{1}{2} \times \text{Stress} \times \text{Strain} \times \text{volume of material}$$

The formula of strain energy can also be written as,

$$U = \frac{1}{2} \times \frac{(\text{Stress})^2}{\text{E}} \times \text{volume of material}$$

DEFORMATION OF METALS

Materials – Alloys will get deformation or change in dimension when it is loaded.

Elastic deformation : If the material retains its original shape and size once the deforming forces are removed

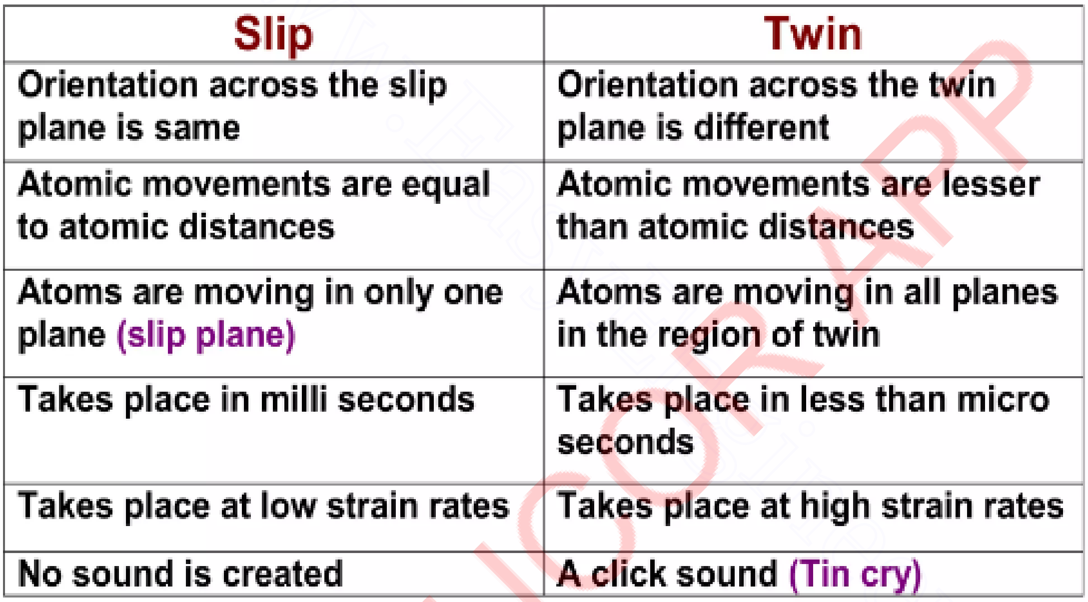
Plastic deformation : permanent deformation.

Plastic deformation depends on Applied stress, Temperature and Strain rate

Plastic deformation mechanisms can happen in two ways

1. Slip
2. Twinning

DIFFERENCES BETWEEN SLIP AND TWINNING



Slip	Twin
Orientation across the slip plane is same	Orientation across the twin plane is different
Atomic movements are equal to atomic distances	Atomic movements are lesser than atomic distances
Atoms are moving in only one plane (slip plane)	Atoms are moving in all planes in the region of twin
Takes place in milli seconds	Takes place in less than micro seconds
Takes place at low strain rates	Takes place at high strain rates
No sound is created	A click sound (Tin cry)

Classical free electron theory - Expression for electrical conductivity – Thermal conductivity, expression - Quantum free electron theory :Tunnelling – degenerate states – Fermi- Dirac statistics – Density of energy states – Electron in periodic potential – Energy bands in solids – tight binding approximation - Electron effective mass – concept of hole. Magnetic materials: Dia, para and ferromagnetic effects – paramagnetism in the conduction electrons in metals – exchange interaction and ferromagnetism – quantum interference devices – GMR devices.

ELECTRICAL PROPERTIES OF MATERIALS

Low resistive materials are known as conducting materials. They have high electric and thermal conductivities. The conducting property of a solid is due to the number of valence electrons, which become free electron when they are detached from the parent atom.

Classification of conducting materials:

Based on their conductivity conducting materials are classified into three types.

- Zero resistivity materials
- Low resistivity materials
- High resistivity materials

ELECTRON THEORY OF SOLIDS: The electron theory of metals aims to explain the structure and properties of solids through their electronic structure. The electron theory is applicable to all solids i.e., both metals and non-metals. It explains the electrical, thermal and magnetic properties of solids etc.
The theory has been developed in three main stages.

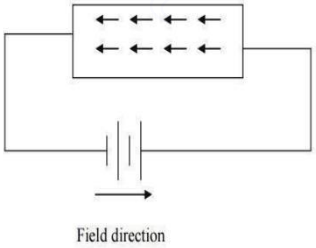
The classical free electron theory: Drude and Lorentz proposed this theory in 1900. According to this theory, the metals containing the free electrons obey the laws of classical mechanics.

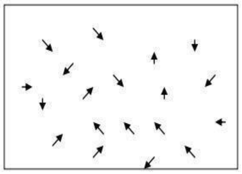
The quantum free electron theory: Somerfield developed this theory in 1928. According to this theory the free electrons obey quantum laws. According to this theory the free electrons are moving in a constant potential.

The zone theory: Bloch stated this theory in 1928. According to this theory, the free electrons move in a periodic field provided by the lattice.

POSTULATES OF CLASSICAL FREE ELECTRON THEORY

In the absence of electrical field: When an electrical field is not applied, the free electrons move everywhere in a random manner. They collide with other free electrons and positive ion core. This collision is known as elastic collision.





In the presence of electric field: When the electrical field is applied, the electrons get some amount of energy from the applied electric field and they begin to move towards the positive potential.

Since electrons are assumed to be a perfect gas, they obey the laws of kinetic theory of gases.

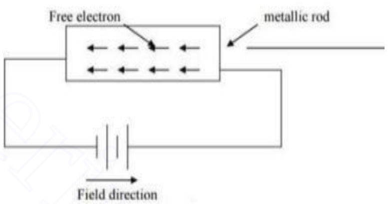
Drift velocity: It is defined as the average velocity acquired by the free electrons in a metal in a particular direction by the application of an electrical field. $\boldsymbol{v_d = \frac{\lambda}{\tau_c}}$

Collision Time: The average time taken by a free electron between any two successive collisions is known as collision time. $\boldsymbol{\tau_c = \lambda / v_d}$

Mean free path: The average distance travelled by a free electron between any two successive collisions in the presence of an applied field is known as mean free path. It is the product of drift velocity of electrons (v_d) and collision time (τ_c). $\boldsymbol{\lambda = v_d \times \tau_c}$

Relaxation time: The average time taken by a free electron to reach its equilibrium position from its disturbed position due to application of an external electric field is called relaxation time. It is approximately equal to 10^{-14} second.

Electrical conductivity of a metal



Definition: It can be defined as the quantity of electric charge (Q) conducted per unit time (t) across unit area (A) of the solid for unit applied electric field (E). $\sigma = \frac{Q}{tAE}\ \Omega^{-1}\text{m}^{-1}$

Derivation: We know in the in the absence of external electric field, the motion of electrons in a metal moves randomly in all directions. When an electric field is applied between the two ends of a metallic rod. The electrons will move towards the positive field direction and produces current in the metallic rod.

If 'E' is the electric field intensity and 'm' is the mass of the electron, then

Force experienced by the electron $\quad F = eE$ -------(1)
According to the Newton's second law $\quad F = ma$ -------(2)
Equating (1) and (2) $\quad eE = ma$

$$a = \frac{eE}{m} \quad \text{---------(3)}$$

Due to the applied electric field, the electron gains acceleration 'a'

$$\text{Acceleration} = \frac{\text{Velocity}}{\text{Time}} = \frac{\text{Drift velocity}}{\text{Relaxation time}}$$

$$a = \frac{v_d}{\tau}$$

$$\boldsymbol{v_d = a\tau} \quad \text{---------(4)}$$

Substituting (3) in (4) $$\mathbf{v_d} = \frac{\mathbf{eE}}{\mathbf{m}}\boldsymbol{\tau} \text{ --------(5)}$$

If 'n' is the free electron density and 'e' is the charge of electron then current density is given by

$$J = nV_d e\text{--------(6)}$$

Sub (5) in (6) $$J = ne\left(\frac{eE}{m}\tau\right)$$

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

According to ohm's law, current density (J) is expressed as $J = \sigma E$ $\frac{J}{E} = \sigma$

$$\frac{J}{E} = \frac{ne^2}{m}\tau$$

$$\sigma = \frac{ne^2}{m}\tau \quad \text{------(8)}$$

Thus the above equation represents the electrical conductivity of metal.

Thermal conductivity of a metal:

In general, the thermal conductivity takes place not only by thermal motion of free electrons but also by thermally excited lattice vibrations called phonons. The total thermal conductivity K $_{tot}$ is given by

$$K_{Tot} = K_{electron} + K_{Phonon}$$

In metals, conductivity due to free electrons is predominant. $K_{Tot} \approx K_{electron}$

In insulators thermal conductivity is due to atomic or molecular vibrations of the lattice is predominant $\therefore K_{Tot} \approx K_{phonon}$

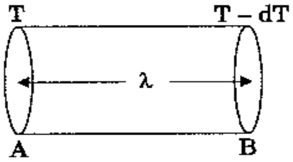
In semiconductors both electron & phonon will contribute for thermal conduction.

$$\therefore K_{Tot} \approx K_e + K_{ph}$$

Definition: Thermal conductivity of the material is defined as the amount of heat conducted per unit area per unit time maintained at unit temperature gradient

$$K = \frac{Q}{tA\left(\frac{dT}{dx}\right)} \quad W/m/K$$

Derivation: Let us consider a uniform rod AB with Temp (Hot) T at end A & T-dT (cold) at end B. Heat flows from hot end to cold end and the distance between A & B isλ. The no of conduction electrons in a metal is ‘n’ their average velocity is v.



At A, Average kinetic energy of an electron = $\frac{3}{2}KT$ ---------(1)

At B, Average kinetic energy of an electron = $\frac{3}{2}K(T-dT)$---------(2)

The number of electrons crossing per unit area per unit time is $\frac{1}{6}\ nv$

Excess of kinetic energy carried by the electron from A to B = $\left[\frac{3}{2}KT - \frac{3}{2}K(T-dT)\right]\frac{1}{6}\ nv$

$= \left[\frac{3}{2}KT - \frac{3}{2}KT + \frac{3}{2}KdT\right]\frac{1}{6}\ nv$

$= \frac{1}{4}nvKdT$ ---------(3)

Similarly the deficient of kinetic energy carried by the electron from A to B per unit area in unit time = - $\frac{1}{4}nvKdT$ ----------(4)

Hence, the net amount of energy transferred from A to B per unit area per unit time

$$Q = \left(\frac{1}{4}nvKdT\right) - \left(-\frac{1}{4}nvKdT\right)$$

$$Q = \frac{1}{2}nvKdT \quad \text{-----------(5)}$$

From basic definition of thermal conductivity

The amount of heat conducted per unit time per unit area is $Q = K\frac{dT}{\lambda}$ ---------(6)

Equate (5) and (6) we get, $\frac{1}{2}nvKdT = K\frac{dT}{\lambda}$

$$K = \frac{1}{2}nvk\lambda \quad \text{--------(7)}$$

For metals Relaxation time (τ) = Collision time (τ_c)

$$\tau v = \lambda \quad \text{---------(8)}$$

Sub (8) in (7) we get $K = \frac{1}{2}nv^2k\tau$ -----------(9)

This is the classical expression for thermal conductivity of a metal.

Weidemann-Franz law:

It states that for the metals, the ratio of thermal conductivity to electrical conductivity is directly proportional to the absolute temperature. This ratio is constant for all metals at a given temperature.

$$\frac{\mathbf{K}}{\boldsymbol{\sigma}}\,\boldsymbol{\alpha}\mathbf{T} \qquad \frac{\mathbf{K}}{\boldsymbol{\sigma}} = \mathbf{LT}$$

Where, L is a constant known as Lorentz number.

We know that,

Electrical conductivity of a metal $\sigma = \frac{ne^2}{m}\tau$ ------ (1)

Thermal conductivity of a metal $K = \frac{1}{2}nv^2k\tau$ ------ (2)

$$\frac{\mathbf{K}}{\boldsymbol{\sigma}} = \frac{\frac{ne^2}{m}\tau}{\frac{1}{2}nv^2k\tau} \qquad \frac{\mathbf{K}}{\boldsymbol{\sigma}} = \frac{1}{2}\frac{mv^2\,k}{e^2} \text{ ---------- (3)}$$

We know that the kinetic energy of an electron $\frac{1}{2}mv^2 = \frac{3}{2}kT$ ---------(4)

Substituting equation (4) in equation (3), we have $\frac{K}{\sigma} = \frac{3}{2}kT\,\frac{k}{e^2}$

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

$$\frac{K}{\sigma} = LT \text{ ------------ (5)}$$

where $L = \frac{3}{2}\frac{k^2}{e^2}$ is a constant and it is known as Lorentz number.

Thus it is proved that, the ratio of thermal conductivity to electrical conductivity of a metal is directly proportional to the absolute temperature of the metal. Weidemann -Franz law clearly shows that if a metal has high thermal conductivity, it will also have high electrical conductivity.

Lorentz number:

The ratio of thermal conductivity (K) of a metal to the product of electrical conductivity (σ) of a metal and absolute temperature (T) of the metal is a constant. It is called Lorentz number and it is given by $\mathbf{L} = \frac{\mathbf{K}}{\boldsymbol{\sigma}\mathbf{T}}$

The value of L can be calculated from the expression $L = \frac{3}{2}\frac{k^2}{e^2}$

$$L = \frac{3}{2}\frac{(1.38 \times 10^{-23})^2}{(1.6 \times 10^{-19})^2}$$

$$L = 1.12 \times 10^{-8}\ W\,\Omega\,K^{-2} \text{ (By theory)}$$

$$L = 2.44 \times 10^{-8}\ W\,\Omega\,K^{-2} \text{ (By Experiment)}$$

This discrepancy in the experimental and theoretical value of Lorentz number is one of the drawbacks of classical theory. It is rectified in quantum theory.

Merits of classical free electron theory

- It is used to verify ohm’s law.
- The electrical and thermal conductivities of metals can be explained by this theory.
- It is used to derive Wiedemann-Franz law.
- It is used to explain the optical properties of metals.

Drawbacks of classical free electron theory

- It is a macroscopic theory
- Classical theory states that all the free electrons will absorb energy, but quantum theory states only few electrons will absorb energy.
- This theory cannot explain the Compton, photo-electric effect, paramagnetic, ferromagnetism, etc.
- The theoretical and experimental values of specific heat and electronic specific heat are not matched.
- The Lorentz number by classical theory does not have good agreement with the experimental value and it is rectified by quantum theory.
- According to this theory, the ratio $\frac{K}{\sigma T}$ is constant at all temperatures. But it is found that it is not constant at low temperatures.
- By this theory, the value of specific heat of a metal is 4.5R, but the experimental value is 3R, where R is a universal gas constant.
- The susceptibility of a paramagnetic material is inversely proportional to temperature. But experimental result shows that Para magnetism of a metal is independent of temperature. Moreover Ferromagnetism cannot be explained by this theory.

Differences between electrical and thermal conductivity

S. No	Electrical Conductivity	Thermal Conductivity
1	Electrical conductivity is based on the no of free electrons	Thermal conductivity is based both on electrons and phonons
2	The quantity of electrical charges flowing per unit time across unit area in the metal for unit applied electric field is called electrical conductivity	It is defined as the amount of heat conducted per unit time through the metal having unit area of cross section maintaining at unit temperature gradient between the two ends
3	Electrical conductivity takes place from higher potential side to lower potential side	Thermal conductivity takes place from hot end to cold end.
4	Unit :Ω^{-1} m^{-1}	Unit :W $m^{-1}K^{-1}$

Quantum free electron theory:

In order to remove the failures of classical free electron theory, **Sommerfield** proposed quantum free electron theory in 1928, based on the quantum concepts.

According to this theory, the ***electrons in a metal move in a constant potential***. He derived an expression for electron energies by using Schrodinger's wave equation and De- Broglie concept of matter waves. He treated the problem quantum mechanically using Fermi – Dirac statistics.

Important assumptions:

- ✓ The potential of an electron is uniform or constant within the crystal.
- ✓ The electrons possess wave nature.
- ✓ The allowed energy levels of an electron are quantized.
- ✓ The electrons have freedom to move within the crystal itself and they are restricted from leaving crystal due to potential barrier at its surface.
- ✓ The free electrons obey Fermi – Dirac statistics.

Merits of quantum free electron theory:

It explains the electrical conductivity, thermal conductivity and specific heat capacity of metals, photoelectric effect, Compton Effect etc.

Demerits of quantum free electron theory:

- ✓ It fails to provide the distinction between metals, semiconductors and insulators.
- ✓ It fails to explain the positive value of Hall co- efficient and some transport properties of metals.

Tunnelling

In quantum mechanics a particle having lesser energy (E) than the barrier potential (V) can easily cross over the potential barrier having a finite width 'l ' even without climbing over the barrier by tunnelling through the barrier. This process is called tunnelling.

Explanation: let us consider a beam of particles having kinetic energy E, less than the barrier potential (V), incident from region 1. According to classical mechanics the probability for the incident particles to cross the barrier is zero, because it has very less energy (E) when compared to the barrier potential (V).

But according to quantum mechanics, the incident wave from region (1) having the wave function Ψ_1 can cross the barrier region (2) by the process of tunnelling, represented by the wave function Ψ_2 and comes out to the region (3), represented by the wave function Ψ_3. However based on the width of the potential barrier there is a probability for the wave, represented by the wave function Ψ_1' to get reflected within the same region (1). The value of transmission coefficient T depends on the mass of the particle (m), thickness of the barrier (*l)* and the energy difference i.e, (V – E).

Examples

1. The tunnelling effect is observed in Josephson junction, in which electron pairs in the superconductor's tunnel through the barrier layer, giving rise to the Josephson current.
2. This effect is also observed in the case of emission of alpha particles by radioactive nuclei. Here, though the 'α' particle has very less kinetic energy they are able to escape from the nucleus whose potential wall is around 2.5 MeV high.
3. Tunnelling also occurs in certain semiconductor diodes called tunnel diodes.
4. Electron tunnels through insulating layer and act as a switch by tunnelling effect.

Degenerate states: For various combinations of quantum numbers '**n**' if we get the same Eigen value (Energy levels) but different Eigen functions, then it is called degenerate state.

The energy of the particle in a 3-dimensional in the ground state is given by

$$E_{n_x n_y n_z} = \frac{\left(n_x{}^2 + n_y{}^2 + n_z{}^2\right)h^2}{8ma^2}$$

Example: For three combination of quantum numbers say (112), (121) and (211), we get same energy values i.e., $E_{112} = E_{121} = E_{211} = \frac{6h^2}{8ma^2}$ but different Eigen functions i.e., $\Psi_{112} \neq \Psi_{121} \neq \Psi_{211}$

$$\psi_{112} = \sqrt{\frac{8}{a^3}}\sin\frac{\pi x}{a}\sin\frac{\pi y}{a}\sin\frac{2\pi z}{a} \qquad \psi_{121} = \sqrt{\frac{8}{a^3}}\sin\frac{\pi x}{a}\sin\frac{2\pi y}{a}\sin\frac{\pi z}{a} \qquad \psi_{211} = \sqrt{\frac{8}{a^3}}\sin\frac{2\pi x}{a}\sin\frac{\pi y}{a}\sin\frac{\pi z}{a}$$

Fermi Distribution Function

Fermi function F (E) represents the probability of an electron occupying a given energy state at absolute temperature. The energy distribution of the particles was found by Fermi – Dirac statistics. Fermi- Dirac Statistics deals with the energy distribution of the particles having half integral spin values called as Fermions or Fermi particles. Example: Electrons.

The Fermi distribution is given by $\mathbf{F(E) = \frac{1}{1 + e^{(E-E_F)/kT}}}$

Where,

E : Energy of the energy level whose occupancy is being considered.
E_F : Energy of the Fermi level (Fermi energy)
k : Boltzmann's constant
T : Absolute temperature

The probability value F (E) lies between 0 and 1.
If F (E) = 1, the energy level is occupied by an electron.

If F (E) = 0, the energy level is vacant.

If F (E) = 0.5, then there is 50% chance for the electron to occupy the given energy level.

Effect of temperature on Fermi function:

The effect of temperature on Fermi function F(E) can be discussed with respect to the above equation.

Case (1) : Probability of occupation for E < E_F at T = 0

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

When T = 0 and **E** < **E**$_F$, we have $F(E) = \frac{1}{1 + e^{(-ve)/0}}$ $\quad F(E) = \frac{1}{1 + e^{-\infty}}$

$$F(E) = \frac{1}{1 + 0} \qquad F(E) = 1$$

Thus at T = 0, there is 100% chance for the given energy level to be filled with electrons. It can also be said that the energy levels below the Fermi energy levels are filled with electrons.

Case (2) : Probability of occupation for E> E_F at T = 0

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

When T = 0 and **E> E_F,** we have

$$F(E) = \frac{1}{1+e^{(+ve)/0}} \qquad F(E) = \frac{1}{1+e^{\infty}}$$

$$F(E) = \frac{1}{1+\infty} \qquad F(E) = \frac{1}{\infty}$$

F (E) = 0

Thus at T = 0, there is 0% chance for the given energy level to be filled with electrons. It can also be said that the energy levels above the Fermi energy level are not occupied by the electrons.

Case (3): Probability of occupation for E = E_F at T > 0K

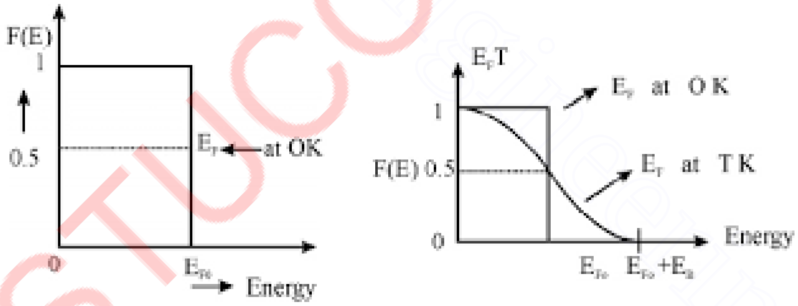
$$F(E) = \frac{1}{1 + e^{(E-E_F)/kT}}$$

When T = 0 and **E = E_F,** we have

$$F(E) = \frac{1}{1+e^{0}} \qquad F(E) = \frac{1}{1+1}$$

$$F(E) = \frac{1}{2} \qquad F(E) = 0.5$$

Here, there is 50% chance for the electrons to occupy Fermi energy level i.e., the value of F(E) becomes 0.5 at E = E_F



(a)At T=0K (b) at T>0K

Case (4): Probability of occupation at any temperature

When the temperature is raised slowly from absolute zero, the Fermi distribution function smoothly decreases to zero. Due to the supply of thermal energy the electrons within the range of kT below the Fermi level alone takes the energy ≈ kT and goes to higher energy state. Hence at any temperature (T), empty states will also be available below E_F. Therefore the fermi distribution reduces to classical Maxwell Boltzmann statistics.

Uses of Fermi distribution function:

- It gives the probability of occupation for a given energy level at a given temperature.
- It gives the idea about filled and unfilled states.
- It is very useful in the calculation of number of free electrons per unit volume at given temperature.
- It is very useful in the calculation of Fermi energy of a metal.

Density of states

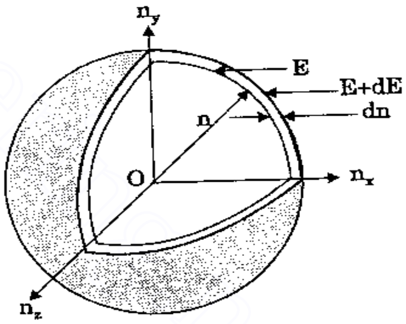
The Fermi function gives only the probability of filling up of electrons in a given energy state, it does not gives information about the number of electrons that can be filled in a given energy state. To know that we should know about the number of available energy states so called density of states.

Definition:

It is defined as the number of available electron states per unit volume in an energy interval E and E+dE. It is denoted by Z (E) and it is given by

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

Derivation: Let us consider a cubical sample with side ‘a’. A sphere is constructed with three quantum numbers n_x, n_y and n_z as coordinate axes in three-dimensional space. A radius vector n is drawn from the origin ‘o’ to a point with coordinates n_x, n_y and n_z in this space. All the points on the surface of that sphere will have the same energy E. thus $n^2 = n_x{}^2 + n_y{}^2 + n_z{}^2$ denotes the radius of the sphere with energy E. This sphere can be further divided into many shells. Each shell represents a particular combination of quantum numbers. Therefore it denotes a particular energy value with a particular radius. In this space, unit volume represents one energy state.



Number of energy states within a sphere of radius ‘n’ = $\frac{4}{3}\pi n^3$ ------------ (1)

Since the quantum numbers can have only positive integer values; we have to take only one octant of the sphere, i.e., $\frac{1}{8}$Th of the spherical volume. Therefore the number of available energy states within one octant of the sphere of radius 'n' corresponding to energy E is

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

Similarly, the number of available energy states within one octant of the sphere of radius 'n+dn' corresponding to energy E+dE is $=\frac{1}{8}\left[\frac{4}{3}\pi(n+dn)^3\right]$ ---------------(3)

Now, the number of available energy states between the shell of radius n and n+dn is determined by subtracting eqn (2) from eqn (3

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

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

$$N(E)dE = \left(\frac{\pi}{6}\right)[n^3 + dn^3 + 3n^2dn + 3ndn^2 - n^3]$$

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

$$N(E)dE = \left(\frac{\pi}{6}\right)[3n^2dn]$$

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

$$N(E)dE = \left(\frac{\pi}{2}\right)n[ndn]\text{ -----------(4)}$$

We know that the energy of the electron in a cubical metal piece of sides 'a' is given by

$$E = \frac{n^2h^2}{8ma^2}\text{ ----------------(5)}$$

$$n^2 = \left[\frac{8ma^2E}{h^2}\right]\text{ -------------(6)}$$

$$n = \left[\frac{8ma^2E}{h^2}\right]^{1/2}\text{ ---------------(7)}$$

Differentiating eqn(6) we get $$ndn = \left[\frac{8ma^2dE}{2h^2}\right]\text{ --------------- (8)}$$

Substituting eqns (7) and (8) in eqn (4), we have

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

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

$$N(E)dE = \frac{\pi}{4}\left[\frac{8ma^2}{h^2}\right]^{1/2}E^{1/2}\left[\frac{8ma^2}{h^2}\right]dE\text{ ------------(9)}$$

$$N(E)dE = \frac{\pi}{4}\left[\frac{8ma^2}{h^2}\right]^{3/2}E^{1/2}dE\text{ ------------(10)}$$

Pauli's exclusion principle states that two electrons of opposite spins can occupy each state and hence the number of energy states available for electron occupancy is given by

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

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

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

$$N(E)dE = \frac{4\pi}{h^3}(2m)^{3/2}a^3E^{1/2}dE \text{ -------------(11)}$$

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

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

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

$$Z(E)dE = \frac{4\pi}{h^3}(2m)^{3/2}E^{1/2}dE \text{ ---------------(12)}$$

This is the expression for the density of charge carriers in the energy interval E and E+dE. It is used to calculate the carrier concentration in metals and semiconductors.

Carrier concentration

Carrier concentration, i.e., the number of electrons per unit volume in a given energy interval is calculated by summing the product of the density of the state's Z(E) and the occupancy probability F(E).

i.e., $$n_c = \int Z(E)F(E)dE$$

Substituting the expressions for Z(E) and F(E), we have

$$n_c = \int \frac{4\pi}{h^3}(2m)^{3/2}E^{1/2}\frac{1}{1+e^{(E-E_F)/kT}}dE \text{ -----------(13)}$$

For a metal at absolute zero temperature, the upper most occupied level is E_F and all the levels are completely filled below E_F.

For a material at absolute zero F(E) = 1.

$$n_c = \int \frac{4\pi}{h^3}(2m)^{\frac{3}{2}}E^{\frac{1}{2}}\,dE \text{ ------------(14)}$$

$$n_c = \frac{4\pi}{h^3}(2m)^{\frac{3}{2}}\int_0^{E_F} E^{\frac{1}{2}}dE$$

$$= \frac{4\pi}{h^3}(2m)^{\frac{3}{2}}\left(\frac{E^{\frac{3}{2}}}{\frac{3}{2}}\right)_0^{E_F}$$

$$= \frac{2}{3}\frac{4\pi}{h^3}(2m)^{\frac{3}{2}}{E_F}_0^{\frac{3}{2}}$$

$$n_c = \frac{8\pi}{3h^3}(2m)^{\frac{3}{2}} E_{F_0}^{\frac{3}{2}} \quad \text{-------------(15)}$$

This eqn is used to calculate the carrier concentration in metals and semi conductors.

Expression for Fermi energy at 0K:

We know $n_c = \frac{8\pi}{3h^3}(2m)^{\frac{3}{2}} E_{F_0}^{\frac{3}{2}}$

$$E_{F_0}^{\frac{3}{2}} = \frac{3n_c}{8\pi}\left(\frac{h^2}{2m}\right)^{\frac{3}{2}}$$

$$E_{F_0} = \left(\frac{3n_c}{8\pi}\right)^{\frac{2}{3}}\left(\frac{h^2}{2m}\right) \quad \text{-------------(16)}$$

This eqn is used to find out the Fermi energy of metals and semiconductors.

Average Energy of an electron at 0K

$$Average\ Energy\ of\ an\ electron\ at\ 0K\ E_{Avg} = \frac{Total\ energy\ of\ electrons\ at\ 0K\ (E_{tot})}{Number\ of\ energy\ states\ at\ 0K\ (N(E)dE)}$$

Here, the $Total\ energy\ of\ electrons\ at\ 0K\ (E_{tot}) =$ $Average\ Energy\ of\ an\ electron\ at\ 0K\ X \quad Number\ of\ energy\ states\ at\ 0K\ (N(E)dE)$

$$E_{tot} = \int_0^{E_F} N(E)dE\,.E$$

$$E_{tot} = \int_0^{E_{F_0}} \frac{4\pi}{h^3}(2m)^{3/2} E_F^{\ 1/2} dE\,.E$$

$$E_{tot} = \int_0^{E_{F_0}} \frac{4\pi}{h^3}(2m)^{3/2} E_F^{\ 3/2} dE$$

$$E_{tot} = \frac{4\pi}{h^3}(2m)^{3/2}\frac{E_{F_0}^{\ 5/2}}{5/2}$$

$$E_{tot} = \frac{8\pi}{5h^3}(2m)^{3/2} E_{F_0}^{\ 5/2} \quad \text{----------(1)}$$

We know $N(E)dE = \frac{8\pi}{3h^3}(2m)^{\frac{3}{2}} E_{F_0}^{\frac{3}{2}}$ ---------- (2)

$$E_{Avg} = \frac{\frac{8\pi}{5h^3}(2m)^{3/2} E_{F_0}^{\ 5/2}}{\frac{8\pi}{3h^3}(2m)^{\frac{3}{2}} E_{F_0}^{\frac{3}{2}}}$$

$$E_{Avg} = \frac{3}{5} E_{F_0}$$

ELECTRONS IN PERIODICAL POTENTIAL

The free electron theory explains the properties of thermal conductivity, electrical conductivity and specific heat of most of the metals. But, it fails to explain why some solids are conductors, some are insulators and others are semiconductors.

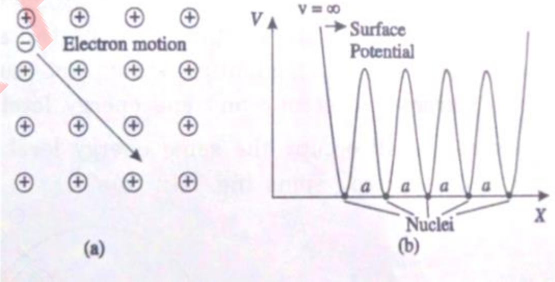
A solution to this problem was given by band theory of solids and is called zone theory.

According to free electron theory, the potential energy of the electron inside the crystal through which an electron moves is supported to be (zero). So it is completely free to move about in the crystal, restrained only by the surface of the crystal.

Postulates

1. According to band theory, potential energy of electron within the crystals is periodic due to periodicity of the crystal i.e., free electron move inside periodic lattice field.
2. The potential energy of the solid of the solid varies periodically with the periodicity of space lattice ‘a’ which is nothing but interatomic spacing.

Inside a real crystal, the electrons (-) move through periodic arrangement of positively charged holes (+) a shown in the fig(a).Fig.(b) shows one dimensional periodic potential distribution for a crystal. It is assumed that the potential energy of the electron at the positive ion site is zero and is maximum when it is half way between the adjacent nuclei.



ENERGY BANDS IN SOLIDS

According to the energy band theory of solids, the free electrons move in a periodic potential produced by positive ion cores. The electrons are treated as weakly perturbed by the periodic potential. A simple qualitative explanation of the formation of energy bands in a solid is given below.

A solid contains an enormous number of atoms packed closely together. Each atom when isolated has a discrete set of electron levels, 1s, 2s, 2p, … If we imagine the N atoms on the solid to be isolated from one another, they would have completely coinciding schemes of energy levels.

The energies of electrons within any one isolated atom obey the following conditions.

(i) There are specific electronic energy levels in each atom (fig. a). Electrons cannot occupy space between these levels

(ii) Electrons fill the lowest energy levels first. A specific quantity of energy, called a quantum of energy must be supplied to move an electron to the next higher level.

(iii) Pauli's, exclusion principle states that no two electrons can occupy the same quantum state. Not more than two electrons can occupy any one energy level. Two electrons shall occupy the same energy level because they have opposite electron spins (fig b).

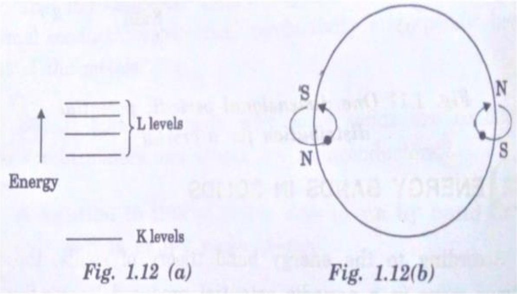


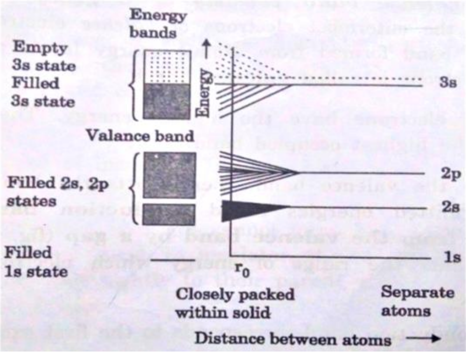
Fig. 1.12 (a) *Fig. 1.12(b)*

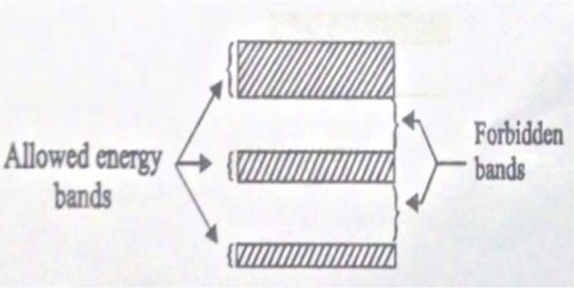
When the atoms are brought in close proximity to form a solid, the valence electrons of common to the entire crystal, and their outermost electronic orbits overlap. Therefore, N electrons will now have to occupy different energy levels, which may be brought about by the electric forces exerted on each electron by all N nuclei. As a result of these forces, each atomic energy level is split up into a large number of closely spaced energy levels. **A set of such closely spaced energy levels is called an energy band.**

Consider 11 electrons of a neutral sodium atom, each occupying specific energy level as indicated in fig. The energy levels of sodium become bands when the atoms lie close together.

In an energy band, allowed energies are almost continuous. These energy bands are separated by ranges of energies that have no allowed energy levels. These regions are known as **forbidden bands** or **energy gaps.**

The amount of splitting is not the same for different levels. The levels filled by valence electrons are disturbed to a greater extent, while this filled by electrons of inner shells are distributed only slightly. If there are N atoms in a solid, there are N allowed quantum states in each band. Each quantum state is occupied by a maximum of two electrons with opposite spins. Thus, each energy band can be occupied by 2N electrons.





The **valence band consists of a group of states** containing the outermost electrons or valence electrons of an atom. The band formed from atomic energy levels contains valence electrons is called **valence band.** These electrons have the highest energy. The band is obviously the highest occupied band.

Above the valence band, there exists the band of next higher permitted energies called **conduction band**. **It is separated from the valence band by a gap.** The gap represents the range of energy which electrons cannot possess.

The conduction band corresponds to the first excited states and it is normally the lowest unfilled energy band. In conduction band, the electrons can move freely and they are generally called **conduction electrons**.

According to free electron theory, the potential energy of the electron inside the crystal through which an electron moves is supposed to be constant which an electron moves is supposed to be constant (zero) and so it is completely free to move throughout the crystal, restrained only by the surface of the crystal.

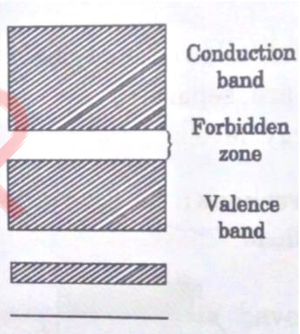
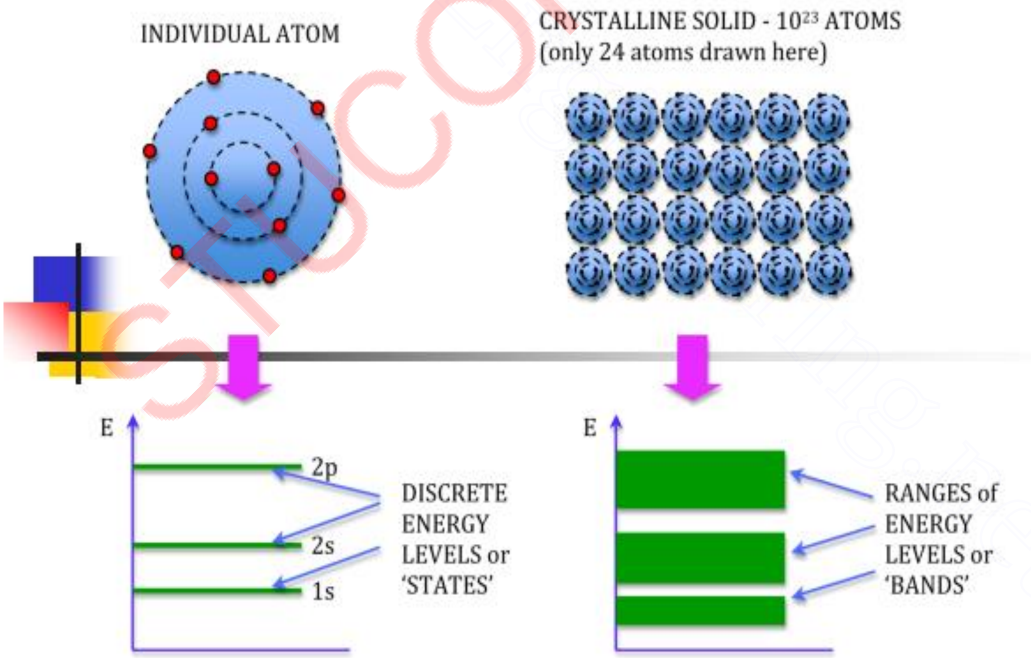


Fig 1.15

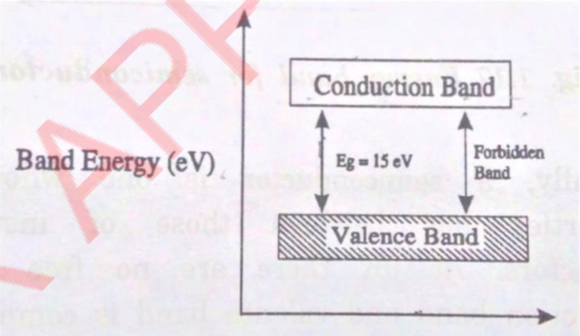


Classification of Metals, Semiconductors and Insulators

On the basis of width of forbidden gap valence and conduction band the solids are classified into insulators, semiconductors and conductors.

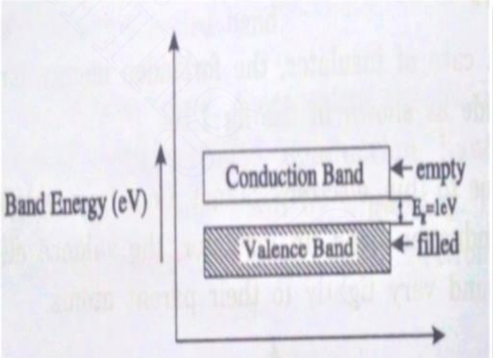
Insulators

- In case of insulator, the forbidden energy band is very wide as shown in the fig. Due to this, electrons cannot jump from valance band to conduction band. In insulator, the valance electrons are bound very tightly to their parent atoms.
- For example, In the case of material like Glass, the valance band is completely full at 0k and the energy gap between valance band and conduction band of the order of 10eV.
- Even in the presence of high electric field, the electrons cannot jump from the valance band to conduction band.
- When a very large energy is supplied, an electron may jump across the forbidden gap. Increase in temperature also enables some electrons to go the conduction band.
- **This explains why certain insulators became conductors at high temperature.** The resistivity of insulators is of the order of 10^7 Ωm. (ohmmeter)

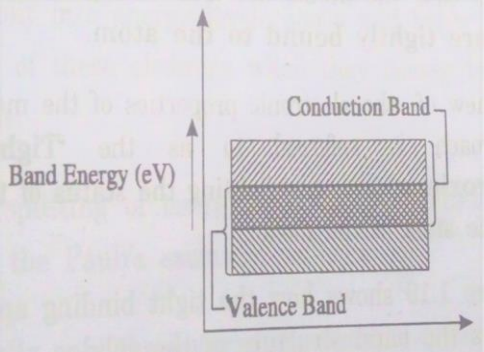


Semiconductor

- In semiconductors**,** the forbidden gap is very small as shown in the fig. Germanium and silicon are the best example semiconductors.
- In germanium, the forbidden gap is of the order of 0.7 eV while in case of silicon, it is the order of 1.1eV.
- Actually, a semiconductor one whose electrical property lies between those of insulators and conductors. At 0k there are no free electrons in conduction band and valence band is completely filled.
- When a small amount of energy is supplied, the electrons can easily jump from valence band to conduction, since the forbidden gap is very small.
- In semiconductors, the conductivities is the order of 10^2 Ωm. (ohm meter)



Conductor



- In case of conductors, there is no forbidden gap both conduction band and valence band overlap each other as shown in the fig.
- In conduction gap, plenty of free electrons available for the process of electric conduction. The electron from the valence band enters into the conduction band.
- The most important fact in conductor is that due to the absence of forbidden gap, there is no structure to establish holes. The total current in conductor is simply the flow of electrons.

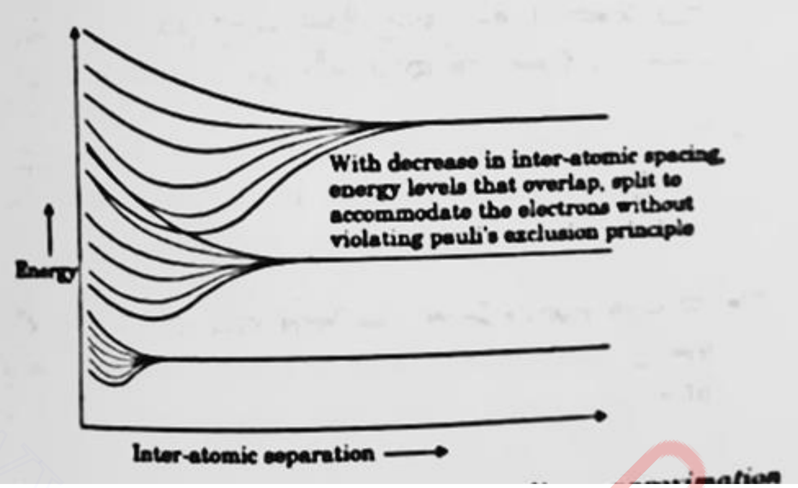
Tight binding approximation

There are usually two approaches to understand the origin of band theory associated with solids. One is the "nearly free electron model" and the other "tight-binding model".

1) Nearly free electron model: In the nearly free electron approximation, interactions between electrons are completely ignored. In solids there exists the ionic core which are tightly bound to the lattice location, while the free electrons are free to move here and there throughout the solid.

2) Tight-binding model: The opposite extreme to the nearly-free electron model assumes the electrons in the crystal behave much like an assembly of constituent atoms.

   - In this approach, the atoms are independent to begin with and they are brought together to build the solid. The electrons are bound to their respective individual atoms to begin with.
   - The atoms are free to begin while the electrons are tightly bound to the atom.
   - When atoms are far apart all the bound electrons have fixed energy levels.
   - When the atoms are brought close to form a solid, the electrons will maintain their original energy levels as long as interatomic separation is large.
   - When atoms are close enough the outer shell electrons begin to overlap and the energy levels begin to split above and below the energy level of individual atoms.
   - Initially the outer shell electrons overlap and as the interatomic spacing keeps on decreasing further, the inner shell electrons overlap and hence the corresponding energy levels also split.



Concept of Effective Mass

The mass of an electron in the periodic potentials of a crystal is different from the free electron mass and is usually referred to as the effective mass. Effective mass of an electron is the mass of the electron when it is accelerated in a periodic potential. It is denoted as m*.

According to de Broglie hypothesis, a moving electron is associated with a wave. The velocity of an electron (*v*) is equal to the group velocity (v_g) of the associated wave.

The group velocity is given by $v_g = \frac{d\omega}{dk}$ ----------(1)

Where ω is the angular frequency ($2\pi v$) and K is the propagation vector of the wave.

In quantum mechanics, the energy, '*E*' of an electron is given by $E = hv$

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

$$E = \hbar\,\omega$$

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

Substituting value of ω from eq (2) to eq (1), we get $\boldsymbol{v_g = \frac{d}{dk}\left(\frac{E}{\hbar}\right)}$

$$\boldsymbol{v_g = \frac{1}{\hbar}\frac{dE}{dk}} \quad \text{------------(3)}$$

Differentiating Equation (3) with respect to '*t*' , we get acceleration of electron as

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

$$a = \frac{d}{dt}\left(\frac{\mathbf{1}}{\hbar}\frac{\boldsymbol{dE}}{\boldsymbol{dk}}\right)$$

$$a = \frac{\mathbf{1}}{\hbar}\left(\frac{\boldsymbol{d^2E}}{\boldsymbol{dk^2}}\right)\frac{dk}{dt} \quad \text{--------------(4)}$$

In quantum theory, the momentum of an electron is given by $p = \frac{h}{\lambda}$

$$p = \frac{h}{2\pi}\frac{2\pi}{\lambda}$$

$$p = \hbar k \quad \text{-----------(5)}$$

Differentiating momentum with respect to t $\frac{dp}{dt} = \hbar\,\frac{\boldsymbol{dk}}{\boldsymbol{dt}}$

Since force acting on the electron $\quad F = \frac{dp}{dt}$

$$F = \hbar\,\frac{\boldsymbol{dk}}{\boldsymbol{dt}} \qquad \frac{\boldsymbol{dk}}{\boldsymbol{dt}} = \frac{\boldsymbol{F}}{\hbar} \quad \text{-----------(6)}$$

Substituting egn (6) in (4) we get, $a = \frac{\mathbf{1}}{\hbar}\left(\frac{\boldsymbol{d^2E}}{\boldsymbol{dk^2}}\right)\frac{\boldsymbol{F}}{\hbar}$

$$a = \frac{\mathbf{1}}{\hbar^2}\left(\frac{\boldsymbol{d^2E}}{\boldsymbol{dk^2}}\right)\boldsymbol{F}$$

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

When an electric field is applied, acceleration of the electron due to this field

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

$$F = m^*a \quad \text{-------------(8)}$$

Comparing equations (7) and (8), we have $\quad m^*a = \left[\frac{\hbar^2}{\left(\frac{\boldsymbol{d^2E}}{\boldsymbol{dk^2}}\right)}\right]\boldsymbol{a}$

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

The above equation indicates the effective mass of an electron is not a constant, but depends on the value of $\left(\frac{d^2E}{dk^2}\right)$

Special cases

Case (1): If $\left(\frac{d^2E}{dk^2}\right)$ is positive, then m^* is also positive

Case (2): If $\left(\frac{d^2E}{dk^2}\right)$ is negative, then m^* is also negative

Case (3) If $\left(\frac{d^2E}{dk^2}\right)$ is large, then the electron behave as a light particle

Case (4) If $\left(\frac{d^2E}{dk^2}\right)$ is very small, then the electron behave as heavy particle

Concept of holes

- Effective mass plays an important role in conduction process of semiconductors & holes – full or filled valence bands.
- Effective mass is –ve near zone edges of filled valence bands.
- Electrons are accelerated in direction opposite to that the applied field direction – negative mass behavior of electrons.
- Electrons with negative effective mass is considered as a new entity having same positive mass as that of an electron but with a positive charge – hole
- Positive hole conduction and negative electron conduction are in equilibrium.

MAGNETIC MATERIALS

INTRODUCTION

Magnetism arises from the magnetic moment or magnetic dipole of the magnetic materials. When an electron revolves around the positive nucleus, orbital magnetic moment arises. Similarly when the electron spins, spin magnetic moment arises. Any material can be magnetized by an external magnetic field is called as magnetic materials. When a magnetic field is applied externally, the magnetic materials can be easily magnetized since they have permanent magnetic moment. Among the different types of magnetic materials, the following five will be having practical application.

1. Dia magnetic materials
2. Para magnetic materials
3. Ferro magnetic materials
4. Anti Ferro magnetic materials
5. Ferrimagnetic materials etc.

BASIC TERMS AND DEFINITIONS

1. Magnetic dipole: Magnetic dipole is a system consisting of two equal and opposite magnetic poles separated by a small distance '$\boldsymbol{l}$'. Where '$\boldsymbol{l}$' is the length of the magnet.

2. Magnetic moment: The product of magnetic pole strength '$\boldsymbol{m}$' and the length of the magnet '$\boldsymbol{l}$' is known as magnetic moment (**M**) $\boldsymbol{M = m.l}$

3. Magnetic flux (ϕ): Total number of magnetic lines of forces passing through a surface is known as magnetic flux. It is represented by ϕ and its unit is weber (WB).

4. Magnetic induction (or) Magnetic Flux density: Magnetic induction is the number of magnetic force passing through unit area perpendicularly. $B = \frac{\phi}{A}$Its unit is 'Wb/m^2'or *Tesla*.

5. Magnetic field intensity (or) Strength (H): It is defined as the force experienced by a unit North Pole placed at the given point in a magnetic field. Its unit is N/Wb or *Ampere/meter.*

6. Intensity of magnetization: Magnetization means the process of converting a Non-magnetic material into the magnetic material. It measures the magnetization of a magnetized specimen. It is defined as the magnetic moment per unit volume.$\boldsymbol{I} = \frac{\boldsymbol{M}}{\boldsymbol{V}}$ Its unit is $\boldsymbol{Wb/m^2}$

7. Magnetic permeability (μ): It is the ratio between magnetic flux density (**B**) and the magnetic field intensity (**H**). $\mu = \mu_0\mu_r$ $\mu = \frac{\mathrm{B}}{\mathrm{H}}$

8. Relative permeability (μ_r): It is the ratio between permeability of the medium to the permeability of free space $\mu_r = \frac{\mu}{\mu_0}$

9. Magnetic Susceptibility, χ: It is the ratio between intensity of magnetization (***I***) and the magnetic field intensity (***H***) $\chi = \frac{I}{H}$

Relation between μ_r and χ:

We know, $B = \mu H$
In other way $B = \mu_0(I + H)$

$$B = \mu_0 H(\frac{I}{H} + 1)$$

$$\frac{B}{H} = \mu_0(1 + \chi)$$

The relative permeability $\mu = \mu_r\mu_0$ and $\frac{B}{H} = \mu$

$$\mu_r\mu_0 = \mu_0(1 + \chi)$$

$$\mu_r = 1 + \chi$$

Where χ is the Susceptibility of the medium.

ORIGIN OF MAGNETIC MOMENT AND BOHR MAGNETON

ORIGIN OF MAGNETIC MOMENT

Any matter is basically made up of atoms. The property of magnetism exhibited by certain materials with the magnetic property of its constituent atoms. We know that electrons in an atom revolve around the nucleus in different orbits.

Basically there are three contributions for the magnetic dipole moment of an atom.

1. The orbital motions of electrons (the motion of electrons in the closed orbits around the Nucleus) are called orbital magnetic moment.
2. Spin motion of the electrons (due to electron spin angular momentum) is called spin magnetic moment.
3. The contribution from the nuclear spin (due to nuclear spin angular momentum) is nearly 10^3 times smaller than that of electron spin; it is not taken into consideration.

BOHR MAGNETRON: The magnetic moment contributed by an electron with angular momentum quantum number n = 1 is known as Bohr Magnetron.

$$\mu_B = \frac{eh}{4\pi m} \mu_B = 9.27 x 10^{-24} \frac{A}{m^2}$$

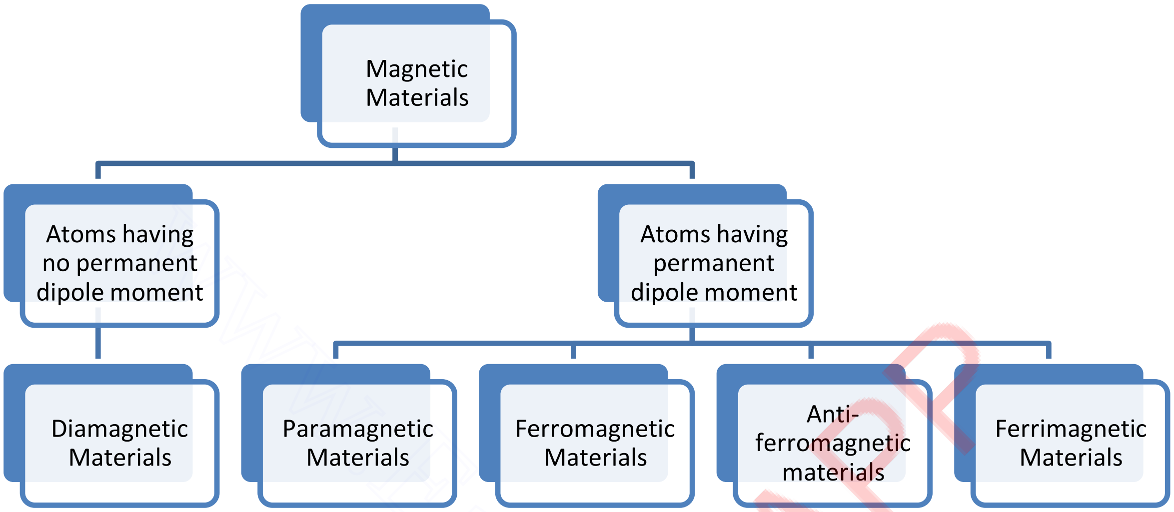
CLASSIFICATION OF MAGNETIC MATERIALS:

(On the basis of magnetic moment)

Magnetic materials are basically divided into two types on the basis of magnetic moments, namely

1. Materials not having any permanent magnetic moment.
    Examples: Dia-magnetic material
2. Materials having permanent magnetic moment
    Examples: Para-magnetic materials
    Ferro magnetic materials
    Ferri magnetic materials

Depending on the interaction between the induced dipoles, magnetic materials having permanent magnetic moment are classified into three.

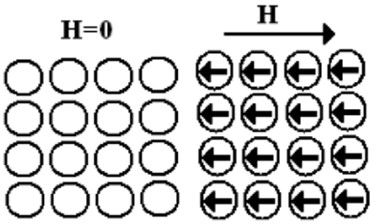


- If the permanent dipoles do not interact among themselves, the materials are known as ***paramagnetic materials***
- If the permanent dipole is strong and all the dipoles line up in parallel, the materials are known as ***Ferromagnetic materials***.
- If the permanent dipoles line up in anti parallel direction, the materials are known as antiferromagnetic or Ferrimagnetic materials.

DIAMAGNETIC MATERIALS:

Diamagnetism is exhibited by all the materials. The atoms in the diamagnetic materials do not possess permanent magnetic moment. However, when a material is placed in a magnetic field, the electrons in the atomic orbits tend to counteract the external magnetic field and the atoms acquire an induced magnetic moment. As a result, the material becomes magnetized. The direction of the induced dipole moment is opposite to that of externally applied magnetic field. Due to this effect, the material gets very weakly repelled, in the magnetic field. This phenomenon is known as diamagnetism.

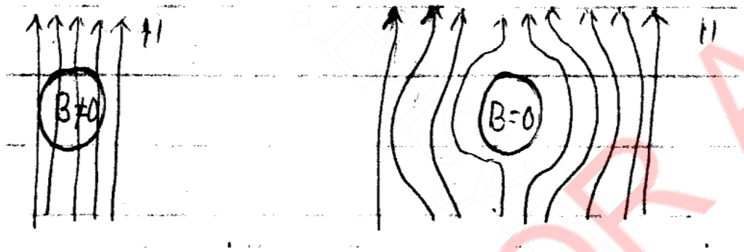
When a magnetic field H_o is applied in the direction shown in fig., the atoms acquire an induced magnetic moment in the opposite direction to that of the field. The strength of the induced magnetic moment is proportional to the applied field and hence magnetization of the material varies directly with the strength of the magnetic field. The induced dipoles and magnetization vanish as soon as the applied field is removed.



Properties:

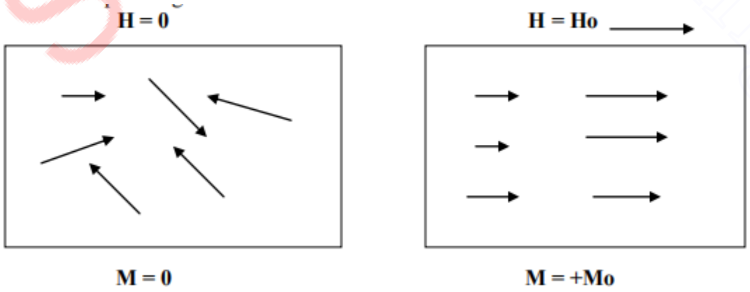
- Permanent dipoles are absent. Therefore the magnetic effects are very small.
- They repel the magnetic lines of force.
- The susceptibility is negative, and is independent of temperature and applied field.
- Permeability is less than unity.
- When temperature is less than critical temperature diamagnets become normal material

  Examples: Gold, germanium, Silicon, water, alcholol, etc.



PARAMAGNETIC MATERIALS:

In certain materials, each atom or molecule possesses a net permanent magnetic moment (due to orbital and spin magnetic moment) even in the absence of an external magnetic field. The magnetic moments are randomly oriented in the absence of external magnetic field. Therefore the net magnetic moment is zero, and hence the magnetization of the material is zero. But, when an external magnetic field is applied, the magnetic dipoles tend to align themselves in the direction of the magnetic field and the material becomes magnetized. As shown in fig. This effect is known as paramagnetism.

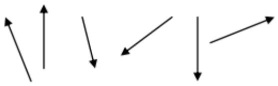


Thermal agitation disturbs the alignment of the magnetic moments. With an increase in Temperature, the increase in thermal agitation tends to randomize the dipole direction thus leading to a decrease in magnetization. This indicates that the paramagnetic susceptibility decreases with increases in temperature. It is noted that the paramagnetic susceptibility varies inversely with temperature.

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

This is known as curie's law of paramagnetism and C is called Curie's constant.

Properties:

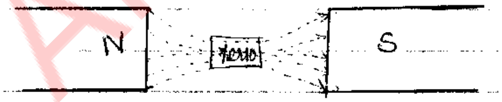


- The magnetic lines of force pass through the material.
- They have permanent magnetic dipoles.
- The susceptibility is positive and it depends on the temperature.
- Permeability is greater than one.
- When the temperature is less than critical temperature, the material becomes diamagnetic.

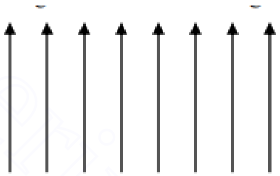
Examples: $CuSO_4$, $MnSO_4$, Platinum, aluminium, etc.

FERROMAGNETIC MATERIALS:

In ferromagnetic material the numbers of unpaired electrons are more. Most of the spin magnetic moment points in one direction. In the absence of magnetic field the dipoles align themselves parallel to each other and give rise to magnetic field called as ***spontaneous magnetization.*** When a small magnetic field is applied, the dipoles get reorient itself along the direction of the magnetic field and they becomes very strong magnets.



Properties:



- All the magnetic lines of force passes through the material, since it has own magnetization.
- They have magnetization, even in the absence of external field.
- They have permanent magnetic dipoles.
- The susceptibility is positive and very high.
  According to Curie Weiss law the susceptibility is given by $\chi = \frac{C}{T-\theta}$
- Permeability is very much greater than I
- When the temperature is greater than Curie temperature, they become paramagnetic.

COMPARISON OF DIAMAGNETIC, PARAMAGNETIC AND FERROMAGNETIC MATERIALS.

S.No	Dia magnetic materials	Paramagnetic materials	Ferromagnetic materials
1	In diamagnetic materials there are equal number of electron spins which are randomly oriented and hence the net magnetic moment is zero.	In paramagnetic materials there is unequal number of electron spins and hence there exists a permanent magnetic moment.	In ferromagnetic materials there is more number of unequal electron spins and hence there exists enormous amount of permanent magnetic moment.

2	When the external magnetic field is applied, the electrons will align perpendicular to the field direction and hence it reduces the magnetic induction present in the material. Thus they are named as weak magnets.	When the external magnetic field is applied, the electrons will align parallel to the field direction and hence the material is magnetized. Thus they are named as strong magnets.	When the external magnetic field is applied, the electrons which are aligned parallel will reorient itself to the field direction and will be easily magnetized. Thus they are named as very strong magnets.
3	When the material is placed in the magnetic field, the magnetic flux lines are repelled away from the material.	When the material is placed in the magnetic field, the magnetic flux lines passes through the material.	When the material is placed in the magnetic field, the magnetic flux lines are highly attracted towards the center of the material.
4	The susceptibility is negative. $(\chi = -ve)$	The susceptibility is positive and small. $(\chi = +ve)$	The susceptibility is positive and large. $(\chi = +ve)$
5	The susceptibility is independent of temperature.	The susceptibility varies inversely with the absolute temperature.	The susceptibility depends upon the temperature.
6	Permeability is less than 1.	Permeability is greater than 1.	Permeability is very much greater than 1.
7	When the temperature is less than critical temperature, the diamagnetism suddenly disappears and becomes a normal material.	When the temperature is less than curie temperature, the paramagnetic material is converted into diamagnetic material.	When the temperature is greater than curie temperature, the ferromagnetic material is converted into paramagnetic material.
8	Examples: gold, bismuth, water, antimony, hydrogen, alcohol, germanium, silicon, etc.	Examples: platinum, chromium, aluminium, copper sulphate, manganese sulphate, etc.	Examples: iron, nickel, cobalt, steel, etc.

ORIGIN OF FERROMAGNETISM AND EXCHANGE INTERACTION

Concept: *Metals contain large number of electrons (i.e.,) free electrons. Each electron posses a magnetic moment. When the magnetic field is applied, then the elementary electrons behave as magnetic dipoles, which tend to orient along the direction of external magnetic field. Thus the electrons affect the paramagnetism volume susceptibility* (χ_C).

Explanation

Langevin showed that paramagnetic susceptibility varies as $\frac{1}{T}$

$$\chi_C = \frac{1}{T}$$

Where χ_C is called paramagnetic susceptibility.

Its value is 10^{-4} at room temperature but experimental observation shows that the paramagnetic susceptibility value has very small value sy, in the order of 10^{-6} and is independent of temperature. Pauli applied Fermi Dirac statistics to explain this disagreement as follows. Each electron has a magnetic moment $I\ \mu_B$ along the direction of magnetic field.

If there are 'n' number of conduction electrons per unit volume, then
The net magnetization is $M = \mu_B n$

$$M = \mu_B (n_+ - n_-) \qquad \text{----------------- (1)}$$

Where $n = n_+ - n_-$
Here n_+ is the number of electrons with magnetic moment parallel to the magnetic field B and n_- is the number of electrons with magnetic moment anti-parallel to the magnetic field B.

The concentration of electrons with magnetic moments parallel to the magnetic field is

$$n_+ = \frac{1}{2}\int_{\mu_B}^{E_F} F(E)\ g\left(E + \mu_B B\right) dE \qquad \text{---------------- (2)}$$

$$n_+ = \frac{1}{2}\int_{0}^{E_F} F(E)\ g\ (E) dE + \frac{1}{2}\ \mu_B B\ g\ (E_F) \qquad \text{---------------- (3)}$$

Similarly,

$$n_- = \frac{1}{2}\int_{\mu_B}^{E_F} F(E)\ g\left(E - \mu_B B\right) dE$$

$$n_- = \frac{1}{2}\int_{0}^{E_F} F(E)\ g\ (E) dE - \frac{1}{2}\ \mu_B B\ g\ (E_F) \qquad \text{---------------- (4)}$$

Where F(E) is called Fermi-Dirac distribution function and $\frac{1}{2}\ g\ (E\ \pm \mu_B B)$ is the density of orbitals of one spin (either + or (or) -) orientation.

Substituting equation (3) and equation (4) in equation (1), we get

The net magnetization

$$M = \mu_B \left\{\frac{1}{2}\int_{0}^{E_F} F(E)\ g\ (E) dE + \frac{1}{2}\ \mu_B B\ g\ (E_F) - \left[\frac{1}{2}\int_{0}^{E_F} F(E)\ g\ (E) dE - \frac{1}{2}\ \mu_B B\ g\ (E_F)\right]\right\}$$

$$M = \mu_B [\mu_B B\ g\ (E_F)]$$

$$M = {\mu_B}^2 B\ g\ (E_F) \qquad \text{---------------- (5)}$$

We know, density of states

$$g\ (E_F) = \frac{3}{2}\ \frac{n}{E_F} \qquad \text{---------------- (6)}$$

Where E_F is the Fermi Energy.

Substituting equation (6) in equation (5), we get

$$M = \mu_B{}^2 B \,\frac{3}{2}\,\frac{n}{E_F} \qquad \text{---------------- (7)}$$

Since $B = \mu_0 H$, we can write equation (7) as

$$M = \mu_B{}^2 \mu_0 H \,\frac{3}{2}\,\frac{n}{E_F}$$

$$\frac{M}{H} = \frac{3}{2}\,\frac{\mu_B{}^2 \mu_0\, n}{E_F} \qquad \text{---------------- (8)}$$

Since $\chi_C = \frac{M}{H}$, we can write equation (8) as

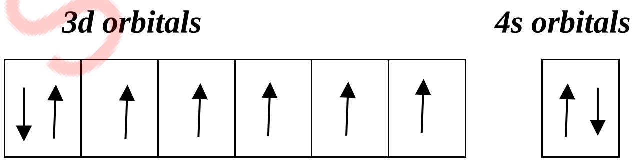
$$\chi_C = \frac{3}{2}\,\frac{\mu_B{}^2 \mu_0\, n}{E_F} \qquad \text{---------------- (9)}$$

Equation (9) is called as the Pauli's paramagnetic susceptibility of a Fermi gas of conduction electrons.

Here in equation (9) we can note that the susceptibility is independent of temperature thus verifying the experimental also.

ORIGIN OF FERROMAGNETISM AND EXCHANGE INTERACTION

The ferromagnetic property is exhibited by transition elements such as iron, cobalt and nickel at room temperature and rare earth elements such as gadolinium and dysprosium. The ferromagnetic materials possess parallel alignment of dipoles. This parallel alignment of dipoles is not due to the magnetic force existing between any two dipoles. The reason is that the magnetic potential energy is very small and it is smaller than thermal energy.



The electronic configuration of iron is $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $3d^6$ and $4s^2$. For iron, the six electrons present in the 3d sub shell occupy the orbitals such that there are four unpaired electrons and two paired electrons. These four unpaired electrons contribute a magnetic moment of 4β. This arrangement shows the parallel alignment of four unpaired electrons. The parallel alignment of dipoles in iron is not due to the magnetic interaction. It is due to the Pauli's exclusion principle and electrostatic interaction energy.

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.

Quantum Interference Devices

A Quantum Interference Device is a very sensitive device which is used to measure very weak magnetic fields at the order of 5 x 10-18 Tesla, using the principle of interference.

Examples

1. Superconducting quantum interference devices
2. GMR devices etc.

Applications

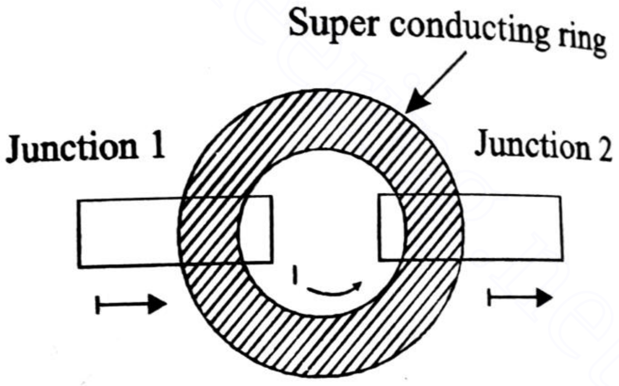
1. These devices are used in research and biological studies.
2. They are used in ultra-sensitive electronic and magnetic measurements.

Superconducting Quantum Interference Devices (SQUID)

SQUID [Superconducting Quantum Interference Devices] are the improved model of Josephson devices. It has high efficiency, sensitivity and quick performance.

Principle: ***Small change in magnetic field, produces variation in flux quantum*.**

Explanation:



It consists of a super conducting rings which can have magnetic fields of quantum values (1,2,3, ….) of flux placed in between the two Josephson junctions.

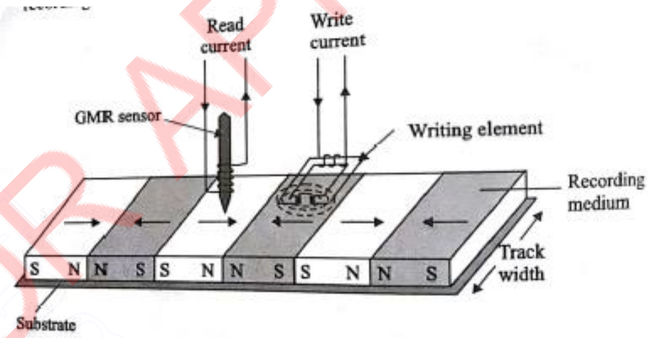
When the magnetic field is applied perpendicular to the plane of the ring, current is induced at the two Josephson junctions and produces interference pattern. The induced current flows around the ring so that the magnetic flux in the ring can have quantum values of flux, which corresponds to the value of magnetic field applied. Therefore SQUIDS are used to detect the variation in very minute magnetic signals in terms of quantum flux. They are used ad storage devices for magnetic flux. They are also used in the study of earthquakes, removing paramagnetic impurities, detection of magnetic signals from the brain, heart etc.

GMR Devices

Giant magnetoresistance (GMR) is a quantum mechanical magnetoresistance effect observed in thin film structures composed of alternating ferromagnetic and nonmagnetic layers. Giant magnetoresistance is a large change in electrical resistance due to spin alignment of electrons in alternating magnetic layers separated by a non-magnetic layer. GMR Devices are widely used as magnetic sensors, read heads in hard disks, magnetometers, compass system, etc.

MAGNETIC HARD DISK DRIVE (HDD) WITH GMR SENSOR

The GMR read head sensor in a hard disk is built using a spin valve. Spin valve resistance demonstrates a steep change in the small field range close to H=0. As the magnetic bits on the hard drive pass under the read head, the magnetic alignment of the sensing layer in the spin valve changes resulting in the resistance change.



As the read head passes over the disk, the free layer shifts its magnetic orientation to match that of the bit. So sometimes the direction of the free layer's magnetic field is aligned with the field of the pinned layer (which never changes), and sometimes it is opposite. When they are aligned, most of their electrons will share the same up or down spin. As some of these electrons pass through the layers in the form of current, there will be minimal scattering. The low resistance means a current will be detected, and the computer computes a 1 bit.

When the free layer's magnetic orientation switches to opposite that of the pinned layer, there's a much different result. The electrons in the two layers have opposing spins. So as the current passes through the magnetized layers, those electrons will scatter in one or the other of them, resulting in a much weaker current and a 0 bit.

PROBLEMS

1. **Calculate the drift velocity of the free electron with a mobility of 3.5×10^{-3} $m^2V^{-1}s^{-1}$ in copper for an electric field strength of 0.5 V/m.**

$$\text{Drift Velocity } v_d = \mu E$$

$$v_d = 3.5 \times 10^{-3} \times 0.5$$

$$v_d = 1.75 \times 10^{-3} \text{ m/s}$$

$$v_d = 0.00175 \text{ m/s}$$

2. A conducting rod contains 8.5x10^{28} electrons per m^3. Calculate the electrical conductivity at room temperature if the collision time for electron is 2 x 10^{-14}s.

$$\sigma = \frac{ne^2\tau}{m}$$

$$\sigma = \frac{(8.5\,x\,10^{28}x\,(1.609\,x\,10^{-19})^2 x\,2\,x\,10^{-14})}{9.11\,x\,10^{-31}}$$

$$\sigma = 4.83\,x\,10^7 mho/m$$

3. The mobility of electron in copper is 3x10^{-3} m^2/Vs. Assuming e = 1.6 x 10^{-19} C and m$_e$= 9.1x10^{-31} kg, calculate the mean free time.

$$\sigma = \frac{ne^2\tau}{m} \quad \text{and} \quad \sigma = \mu\, n\, e$$

Equating above eqns we can write $\tau = \frac{\mu m}{e}$

$$\text{Mean free time } \tau = \frac{3\,x\,10^{-3}\,x\,9.1\,x\,10^{-31}}{1.6\,x\,10^{-19}}$$

Mean free time τ = 1.70625x10^{-14} seconds

4. Evaluate the Fermi function for energy K$_B$T above the Fermi energy.

$$E-E_F = K_B\,T$$

$$F(E) = \frac{1}{1+e^{E-E_F/k_BT}} \qquad F(E) = \frac{1}{1+e^{k_BT/k_BT}} \qquad F(E) = \frac{1}{1+\exp(1)}$$

$$F(E) = \frac{1}{1+\ 2.78} \qquad \mathbf{F(E) = 0.269}$$

5. The Fermi temperature of a metal is 24600 K. Calculate the Fermi velocity.

The relation between Fermi energy, Fermi velocity and Fermi temperature is given by

$$E_F = K_BT_F = \frac{1}{2}mv_F{}^2$$

$$v_F = \sqrt{\frac{2K_BT_F}{m}} = \sqrt{\frac{2\,x\,1.38\,x\,10^{-23}\,x\,24600}{9.11\,x\,10^{-31}}}$$

$$v_F = 0.8633\,X\,10^6 m/s$$

6. Calculate the electrical and thermal conductivities for a metal with a relaxation time 10^{-14} second at 300 K. Also calculate Lorentz number using the above result. (Density of electrons = 6x10^{28} m^{-3}).

$$\sigma = \frac{ne^2\tau}{m}$$

$$\sigma = \frac{6 X 10^{28} X (1.6 X 10^{-19})^2 X 10^{-14}}{9.11 X 10^{-31}}$$

$$\sigma = 1.686 X 10^7 \text{ mho m}^{-1}.$$

$$\text{Thermal conductivity } K = \frac{\pi^2}{3}\frac{n k^2 \tau T}{m}$$

$$K = \frac{3.14^2}{3}\frac{6 X 10^{28} X (1.38 X 10^{-23})^2 X 10^{-14} X 300}{9.11 X 10^{-31}}$$

$$K = 123.80 \text{ W/m/K}$$

$$\text{Lorentz Number } L = \frac{K}{\sigma T}$$

$$L = \frac{123.92}{1.686 X 10^7 X 10^{-14}}$$

$$L = \mathbf{2.45 X 10^{-8} W\Omega K^{-2}}$$

7. The density of silver is 10.5x10^3 kg/m^3. The atomic weight of silver is 107.9. Each silver atom provides one conduction electron. The conductivity of silver at 20 °C is 6.8 x 10^7 Ω^{-1}m^{-1}. Calculate the density of electron and also the mobility of electrons in silver.

$$\text{Number of atoms present per m}^3 = \text{Avagadro No.}, X \frac{\text{Density}}{\text{Atomic weight}}$$

$$= \frac{6.023 X 10^{23} X 10.5 X 10^3}{107.9 X 10^{-3}}$$

$$\text{Number of atoms present per m}^3 = 5.86 X 10^{28} \text{atoms/m}^3$$

$$\mu = \frac{\sigma}{ne}$$

$$\mu = \frac{6.8 X 10^7}{5.86 X 10^{28} X 1.6 X 10^{-19}} \qquad \mathbf{\mu = 0.72 X 10^{-2} m^2 V^{-1} s^{-1}}$$

8. Use the Fermi distribution function to obtain the value of F (E) for the level just 0.01eV above the Fermi level at 200 K.

$$E-E_F = 0.01\text{eV}$$

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

$$F(E) = \frac{1}{1 + \exp\left(\frac{0.01 X 1.6 X 10^{-19}}{1.38 X 10^{-23} X 200}\right)}$$

$$F(E) = \frac{1}{1 + e^{0.05797}}$$

$$\mathbf{F(E) = 0.3589}$$

9. The Fermi energy of silver is 5.51 eV. What is the average energy of a free electron at 0K?

$$\overline{E_{avg}} = \frac{3}{5} E_F$$

$$\overline{E_{avg}} = \frac{3}{5}(\,5.51 \text{ X } 1.6 \text{ X } 10^{-19})$$

$$\overline{E_{avg}} = 5.2896 \text{ X } 10^{-19} \text{J}$$

$$\overline{\mathbf{E_{avg}}} = \mathbf{3.306\ eV}$$

10. **Magnetic field Intensity of a paramagnetic material is 104 A/m. At room temperature, its susceptibility is 3.7 x 10^{-3}. Calculate the magnetization in the material.**

$$\chi = \frac{I}{H} \qquad I = \chi H \qquad I = 3.7\ X\ 10^{-3}\ X\ 10^{4}$$

$$I = 37\ Am^{-1}$$

11. **A magnetic field of 1800 ampere/meter produces a magnetic flux of 3 x 10^{-5} weber in an iron bar of cross sectional area 0.2 cm^2. Calculate permeability.**

$$B = \frac{\Phi}{A} \qquad B = \frac{3 \text{ x } 10^{-5}}{0.2 \text{ x } 10^{-4}} \qquad B = 1.5\, Wb/m^2$$

$$\mu = \frac{B}{H} \qquad \mu = \frac{1.5}{1800} \qquad \mu = 8.333 \text{ x } 10^{-4} Hm^{-1}.$$

12. **A magnetic field of 2000 A/m is applied to a material which has a susceptibility of 1000. Calculate the (i) Intensity of Magnetization and (ii) Flux density.**

$$\text{Intensity of Magnetization} \quad I = \chi_m H \qquad I = 1000\ X\ 2000$$

Rotate Left 90°.

$$I = 2\ X\ 10^{6}\ A/m.$$

$$\text{Flux Density} \quad B = \mu_0 (I + H)$$

$$B = 4\ X\ 3.14\ X\ 10^{-7}\ X\ (2\ X\ 10^{6} + 2000)$$

$$B = 2.514\ Wb/m^2.$$

13. **The magnetic susceptibility of a medium is 940 x 10^{-4}. Calculate its absolute and relative permeability.**

$$Relative\ permeability\ \mu_r = 1 + \chi$$

$$Relative\ permeability\ \mu_r = 1 + (940 \text{ x } 10^{-4})$$

$$Relative\ permeability\ \mu_r = 1 + (0.094)$$

$$Relative\ permeability\ \mu_r = 1.094$$

$$Absolute\ \ permeability\ \mu = \mu_0 \mu_r$$

$$Absolute\ \ permeability\ \mu = 4\pi \text{ x } 10^{-7} \text{ x } 1.094$$

$$Absolute\ \ permeability\ \mu = 13.74 \text{ x } 10^{-7}\ \mathrm{N}/A^2$$

14. **Iron has relative permeability of 5000. Calculate its magnetic susceptibility.**

$$\chi = \mu_r - 1$$

$$\chi = 5000 - 1$$

$$\chi = 4999$$

15. **The magnetic field strength of silicon is 1500 A/m. if the magnetic susceptibility is , calculate the magnetization and flux density in Silicon.**

Intensity of magnetization $I = \chi_m H$

$$I = -0.3 \text{ x } 10^{-5}\ x\ `1500$$

$$I = -4.5 \text{ x } 10^{-3} A\ /m$$

$Flux\ density\ B = \mu H$

$$B = \mu H$$

$$B = (1 + \chi_m)H$$

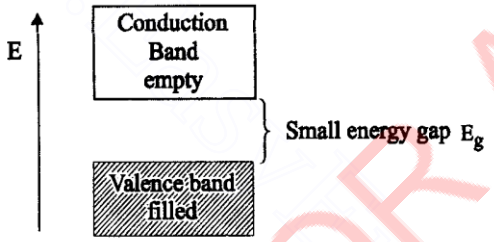
$$B = (1 - 0.3 \text{ x } 10^{-5})1500$$

$$B = (0.999997)1500$$

$$\boldsymbol{B = 1499.9\ Wb/m^2}$$

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.

A semiconductor is a solid which has the resistivity in between the conductor and the insulator. It act as insulator at low temperature and act as conductors at high temperature. Examples: Germanium, Silicon, GaAs, InP, etc. The resistivity of semiconductors are from 10^{-4} to 0.5 ohm – metre. The study of semiconducting materials is essential for engineers due to their wide application in semiconductor devices in engineering and technology.



Energy band diagram of a semiconductor

Properties of semiconductors:

- ✓ The resistivity lies between 10-4 to 0.5 ohm meters.
- ✓ At 0K, they behave as insulators.
- ✓ They empty conduction band and almost filled valence band.
- ✓ The conductivity of a semiconductor increases both due to the temperature and impurities.
- ✓ They have negative temperature coefficient of resistance.
- ✓ In semiconductors both the electron and holes are charge carriers and will take part in conduction.

Classification of semiconductors:

Based on composition they are classified as

(i) Elemental semiconductors (ii) Compound semiconductors

(i) Elemental semiconductors: They are made from a single element of fourth group elements of the periodic table. They are also called as indirect band gap semiconductors. ***Examples:*** Germanium, Silicon, Diamond.

(ii) Compound semiconductors: They are formed by combining third and fifth group elements or second and sixth group elements in the periodic table. They are also called as direct band gap semiconductors. ***Examples:*** GaP, GaAs, MgO, ZnO, ZnS.

S.No	Elemental semiconductors	Compound semiconductors
1	They are made up of single element.	They are made up of compounds.
2	They are made from a single element of fourth group elements of the periodic table.	They are formed by combining third and fifth group elements or second and sixth group elements in the periodic table.
3	They are called indirect band gap semiconductors.	They are called as direct band gap semiconductors.
4	Here heat is produced during recombination.	Here the photons are emitted during recombination.
5	Life time of charge carriers is more.	Life time of charge carriers is less.
6	Current amplification is more.	Current amplification is less.
7	They are used in the manufacture of diodes and transistors, etc.	They are used for making LED's, laser diodes, IC's, etc.
8	Examples: Ge, Si, etc.	Examples: GaAs, GaP, CdS, MgO, etc.

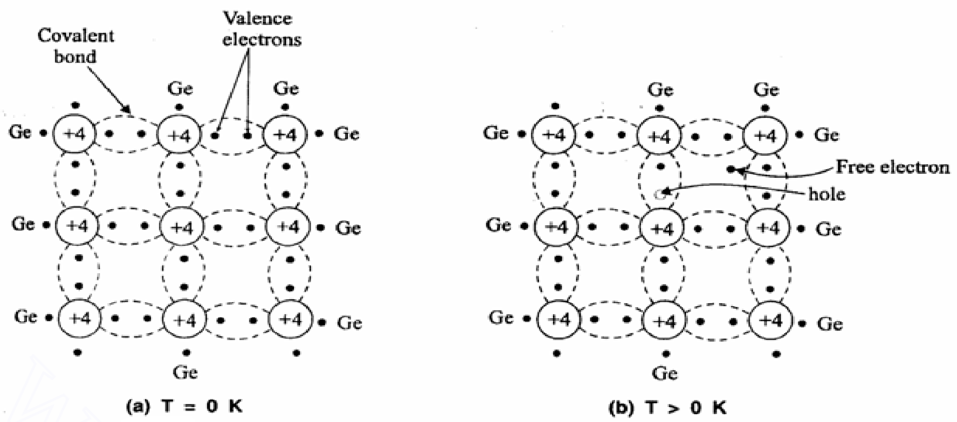
Types of semiconductors:

Depending on the impurity added, there are two types.

(i) Intrinsic semiconductor (or) pure semiconductors
(ii) Extrinsic semiconductor (or) impure semiconductors
    (a) N-type semiconductor
    (b) P-type semiconductor

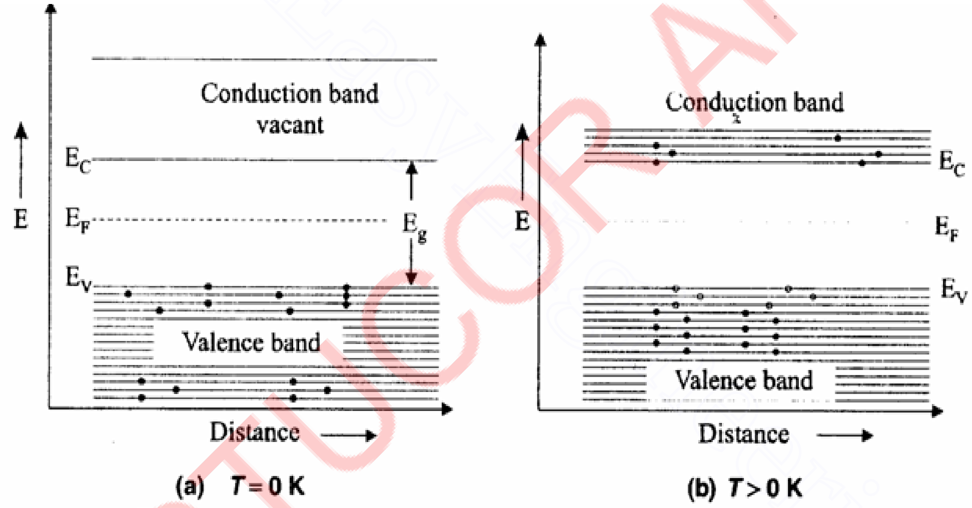
Intrinsic semiconductor:

The semiconductor in extremely pure form, without addition of impurities is known as an intrinsic semiconductor. In intrinsic semiconductor, holes and electrons are created by thermal agitation. As there are no impurities the number of free electrons must be equal to the number of holes. ***Examples***: silicon and germanium.



Germanium Crystal Structure and its Covalent Bond Linkage

They belong to the fourth group element in the periodic table. They are tetravalent atoms since they have four valence electrons. The neighboring atoms form covalent bonds by sharing four electrons with each other so as to form a stable structure. At very low temperatures say 0 K, no free electrons are available for conduction. Hence this semiconductor behaves as an insulator.



Free Electrons and Holes in Intrinsic Semiconductor

Carrier concentration in intrinsic semiconductors:

The number of electrons in the conduction band per unit volume of the material or the number of holes in the valence band of the material is known as carrier concentration. It is also known as density of charge carriers.

Calculation of density of electrons in conduction band:

The number of electrons in the energy interval E and E + dE is given by

$$dn = Z(E)\,F(E)\,dE \qquad \ldots\ldots\ldots\ldots\ldots(1)$$

Where Z (E) dE → Density of energy states

F(E) → Electron probability occupancy.

The number of electrons in the conduction band for the entire region is calculated by integrating the equation (1) from energy E_c to $+\infty$.

$$\therefore \qquad n = \int dn = \int_{Ec}^{+\infty} Z(E)F(E)dE \ldots\ldots \ldots (2)$$

Where

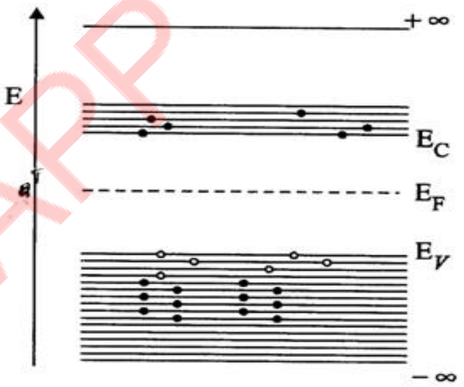
$$Z(E)\,dE = \frac{4\pi}{h^3}\,(2m_e^*)^{3/2}E^{1/2}dE \ldots\ldots\ldots\ldots(3)$$

The electrons in the conduction band are move in a periodic potential , so $m = m_e^*$

Where m_e^* → Effective mass.

E_c → The potential energy of an electron at rest.

$E-E_c$ → The kinetic energy of the conduction electron at higher energy levels.



Energy band diagram of an intrinsic semiconductor

∴ Equation (3) is modified as

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

$$\text{Where } F(E) = \frac{1}{1+e^{(E-E_F)/kT}} \qquad \ldots\ldots\ldots\ldots(5)$$

Substitute equation (4) and (5) in equation (2) we have

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

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

Since kT is very small and $e^{(E-E_F)/kT}$ is very large compared to 1. ∴ 1 from the denominator of equation (6) is neglected.

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

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

$$n = \frac{4\pi}{h^3}(2m_e^*)^{\frac{3}{2}} e^{E_F/kT}\int_{Ec}^{+\infty}(E - E_c)^{\frac{1}{2}}\, e^{-\frac{E}{kT}}\, dE \qquad \text{……….(7)}$$

Take $E - E_c = x$, $dE = dx$, $E = E_c + x$

When $E = E_c$, $E_c - E_c = x$, $x=0$

When $E = +\infty$, $+\infty - E_c = x$, $x = +\infty$

Substituting the above values in equation (7) we have

$$n = \frac{4\pi}{h^3}(2m_e^*)^{\frac{3}{2}} e^{E_F/kT}\int_0^{+\infty}(x)^{\frac{1}{2}} e^{-(E_c+x)/kT}dx$$

$$n = \frac{4\pi}{h^3}(2m_e^*)^{\frac{3}{2}} e^{(E_F-E_c)/kT}\int_0^{+\infty}(x)^{\frac{1}{2}}\, e^{-x/kT}dx \qquad \text{… … … (8)}$$

Using the gamma function, $\int_0^{+\infty}(x)^{\frac{1}{2}}e^{-\left(\frac{x}{kT}\right)}dx = \frac{(kT)^{\frac{3}{2}}\pi^{\frac{1}{2}}}{2}$ … … … (9)

Substituting equation (9) in equation (8) we have $n = \frac{4\pi}{h^3}(2m_e^*)^{\frac{3}{2}}\, e^{(E_F-E_c)/kT}\,\frac{(kT)^{\frac{3}{2}}\pi^{\frac{1}{2}}}{2}$

$$n = 2\left(\frac{2\pi m_e^* kT}{h^2}\right)^{3/2} e^{(E_F-E_c)/kT} \qquad \text{……..(10)}$$

This is the expression for the concentration of electrons in the conduction band of an intrinsic semiconductor.

Calculation of density holes in the valence band:

If an electron is transferred from valence band to conduction band, a hole is created in the valence band. Let dP be the number of holes in the valence band for the energy range E and E+dE

$$dP = Z(E)\,(1-F(E))dE \qquad \text{…………(1)}$$

Where 1-F(E) → Probability of an unoccupied electron state i.e., presence of a hole

$$1\text{-}F(E) = 1 - \left[\frac{1}{1+e^{\frac{(E-E_F)}{kT}}}\right] \qquad 1\text{-}F(E) = \frac{1+e^{\frac{(E-E_F)}{kT}} - 1}{1+e^{\frac{(E-E_F)}{kT}}} \qquad 1\text{-}F(E) = \frac{e^{\frac{(E-E_F)}{kT}}}{1+e^{\frac{(E-E_F)}{kT}}} \qquad \text{…………(2)}$$

E is very small compared to E_F, $e^{\frac{(E-E_F)}{kT}}$ is very small. So the second term in the denominator of equation (2) is neglected. ie, $1 + e^{\frac{(E-E_F)}{kT}} \approx 1$

$$\therefore \quad 1\text{-}F(E) = e^{\frac{(E-E_F)}{kT}} \qquad \text{…………(3)}$$

Density of states in the valence band $\quad Z(E)\,dE = \frac{4\pi}{h^3}\,(2m_h^*)^{3/2}\,E^{1/2}\,dE$ …………(4)

Where m_h^* → Effective mass of the hole in the valence band.

E_v → the potential energy of a hole at rest.

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

∴Equation (4) is modified as $\quad Z(E)dE = \frac{4\pi}{h^3}\,(2m_h^*)^{3/2}\,(E_v - E)^{1/2}\,dE$ …………(5)

Substitute equation (3) and (5) in equation (1) we have

$$dP = \frac{4\pi}{h^3}(2m_h^*)^{\frac{3}{2}}(E_v - E)^{\frac{1}{2}}e^{\frac{(E-E_F)}{kT}}dE \qquad \text{…………(6)}$$

Integrating equation (6) with respect to limit -∞ to E_v

$$\int dP = \int_{-\infty}^{E_v} \frac{4\pi}{h^3}(2m_h^*)^{\frac{3}{2}}\,(E_v - E)^{\frac{1}{2}}\;e^{\frac{(E-E_F)}{kT}}\,dE$$

$$P = \frac{4\pi}{h^3}(2m_h^*)^{\frac{3}{2}}\,e^{-E_F/kT}\int_{-\infty}^{E_v}(E_v - E\,)^{\frac{1}{2}}\,e^{\frac{E}{kT}}dE \qquad \text{… … ……(7)}$$

Take $E_v - E = x$, $\quad dE = -\,dx$, $E = -\,x + E_v$

When $E = E_v$, $x = E_v - E_v$, $x = 0$

When $E = -\infty$, $x = E_v + \infty$, $x = +\infty$

Substituting the above values in equation (7) we have

$$P = \frac{4\pi}{h^3}(2m_h^*)^{\frac{3}{2}}\,e^{-E_F/kT}\int_{\infty}^{0}(x)^{\frac{1}{2}}\,e^{\frac{(-x+E_V)}{kT}}\,(-dx) \qquad \text{………(8)}$$

$$P = \frac{4\pi}{h^3}(2m_h^*)^{\frac{3}{2}}\,e^{(E_v-E_F)/kT}\int_{0}^{\infty}(x)^{\frac{1}{2}}\,e^{\frac{(-x)}{kT}}\,(dx) \qquad \text{………(9)}$$

Using the gamma function, $\int_0^{+\infty}(x)^{\frac{1}{2}}\,e^{-\left(\frac{x}{kT}\right)}dx = \frac{(kT)^{\frac{3}{2}}\pi^{\frac{1}{2}}}{2}$ ……..(10)

Substituting equation (10) in equation (9) we have $\quad P = \frac{4\pi}{h^3}(2m_h^*)^{\frac{3}{2}}\,e^{(E_v-E_F)/kT}\,\frac{(kT)^{\frac{3}{2}}\pi^{\frac{1}{2}}}{2}$

$$P = 2\left(\frac{2\pi m_h^* kT}{h^2}\right)^{3/2} e^{(E_v-E_F)/kT} \qquad \text{…………(11)}$$

This is the expression for the concentration of holes in the valence band of an intrinsic semiconductor.

Intrinsic carrier concentration:

In an intrinsic semiconductor, the concentration of electrons in the conduction band is equal to the concentration of the holes in the valence band. We can rewrite $n = p = n_i$

Where n_i → Intrinsic carrier concentration

$$np = n_i \times n_i \quad \text{and} \quad np = n_i^2$$

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

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

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

where $E_c - E_v = E_g$, E_g → Forbidden energy gap

$$\therefore n_i = 2\left(\frac{2\pi kT}{h^2}\right)^{3/2} (m_e^* m_h^*)^{3/4} e^{(-E_g)/2kT} \qquad \text{……….(12)}$$

Limitations of intrinsic semiconductor

Intrinsic semiconductors cannot be directly used to fabricate devices due to the following limitations;

(i) 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.

(ii) Electrical conductivity is a function of temperature and increases exponentially as the temperature increases.

In intrinsic or pure semiconductors, the carrier concentration of both electrons and holes is very low at normal temperatures. In order to get sufficient current density through semiconductor, a large electrical field should be applied. This problem is overcome by adding suitable impurities into intrinsic semiconductors.

Extrinsic semiconductor:

Impure semiconductors in which charge carriers are produced due to the impurity atoms are called extrinsic semiconductors. It is also known as doped semiconductor. The addition of impurities to a pure semiconductor is known as doping and added impurity is called as doping agent or dopant. The addition of impurities increases the number of free electrons and holes in semiconductor and hence increases its electrical conductivity. Some of the common doping agents are arsenic, aluminium and boron.

Depending on the impurity atom they are classified in to two types

(i) n- type semiconductor and (ii) p- type semiconductor

n- type semiconductor: They are obtained by doping an intrinsic semiconductor with pentavalent impurity atoms like phosphorous and arsenic. The four valence electron of impurity atom will be bonded with four valence electrons of semiconducting atom and one electron is free which is responsible for conduction. Majority carriers are electrons.

p- type semiconductor: They are formed by doping an intrinsic semiconductor with trivalent impurity atoms like Galium and Indium. The three valence electrons of the impurity atom pairs with three valence electrons of the semiconductor and one position of the impurity atom is left free (vacant). The excess holes produced are the majority carriers.

S.no	Intrinsic Semiconductor	Extrinsic semiconductor
1	Semiconductor in a pure form is called intrinsic semiconductor. Example: Si, Ge	Semiconductor which are doped with impurity is called Extrinsic semiconductor Example: Si, Ge doped with Al, In,P
2	The charge carriers are produced only due to thermal agitation.	The charge carriers are produced due to impurities and may also be produced due to thermal agitation.
3	They have low electrical conductivity	They have high electrical conductivity.
4	They have low operating temperature.	They have high operating temperature.
5	At 0 K, Fermi level exactly lies between conduction band and valence band.	At 0 K, Fermi level lies closer to conduction band in n-type semiconductor and lies near valence band in p-type semiconductor.

S.no	n- type Semiconductor	p-type semiconductor
1	n-type semiconductor is obtained by doping an intrinsic semiconductor with pentavalent impurity.	p-type semiconductor is obtained by doping an intrinsic semiconductor with trivalent impurity.
2	Here electrons are majority carriers and holes are minority carriers.	Here holes are majority carriers and electrons are minority carriers.
3	It has donor energy level very close to conduction band.	It has acceptor energy level very close to valence band.
4	When the temperature is increased, these semiconductors can easily donate an electron from the donor energy level to the conduction band.	When the temperature is increased, these semiconductors can easily accept an electron from the valence band to acceptor energy level.

5	Fermi level lies exactly at the middle of the donor level and the bottom of the conduction band $E_F = \frac{(E_d+E_c)}{2}$	Fermi level lies exactly at the middle of the acceptor level and the top of the valence band $E_F=\frac{(E_a+E_v)}{2}$
6	Fermi level decreases with increase of temperature.	Fermi level increases with increase of temperature.

n- type semiconductor:

When a small amount of pentavalent impurity is added to a pure semiconductor. Such impurities are known as donor impurities because they donate free electrons to the semiconductor crystal. In n- type semiconductor electrons are majority charge carriers and holes are minority charge carriers.

Let us consider, pentavalent impurity phosphorus is added to silicon as shown in below figure. Phosphorus atom has 5 valence electrons and silicon has 4 valence electrons. Phosphorus atom has one excess valence electron than silicon. The four valence electrons of each phosphorus atom form 4 covalent bonds with the 4 neighboring silicon atoms. The fifth valence electron of the phosphorus atom cannot able to form the covalent bond with the silicon atom because silicon atom does not have the fifth valence electron to form the covalent bond.

Thus, fifth valence electron of phosphorus atom does not involve in the formation of covalent bonds. Hence, it is free to move and not attached to the parent atom. This shows that each phosphorus atom donates one free electron. Therefore, all the pentavalent impurities are called donors. The number of free electrons are depends on the amount of impurity (phosphorus) added to the silicon. A small addition of impurity (phosphorus) generates millions of free electrons.

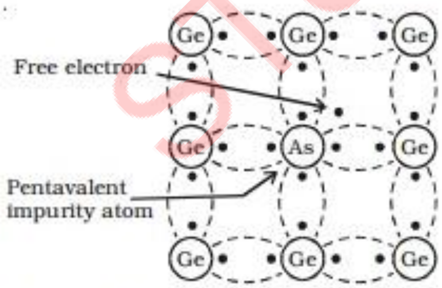


Fig a N-type semiconductor

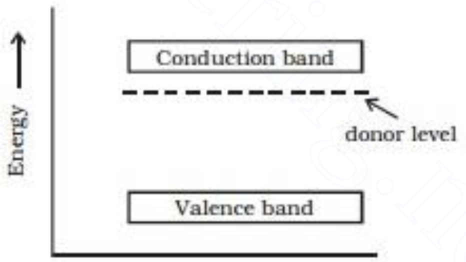


Fig b Energy band diagram of N-type semiconductor

Carrier concentration in n- type semiconductor:

In an n-type semiconductor, the donor level is just below the conduction band. N_d denotes the donor concentration and E_d denotes the energy of donor level.

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

$$n = 2\left(\frac{2\pi m_e^* kT}{h^2}\right)^{3/2} e^{(E_F - E_c)/kT} \qquad \text{……….(1)}$$

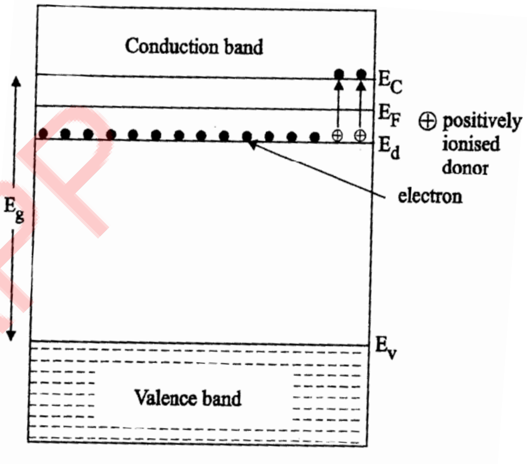
Density of ionized donors $= N_d(1 - F(E_d))$

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

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

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

If E_F lies more than a few kT above donor levels. So the denominator may be neglected.



Energy band diagram of a *n*-type semiconductor

$$\therefore \text{Density of ionized donors} = N_d\left[e^{\frac{(E_d-E_F)}{kT}}\right] \qquad \text{………(2)}$$

At equilibrium density of electrons in the conduction band is equal to the density of ionized donors.

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

Taking log on both sides, we get

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

Rearranging,

$$\frac{E_F - E_c - E_d + E_F}{kT} = \log\left[\frac{N_d}{2\left(\frac{2\pi m_e^* kT}{h^2}\right)^{\frac{3}{2}}}\right]$$

$$\frac{2E_F - (E_d + E_c)}{kT} = \log\left[\frac{N_d}{2\left(\frac{2\pi m_e^* kT}{h^2}\right)^{\frac{3}{2}}}\right]$$

$$2E_F = (E_d + E_c) + kT \log\left[\frac{N_d}{2(\frac{2\pi m_e^* kT}{h^2})^{\frac{3}{2}}}\right]$$

$$E_F = \frac{E_d+E_c}{2} + \frac{kT}{2}\log\left[\frac{N_d}{2(\frac{2\pi m_e^* kT}{h^2})^{\frac{3}{2}}}\right] \qquad \text{……..(4)}$$

Substituting the expression of E_F from equation (5) in (1)

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

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

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

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

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

$$n = (2N_d)^{\frac{1}{2}}\left(\frac{2\pi m_e^* kT}{h^2}\right)^{\frac{3}{4}} \exp\left[\frac{-\Delta E}{2kT}\right] \qquad \text{where } \Delta E = E_c - E_d$$

ΔE → Ionisation energy of the donor. ie, The amount of energy required to transfer an electron from donor energy level E_d to conduction band E_c.

$$n = (2N_d)^{\frac{1}{2}}\left(\frac{2\pi m_e^* kT}{h^2}\right)^{\frac{3}{4}} \exp\left[\frac{-\Delta E}{2kT}\right]$$

It is clear that the density of electrons in the conduction band is directly proportional to the square root of donor concentration.

p- type semiconductor:

When a small amount of trivalent impurity is added to a pure semiconductor, it becomes p- type semiconductor typical examples of trivalent impurities are gallium and indium. Such impurities are known as acceptor impurities because the holes they create can accept electrons. In p- type semiconductor holes are majority charge carriers and electrons are minority charge carriers.

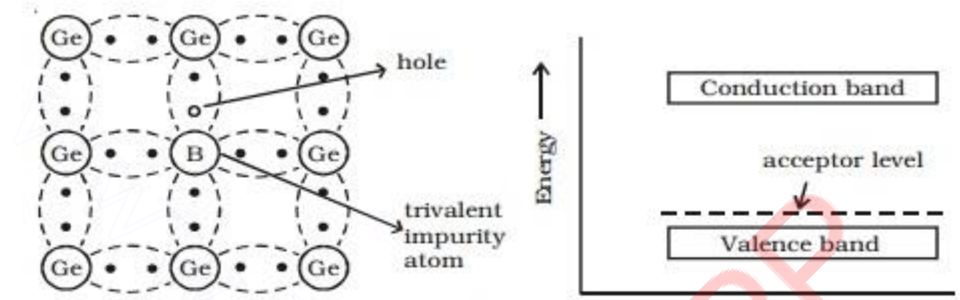


Fig a P-type semiconductor *Fig b Energy band diagram of a P-type semiconductor*

Let us consider, trivalent impurity boron is added to silicon as shown in below figure. Boron atom has three valence electrons and silicon has four valence electrons. The three valence electrons of each boron atom form 3 covalent bonds with the 3 neighboring silicon atoms. In the fourth covalent bond, only silicon atom contributes one valence electron, while the boron atom has no valence electron to contribute. Thus, the fourth covalent bond is incomplete with shortage of one electron. This missing electron is called hole. This shows each boron atom accept one electron to fill the hole. Therefore, all the trivalent impurities are called acceptors. A small addition of impurity (boron) provides millions of holes.

Carrier concentration in p- type semiconductor:

In p-type semiconductors, the acceptor level is just above the valence band. LetE_a represent the energy of the acceptor level, and N_a represent the number of acceptor atoms per unit volume.

Density of holes per unit volume in the valence band is given by

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

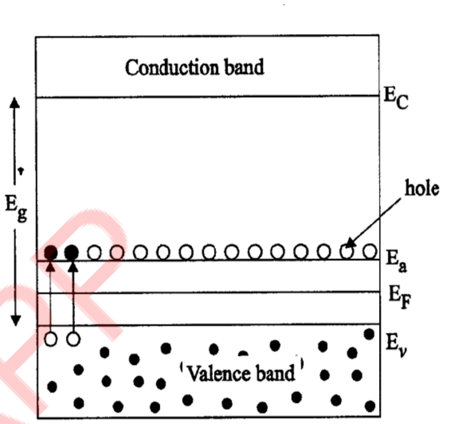
Density of ionized acceptors $= N_a F(E_a)$ $= N_a \left[\frac{1}{1+e^{\frac{(E_a-E_F)}{kT}}}\right]$

Since $E_a - E_F >> \mathrm{kT}$, $e^{\frac{(E_a-E_F)}{kT}}$ is very large quantity and thus 1 can be neglected from the denominator.

∴ Density of ionized acceptors $= N_a\left[e^{\frac{(E_F-E_a)}{kT}}\right]$ ………(2)

At equilibrium density of holes in the valence band is equal to the density of ionized acceptors.

$$2\left(\frac{2\pi \mathrm{m}_\mathrm{h}^*\mathrm{kT}}{h^2}\right)^{3/2} e^{(E_v-E_F)/kT} = N_a\left[e^{\frac{(E_F-E_a)}{kT}}\right]$$



Energy band diagram for *p*-type semiconductor

Taking log on both sides, we get

$$\log\left(2\left(\frac{2\pi \mathrm{m}_\mathrm{h}^*\mathrm{kT}}{h^2}\right)^{3/2} e^{(E_v-E_F)/kT}\right) = \log\left(N_a\left[e^{\frac{(E_F-E_a)}{kT}}\right]\right)$$

Rearranging,

$$\frac{E_v-E_F-E_F+E_a}{kT} = \log\left[\frac{N_a}{2(\frac{2\pi \mathrm{m}_\mathrm{h}^*\mathrm{kT}}{h^2})^{\frac{3}{2}}}\right]$$

$$\frac{-2E_F+(E_a+E_v)}{kT} = \log\left[\frac{N_a}{2(\frac{2\pi \mathrm{m}_\mathrm{h}^*\mathrm{kT}}{h^2})^{\frac{3}{2}}}\right]$$

$$-2E_F = -(E_a+E_v) + kT\log\left[\frac{N_a}{2(\frac{2\pi \mathrm{m}_\mathrm{h}^*\mathrm{kT}}{h^2})^{\frac{3}{2}}}\right]$$

$$E_F = \frac{(E_a+E_v)}{2} - \frac{kT}{2}\log\left[\frac{N_a}{2(\frac{2\pi \mathrm{m}_\mathrm{h}^*\mathrm{kT}}{h^2})^{\frac{3}{2}}}\right] \quad \text{........(3)}$$

Substituting the expression of E_F from equation (3) in (1)

$$\mathrm{p} = 2\left(\frac{2\pi \mathrm{m}_\mathrm{h}^*\mathrm{kT}}{h^2}\right)^{3/2} \exp\left[\frac{E_v - \frac{(E_a+E_v)}{2} - \frac{kT}{2}\log\left[\frac{N_a}{2(\frac{2\pi \mathrm{m}_\mathrm{h}^*\mathrm{kT}}{h^2})^{\frac{3}{2}}}\right]}{kT}\right]$$

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

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

$$p = 2\left(\frac{2\pi m_h^* kT}{h^2}\right)^{3/2} \exp\left[\log\frac{(N_a)^{\frac{1}{2}}}{(2)^{\frac{1}{2}}\left(\frac{2\pi m_h^* kT}{h^2}\right)^{\frac{3}{4}}} + \frac{E_v - E_a}{2kT}\right]$$

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

$$p = (2N_a)^{\frac{1}{2}}\left(\frac{2\pi m_h^* kT}{h^2}\right)^{\frac{3}{4}} \exp\left[\frac{-\Delta E}{2kT}\right] \quad \text{where } \Delta E = E_a - E_v$$

ΔE → Ionisation energy of the acceptor.

ie, The amount of energy required to transfer an holes from acceptor energy level E_a to valence band E_v.

$$p = (2N_a)^{\frac{1}{2}}\left(\frac{2\pi m_h^* kT}{h^2}\right)^{\frac{3}{4}} \exp\left[\frac{-\Delta E}{2kT}\right]$$

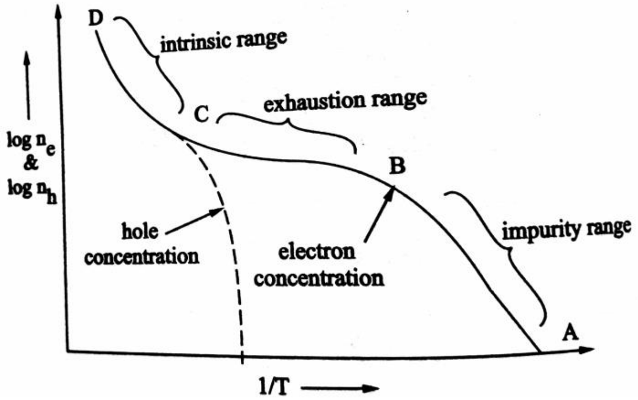
It is clear that the density of holes in the valence band is directly proportional to the square root of acceptor concentration.

Variation of carrier concentration with temperature

In extrinsic semiconductors, the resistivity decreases linearly with increase in temperature. This variation is considered under three different regions.

(i) Extrinsic or impurity range
(ii) Exhaustion range
(iii) Intrinsic range

For an n-type semiconductor, the variation of carrier concentration n and p with temperature is shown in the graph. At 0 K, both conduction and valence bands are free from any charge carriers and hence the electrical conductivity is zero.



Now when the temperature is slowly increased, the donor atom gets ionized and the electrons move towards the conduction band. Here the carrier concentration (n_e) increases slowly in the conduction band for electrons. Since this range is obtained due to impurity atoms, it is called **impurity range** shown by the curve AB.

When the temperature is further increased to reach upto say room temperature, all donor atoms is ionized and hence the carrier concentration increases in the conduction band and reaches to a steady state. Since this range is obtained due to exhaustion of donor atoms, it is called **exhaustion range** shown by the curve BC.

When the temperature is still further increased, due to thermal ionization, the electron from the valence band is lifted up to go to the conduction band and hence there is an increase in the carrier concentration (n_e). In this case the number of electrons in the donor energy level is almost exhausted, many number of electrons are shifted from valence band to conduction band and hence the carrier concentration increases rapidly, tracing the curve CD. Since the material practically becomes intrinsic in this range, this range is known as **intrinsic range**.

The dotted curve indicates the hole concentration in an intrinsic range.

Carrier transport in semiconductor

Random motion and mobility

In absence of an electrical field the free electrons move in all directions in an random manner. They collide with other free electrons and positive ion core during the motion. This collision is known as elastic collision.

As the motion is random the resultant velocity in any particular direction is zero. When an electrical field is applied in a semiconducting material the free charge carriers such as free electrons and holes attain drift velocity V_d. The drift velocity attained by the carriers is proportional to the electric field $strength\ E$.

$$V_d \,\alpha\, E \qquad\qquad V_d = \mu E$$

Where μ is a proportionality constant and it is known as the mobility of the charge carrier. This velocity V_d is different for different semiconductors and for different type of charge carriers.

$$\text{If } E = 1 \text{ V/m then } \mu = V_d.$$

Thus ***mobility μ is defined as the velocity of charge carrier per unit electrical field strength.*** μ_n and μ_p denote electron mobility and hole mobility respectively. Since the types of drift of electrons and of holes are different the mobility of an electron at any temperature is different from that of hole.

The electrical conductivity σi of an intrinsic semiconductor having n_i electron – hole pairs per unit volume is given by

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

Drift and diffusion Transport

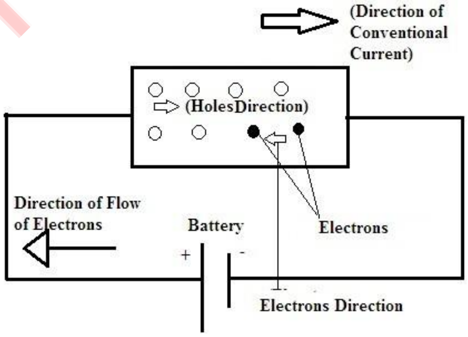
The net current flow across a semiconductor has two components:

(i) Drift current (ii) Diffusion current.

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.

When electrical voltage is applied to a material, electric field is produced at every point within the material. The charge carriers are forced to move in a particular direction due to the electric field. This is known as the drift motion and the current is known as drift current.



Drift current in a semiconductor due to electrons $J_n(drift) = n\mu_n eE$

Drift current in a semiconductor due to holes $J_p(drift) = p\mu_p eE$

Where n and p are number of electrons and holes per unit volume. μ_n and μ_p are the nobilities of electrons and holes respectively, e is charge of electrons and E is electric field.

So total drift current density J = $J_n(drift) + J_p(drift)$

$$J = n\mu_n eE + p\mu_p eE$$

For Intrinsic semiconductor

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

Diffusion current

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

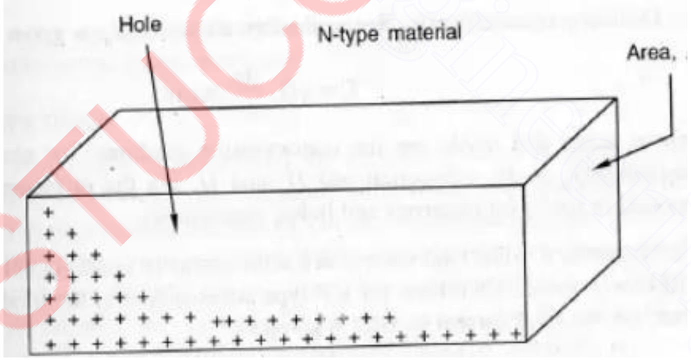
The charge carriers move from the regions of higher concentration to the regions of lower concentration. This process is known as diffusion. The current is known as diffusion current. Consider a semiconductor having a concentration gradient of electrons $\frac{dn}{dx}$ within the semiconductor. The electrons diffuse from high concentration to low concentration due to the concentration gradient.

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

Here negative sign denotes that the electrons are diffusing from higher concentration to lower concentration region.

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

Where D_n is a proportionality constant and it is known as diffusion coefficient of electrons.



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

Rate of flow of electrons through unit area is the diffusion current density of electrons

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

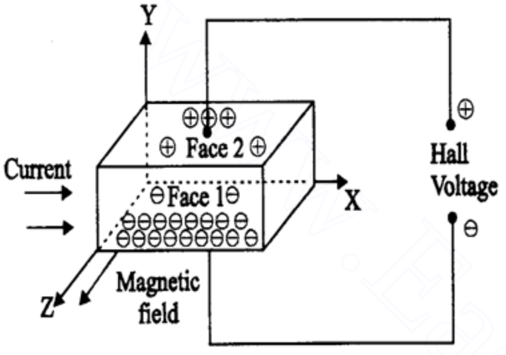
Similarly, the diffusion current density of holes is given by $J_p(\text{diffusion}) = -e\,D_p\left(\frac{dn}{dx}\right)$

Where D_p is diffusion constant of holes.

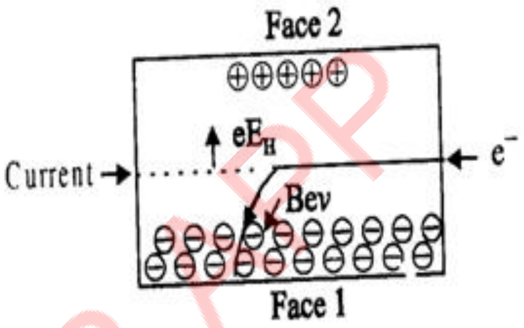
Hall Effect

Hall Effect is used to distinguish between the two types of charge carriers. It is also used to determine the charge carrier densities and the mobility of charge carriers.

Statement: When a conductor (metal or semiconductor) carrying a current (I) is placed in a perpendicular magnetic field (B) , a potential difference (electric field) is produced inside the conductor in a direction normal to the directions of both the current and the magnetic field.



Hall effect



Hall effect in n-type semiconductor:

Let us consider a n-type semiconductor material in the form of rectangular slab. In such a material current flows in the X-direction, magnetic field B is applied in the Z direction. As a result Hall voltage is developed along Y-direction. The current flow is entirely due to the flow of electrons moving from right to left. When a magnetic field is applied, the electrons moving with velocity *v* will experience a downward force Bev.

Where B → Applied magnetic field

e → Charge of an electron

The downward force deflects the electrons in downward direction and therefore there is an accumulation of negatively charged electrons on the bottom face of the slab.

∴ A potential difference is established between top and bottom of the specimen. This potential difference causes an electric field E_H called Hall field.This field will give rise to a force eE_H acting in the upward direction on each electron.

At equilibrium, downward force Bev will balance the upward force eE_H.

$$\therefore \text{Bev} = eE_H$$

$$E_H = Bv \qquad \text{……..(1)}$$

The current density J_x = nev

$$\therefore\ v = -\frac{J_x}{ne} \qquad \text{……..(2)}$$

Where n → concentration of current carrier (electrons)

Substitute equation (2) in (1) we have

$$E_H = -\frac{BJ_x}{ne} \qquad \text{…….(3)}$$

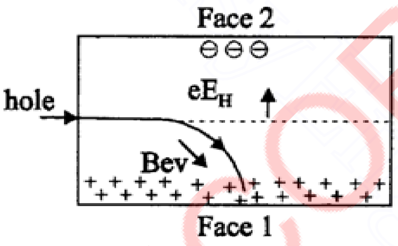
$$E_H = R_H J_x B \qquad \text{……..(4)}$$

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

$$\text{Where } R_H = -\frac{1}{n_e} \qquad \text{….(5)}$$

Where R_H → Hall coefficient or Hall constant.

Hall effect in p type semiconductor:



Hall effect in *p*-type semiconductor

Consider a rectangular slab of p-type semiconducting material and the current flow in this case is entirely due to the flow of positive holes from left to right. The current flow is along x- direction and the magnetic field is applied in the z- direction. Due to applied magnetic field, the holes are accumulated in the bottom of the slab and thus produce a potential difference.

Hall coefficient can be written as $R_H = +\frac{1}{p_e}$ …….(6)

Where p → Concentration of current carriers(holes)

Hall coefficient in terms of Hall voltage:

If t is the thickness of the sample and V_H is the Hall voltage, then $V_H = E_H t$ ….(7)

Where E_H is the Hall field

Substitute equation (4) in (7) we $V_H = R_H J_x Bt$ ……(8)

If b is the breadth of the sample, then Area of the sample (A) = Breadth (b) x Thickness (t)

= bt

Current density $Jx = \frac{I_x}{Area\ of\ the\ sample(A)}$ $Jx = \frac{I_x}{bt}$ ……..(9)

Substituting equation (9) in (8) we have $V_H = \frac{R_H I_x Bt}{bt}$

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

Hall coefficient, $R_H = \frac{V_H b}{I_x B}$ ………(10)

Mobility of charge carriers:

Electrical conductivity of a n-type semiconductor $\sigma_e = n\, e\, \mu_e$

$$\therefore R_H = \frac{-1}{ne} \quad \text{……… (11)}$$

Where μ_e → mobility of charge carriers (electrons)

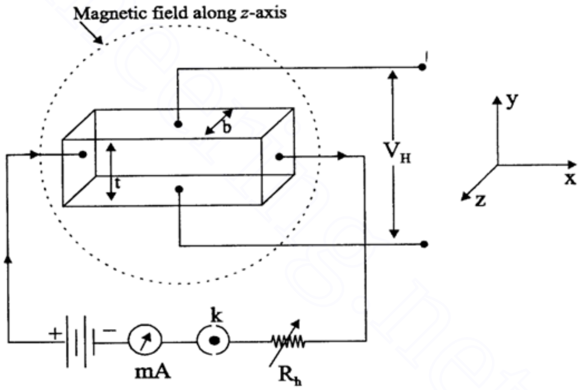
Electrical conductivity of a p-type semiconductor $\sigma_h = p\, e\, \mu_h$

$$\therefore R_H = \frac{-1}{pe} \quad \text{……… (12)}$$

Where σ_h→ mobility of charge carriers(holes)

Determination of Hall coefficient:

A semiconductor material is taken in the form of a rectangular slab of thickness t and breadth b. A suitable current I_x ampere is allowed to pass through this sample along x- axis by connecting it to a battery.The sample is placed in between two poles of an electromagnet such that the applied magnetic field is along the z-axis ie, perpendicular to the plane of paper.



Experimental arrangement to measure Hall coefficient

Hall voltage V_H is developed in the sample 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 from the formula

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

Applications of Hall Effect:

(i) Determination of semiconductor type: the sign of the hall coefficient is used to find whether a given semiconductor is n-type or p-type.

(ii)Calculation of carrier concentration: by measuring hall coefficientR_H, carrier concentration is determined from the relation $n = \frac{1}{eR_H}$

(iii) Determination of mobility: we know that electrical conductivity

$$\sigma_e = ne\mu_e \qquad \mu_e = \frac{\sigma_e}{ne} \qquad \mu_e = \sigma_e R_H$$

(iv) Magnetic field meter: Hall voltage V_H for a given current is proportional to B. Hence V_H measures the magnetic field B.

(v) Hall effect multiplier: It can give an output proportional to the product of two signals. If current I proportional to one input and if B proportional to the second input, then V_H is proportional to the product of two inputs.

Hall Devices

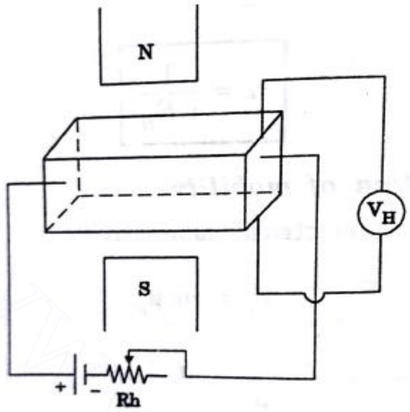
The devices which uses the Hall Effect for its applications is known as hall device. There are 3 types of hall devices.

1. Gauss meter
2. Electronic Multiplier
3. Electronic Wattmeter

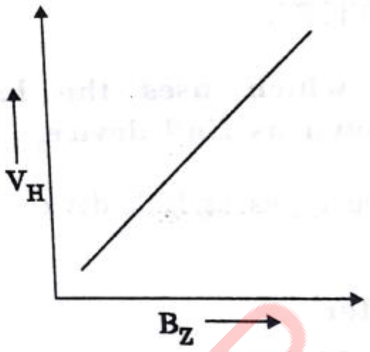
a) Gauss meter

The hall voltage $V_H = \frac{R_H B_Z I_x}{t}$. In this $V_H \propto \boldsymbol{B}_Z$ for a given hall element; R_H and t are constant. The current I through Hall element is also kept constant.

This principle is used in Gauss meter. It is used for measuring magnetic field. The variation of Hall voltage with magnetic field is shown in fig. the voltmeter which is used to measure V_H can be directly calibrated in terms of gauss. The graph can also be used to measure any unknown magnetic fields.



Gauss Meter



B_Z *Verses* V_H

b) Electronic Multipliers

From Hall Effect, we have

$$V_H = \frac{R_H B_Z I_1}{t}$$

Since R_H and t are constant for an element.

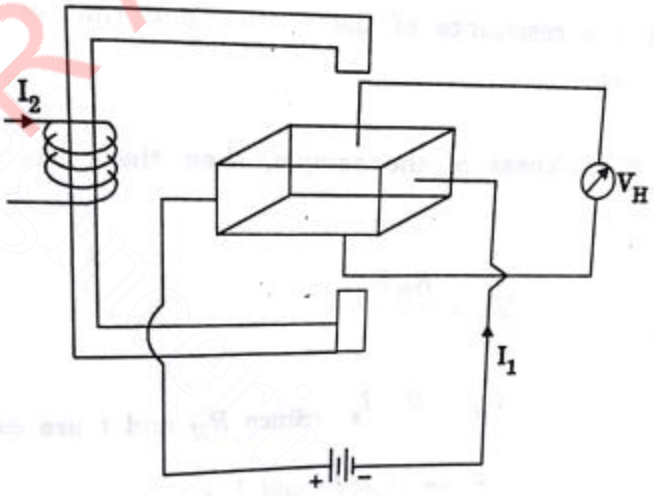
$$V_H = B_Z I_1$$

But, the magnetic field B_Z is proportional to current (I_2) through the coil.

i.e; $B_Z \propto I_2$

$$\therefore V_H \propto I_1 I_2$$

V_H is a measure of the product of two currents. This is the basic principle used in analog electronic multipliers.

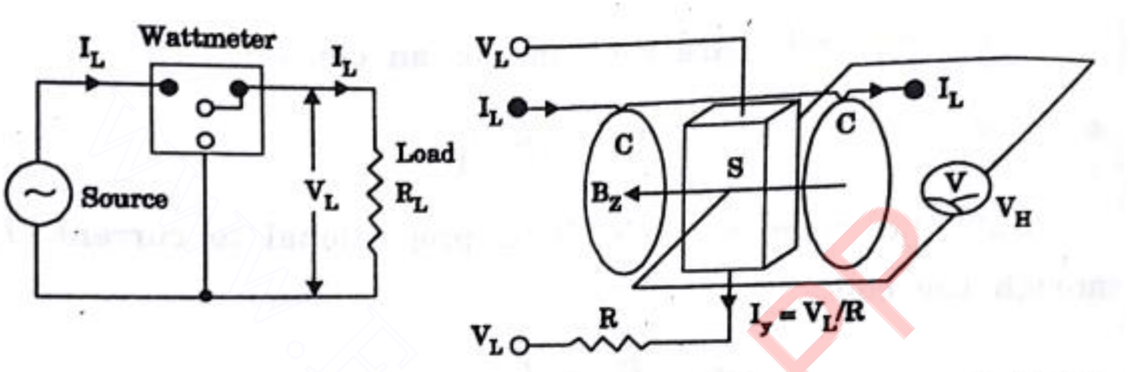


Electronic multiplier

c) Electronic Wattmeter

Hall Effect is used to measure electrical power dissipated in a load. The instrument used to measure the power in a circuit using Hall Effect principle is known as Hall Effect – Watt meter. S is Hall Effect sample. It is placed in a magnetic field B_Z produced by the load current I_L passing through the coils CC.

The voltage across the load V_L drives the current $I_y = \frac{V_L}{R}$ through the sample. R is a series resistance which is >> than the resistance of the sample and that of the load. Also $I_y \ll I_L$



V_L - Load voltage I_L - Load Current C, C - Coils to set magnetic field B

Hall effect wattmeter

If "t" thickness of the sample, then the measured hall voltage

$$V_H = \frac{R_H B_Z I_1}{t}$$

$V_H \propto B_Z I_y$ (Since R_H and t are constant).

Since $B_Z \propto I_L$ and $I_y \propto V_L$ $\qquad V_H \propto V_L I_L$

This is the electric power dissipated by the load. The voltmeter that measures V_H can be calibrated directly to read power.

Metal – Semiconductor Contact

Metal – semiconductor contact plays e very important role in the present day electronics devices and integrated circuit technology.

When a metal and a semiconductor are brought into contact, there are 2 types of junctions formed depending on the work functions of the metal and semiconductor.

Types of Metal – Semiconductor junction

(i) Schottky junction - $\phi_m > \phi_{semi}$

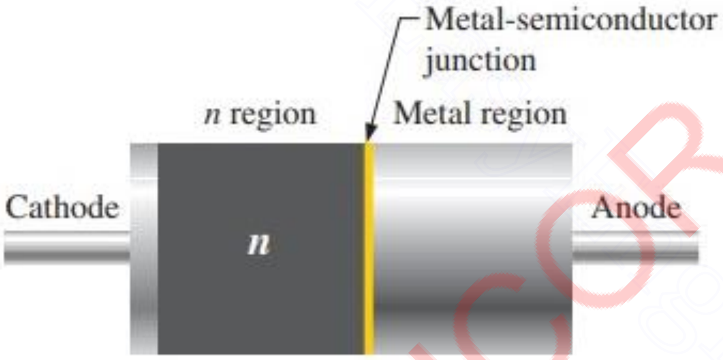
(ii) Ohmic junction - $\phi_m < \phi_{semi}$

Work function: energy required to raise the electron from the metal or the semiconductor to the vacuum level.

Schottky Diode

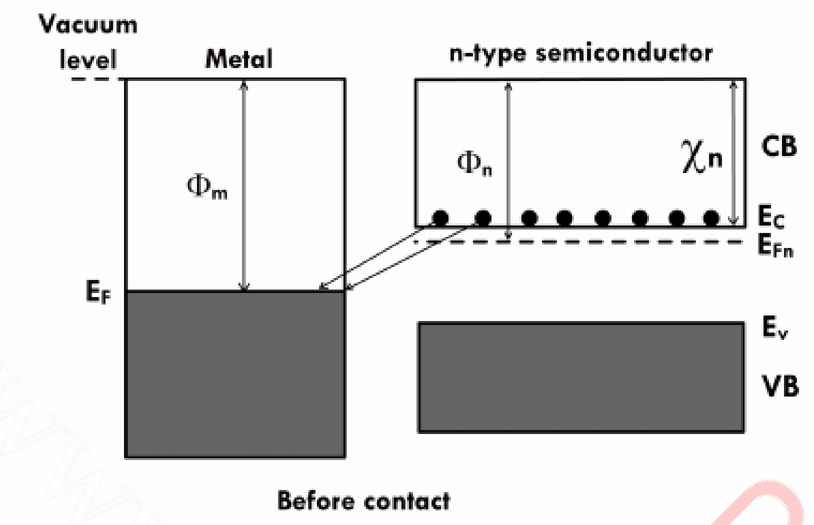
When the metal has high work function than that of n-type semiconductor then the junction formed is called Schottky diode.

Principle: Schottky diode is a unilateral device in which current flows from metal to semiconductor (n-type) in one direction.

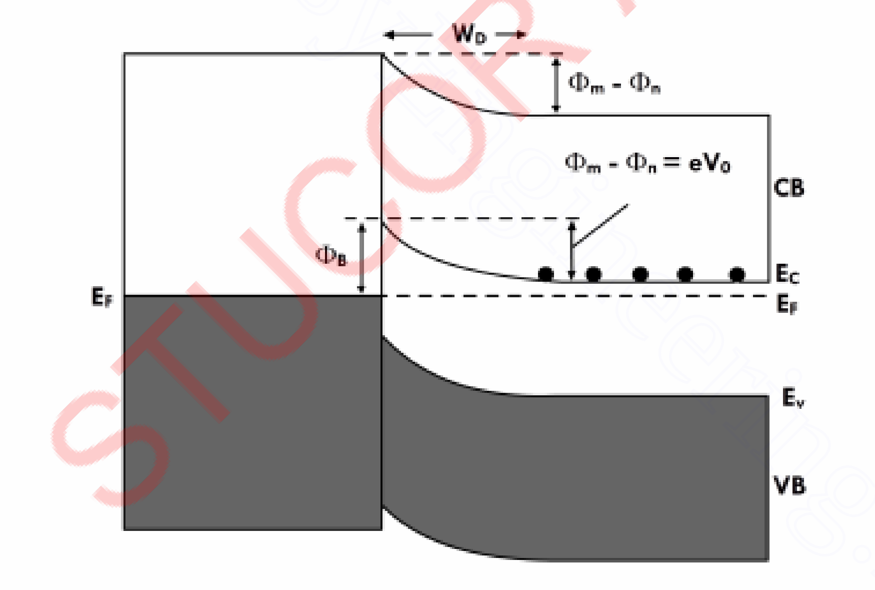


Schottky Diode Symbol

Consider a junction formed between a metal and n-type semiconductor. The Fermi level of the semiconductor is higher (since its work function is lower) than the metal. The electrons in the conduction level of the semiconductor move to the empty energy states above the Fermi level of the metal. This leave a positive charge on the semiconductor side and due to the excess electrons, a negative charge on the metal side, leading to a contact potential.



When a Schottky junction is formed between the metal and semiconductor, the Fermi level lines up and also a positive potential is formed on the semiconductor side. Because the depletion region extends within a certain depth in the semiconductor there is bending of the energy bands on the semiconductor side. Bands bend up in the direction of the electric field.



The Schottky junction can be biased by application of an external potential.

There are two types of bias

1. Forward bias - metal is connected to positive terminal and n-type semiconductor connected to negative terminal

2. Reverse bias - metal is connected to negative terminal and n-type semiconductor connected to positive terminal

The current flow depends on the type of bias and the amount of applied external potential.

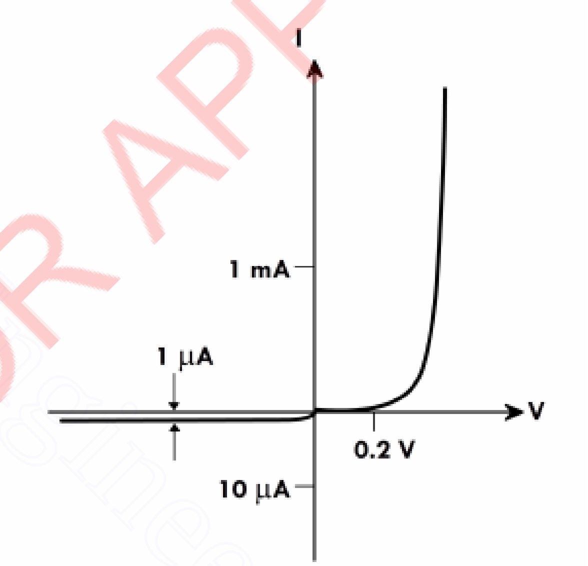
Forward bias:

In a forward biased Schottky junction the external potential is applied in such a way that it opposes the in-built potential. The electrons injected from the external circuit into the n-type semiconductor have a lower barrier to overcome before reaching the metal. This leads to a current in the circuit which increases with increasing external potential.

Reverse bias:

In the case of a reverse bias the external potential is applied in the same direction as the junction potential. This increases the width of depletion region further and hence there is no flow of electron from semiconductor to metal. So a Schottky junction acts as a rectifier i.e. it conducts in forward bias but not in reverse bias

The I – V characteristics of the junction is shown in figure. There is an exponential increase in current in the forward bias (I quadrant) while there is a small current in reverse bias.



Advantages of Schottky diode

- In Schottky diode, stored charges or depletion region is negligible. So a Schottky diode has a very low capacitance.
- The Schottky diode will immediately switch from ON state to OFF state since the depletion region is negligible.
- A small voltage is enough to produce large current.
- It has high efficiency.
- It operates at high frequencies.
- It produces less noise.

Applications of Schottky diode

- It can be used for rectification of signals of frequencies even exceeding 300 MHz.

- It is commonly used in switching device at frequencies of 20GHz.
- It is used in radio frequency applications.
- It is widely used in power supplies.
- It is used in logic circuits.
- Its low noise figure finds application in sensitive communication receivers like radars.
- It is also used in clipping and clamping circuits and in computer grating.

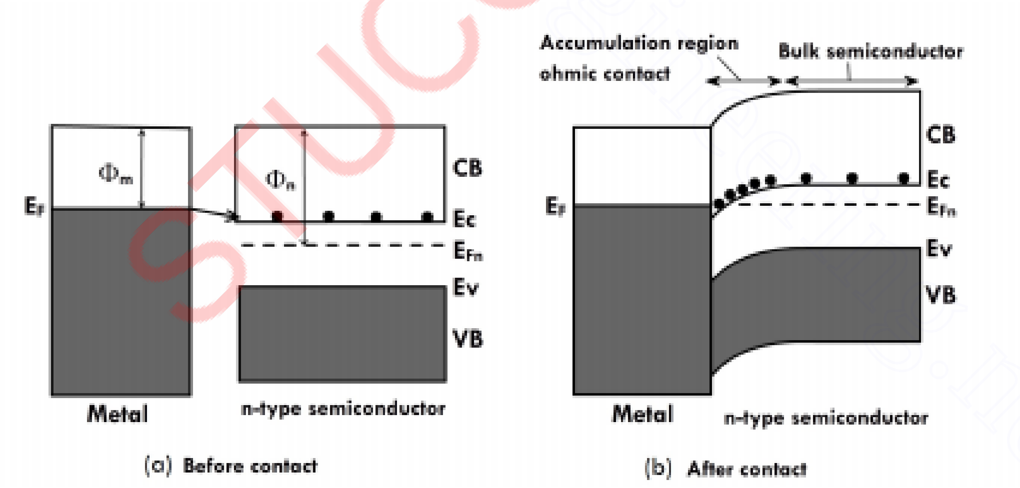
Ohmic Contacts

When the semiconductor has a higher work function the junction formed is called the Ohmic junction.

Principle: An Ohmic contact is an non-rectifying contact which obeys Ohm's law (V=IR). The resistance of the Ohmic contact should always be low i.e., conductivity should be large.

Here, the current is conducted equally in both directions and there is a very little voltage drop across the junction. Before contact, fermi level of the metal and semiconductor are at different positions.

At equilibrium, electrons move from the metal to the empty states in the conduction band so that there is an accumulation region near the interface (on the semiconductor side) from the metal to the empty states in the conduction band so that there is an accumulation region near the interface (on the semiconductor side).



Applications

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

PROBLEMS

1. **Find the resistance of an intrinsic Ge rod 1 cm long, 1 mm wide and 0.5 mm thick at 300 K. For Ge, n_i= 2.5 x 10^{19}/m^3, 0.39 m^2V^{-1} s^{-1} and 0.19 m^2V^{-1} s^{-1} at 300 K.**

Given:

n_i= 2.5 x 10^{19}/m^3, μ_e =0.39 m^2V^{-1} s^{-1},μ_h =0.19 m^2V^{-1} s^{-1}, e $= 1.6 \times 10^{-19}$J

l =1 cm = 1×10^{-2}m, Width = 1 mm, thickness = 0.5 mm

Conductivity $\sigma = n_i e(\mu_e + \mu_h)$

$$\sigma = 2.5 \times 10^{19} \times 1.6 \times 10^{-19}(0.39 + 0.19)$$

$$\sigma = 2.32\ \Omega^{-1}m^{-1}$$

$$Area = width \times thickness = 1 \times 10^{-3} \times 0.5 \times 10^{-3}$$

$$R = \frac{l}{\sigma A} = \frac{1\times10^{-2}}{2.32\times(1\times10^{-3}\times0.5\times10^{-3})}$$

$$R = 8620.6\ \Omega$$

2. **The intrinsic carrier density is 1.5×10^{16}/m^3.If the mobility of electron and hole are 0.13 and 0.05 $m^2V^{-1}s^{-1}$calculate the conductivity.**

Given: n_i =1.5×10^{16}/m^3, μ_e =0.13$m^2V^{-1}s^{-1}$,μ_h =0.05 $m^2V^{-1}s^{-1}$

$$\sigma = n_i e(\mu_e + \mu_h)$$

$$\sigma = 15 \times 10^{16} \times 1.6 \times 10^{-19}(0.13 + 0.05)$$

$$\sigma = 4.32 \times 10^{-4}\Omega^{-1}m^{-1}$$

3. **The donor density of an n-type germanium sample is 10^{21} /m^3.The sample is arranged in a Hall experiment having magnetic field of 0.5 Tesla and the current density is 500 ampere/m^2. Find the Hall voltage if the sample is 3 mm wide.**

Given: n_e =10^{21} /m^3, B = 0.5 Tesla, t =3 mm =3×10^{-3}m, J_x =500 ampere/m^2

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

$$R_H = \frac{1}{10^{21} \times 1.6 \times 10^{-19}}$$

$$R_H = 6.25 \times 10^{-3}$$

$$V_H = R_H J_x B t$$

$$V_H = 6.25 \times 10^{-3} \times 500 \times 0.5 \times 3 \times 10^{-3}$$

$$Hall\,Voltage\ V_H = 4.6875 \times 10^{-3} Volts$$

4. **In a p-type germanium, n_i = 2.1x 10^{19} m^{-3}, density of boron = 4.5 x 10^{23} atoms m^{-3}. The electrons and hole mobility are 0.4 and 0.2 m^2/volt sec respectively. What is its conductivity before and after the addition of boron atoms?**

Given: $n_i = 2.1 \times 10^{19}/m^3$; $\mu_e = 0.4 m^2$/volt; $\mu_h = 0.2 m^2$/volt.sec

(i) Before including boron atoms, the semiconductor is an intrinsic semiconductor.

Therefore, Conductivity (σ) = $n_i e(\mu_e + \mu_h)$

$= 2.1\text{x}10^{19}\text{x}1.6\text{x}10^{-19}(0.4+0.2)$

$\sigma = 2.016\ \Omega^{-1}\ m^{-1}$

(ii) After the boron atoms are included, each boron atoms are ready to accept one electron.

Therefore, Conductivity of p type semiconductor after boron atoms are included.

$\sigma' = pe\mu_h$

$\sigma' = 4.5\text{x}10^{23}\text{x}1.6\text{x}10^{-19}\text{x}0.2$

$\sigma' = 1.44\text{x}10^4\ \Omega^{-1}m^{-1}$

5. **A n-type semiconductor has Hall coefficient = $4.16 \times 10^{-4} m^{-3} c^{-1}$ .The conductivity is 108 $ohm^{-1}m^{-1}$. Calculate its charge carrier density n_e and electron mobility at room temperature.**

Given: $R_H = 4.16 \times 10^{-4} m^{-3} c^{-1}$, σ = 108 $\Omega^{-1}m^{-1}$

For n-type the charge carrier density is $n_e = -\frac{1}{eR_H}$

$$n_e = \frac{3\pi}{8}\frac{1}{eR_H}$$

$$n_e = \frac{3 \times 3.14}{8}\frac{1}{1.6 \times 10^{-19} \times 4.16 \times 10^{-4}}$$

$$n_e = 1.7690 \times 10^{22}/m^3.$$

i) Electron mobility $\mu_e = \frac{\sigma_e}{n_e e}$ $\mu_e = \frac{108}{1.769\times10^{22}\times1.6\times10^{-19}}$

$$\mu_e = 0.03816\ \text{m}^2\text{V}^{-1}\text{s}^{-1}$$

6. **The Hall co-efficient of certain silicon was found to be -7.35 x10^{-5} m^{3}C^{-1} from 100 to 400 K. Determine the nature of the semiconductor. If the conductivity was found to be 200 m^{-1} Ω^{-1}, calculate the density and mobility of the charge carriers.**

Since Hall coefficient is negative the given semiconductor is an ‘n’ type semiconductor.

For an n-type semiconductor, Conductivity $\sigma = n_e e\ \mu_e$

$$\text{Mobility}\mu_e = \frac{\sigma}{n_e e}$$

$$\text{Here } n_e = -\frac{1}{eR_H} \qquad n_e = -\frac{1}{1.6\times10^{-19}\times-7.35\times10^{-5}}$$

Charge density of electrons $n_e = 8.503\text{x}10^{22}/\text{m}^3$

$$\text{Therefore}\mu_e = \frac{200}{8.503\times10^{22}\times1.6\times10^{-19}}$$

Mobility of charge carriers $\mu_e = 0.0147\text{m}^2\text{V}^{-1}\text{s}^{-1}$.

7. **The energy gap of Si is 1.1 eV. Its electron and hole mobilities at room temperature are 0.48 and 0.013 m^{2}V^{-1}s^{-1}.Evaluate its conductivity.**

$\mu_e = 0.48\ \text{m}^2\text{V}^{-1}\text{s}^{-1}$ $\mu_h = 0.013\ \text{m}^2\text{V}^{-1}\text{s}^{-1}$

$$n_i = 2\left[\frac{2\pi m_e k_B T}{h^2}\right]\exp\frac{-E_g}{2k_B T}$$

$$n_i = 2\left[\frac{2\times3.14\times9.11\times10^{-31}\times1.38\times10^{-23}\times300}{(6.625\times10^{-34})^2}\right]\exp\frac{-1.1\times1.6\times10^{-19}}{2(1.38\times10^{-23}\times300)}$$

$$n_i = 1.4707\times10^{16}\ /m^3$$

$$\text{Conductivity } \sigma = n_i e(\mu_e+\mu_h)$$

$$\sigma = 1.4707\times10^{16}\times1.6\times10^{-19}\times(0.48+0.013)$$

$$\sigma = 1.160 \times 10^{-3}\Omega^{-1}m^{-1}.$$

8. **A patient with a pacemaker is mistakenly being scanned for an MRI image. A 10 cm long section of pacemaker wire moves at a speed of 10 cm/s perpendicular to the MRI unit's magnetic field and a 20mV Hall voltage is induced. What is the magnetic field strength?**

   Length of the path $l = 10\ cm = 0.1\ m$, Velocity $V = 10cm/s = 0.1m/s$

   Induced voltage $V = 20\ \text{mV} = 20 \times 10^{-3}\text{V}$

   Induced Hall voltage $V = Bvl$

$$B = \frac{V}{vl}$$

$$B = \frac{20 \times 10^{-3}}{0.1 \times 0.1}$$

$$B = 2\ Tesla$$

9. **The Hall Co-efficient of a specimen of doped silicon is found to be3.66 ×10^{-4} m^{-3}/C. The resistivity of specimen is 8.93×10^{-3} Ωm. Find the mobility and density of charge carriers.**

$$\text{Charge carrier density}\ \ n_e = \frac{3\pi}{8}\frac{1}{eR_H}$$

$$n_e = \frac{3\ X\ 3.14}{8}\ \frac{1}{1.6\ X\ 10^{-19}\ X\ 3.66\ X\ 10^{-4}}$$

$$n_e = 2.0107\ X\ 10^{22}/m^3$$

$$\text{Electron mobility}\ \ \mu_e = \frac{\sigma_e}{n_e e}\mu_e = \frac{1}{\rho_e n_e e}$$

$$\mu_e = \frac{1}{8.93\ X\ 10^{-3} X 2.0107\ X\ 10^{22}\ X\ 1.6\ X\ 10^{-19}}$$

$$\mu_e = 0.0348\ m^2/Vs.$$

10. **A silicon plate of thickness 1mm, breadth 10 mm and length 100 mm is placed in a magnetic field of 0.5 Wb/m^2 acting perpendicular to its thickness. If 10^{-2} A current flows**

along its length, calculate the Hall voltage developed, if the Hall coefficient is 3.66 × 10^4 m^3/coulomb.

$V_H = \frac{R_H I_H B}{t}$ $V_H = \frac{3.66\times10^{-4}\times10^{-2}\times0.5}{1\times10^{-3}}$ $V_H = 1.83 \times 10^{-3}$ Volts.

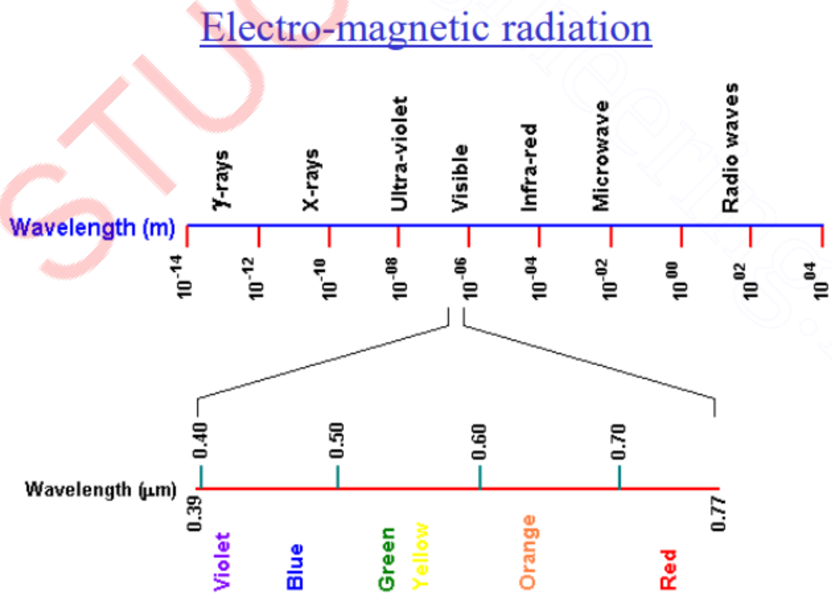
UNIT - IV OPTICAL PROPERTIES OF MATERIALS

Classification of optical materials – Optical processes in semiconductors: 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 –excitonic state – Electro-optics and nonlinear optics: Modulators and switching devices – plasmonics.

INTRODUCTION:

Engineering materials are important in everyday life because of their versatile structural properties. Other than these properties, they do play an important role because of their physical properties. Prime physical properties of materials include: electrical properties; thermal properties; magnetic properties and optical properties. The optical properties of engineering materials are useful in different applications. Ex.: domestic, medicine, astronomy, manufacturing.

Optical property of a material is defined as its interaction with electro-magnetic radiation in the visible. Electromagnetic spectrum of radiation spans the wide range from γ-rays with wavelength as 10^{-12}m, through x-rays, ultraviolet, visible, infrared, and finally radio waves with wavelengths as along as 10^{5}m. Visible light is one form of electromagnetic radiation with wavelengths ranging from 0.39 to 0.77 µm. Light can be considered as having waves and consisting of particles called photons.



MATERIAL – LIGHT INTERACTION

- **Interaction of photons** with the **electronic or crystal structure** of a material leads to a number of phenomena.
- The photons may give their energy to the material (**Absorption**);
- Photons give their energy, but photons of identical energy are immediately emitted by the material (**Reflection**);
- Photons may not interact with the material structure (**Transmission**); or during transmission photons are changes in velocity (**Refraction**).
- At any instance of light interaction with a material, the total intensity of the incident light striking a surface is equal to sum of the absorbed, reflected, and transmitted intensities i.e.

$$I_0 = I_A + I_R + I_T$$

CLASSIFICATION OF OPTICAL MATERIALS

Materials are classified on the basis of their interaction with visible light into three categories.

(1) **Transparent Materials:** Materials that are capable of transmitting light with relatively little absorption and reflection are called transparent materials i.e. we can see through them.

Examples: Plain glass, clear water, etc.

(2) **Translucent materials:** Materials through which light is transmitted diffusely i.e. objects are not clearly distinguishable when viewed through.

Examples: Butter paper, plastic covers, frosted glass, hydrogel and colloidal materials. Smoke, fog and cloud can also be considered as translucent materials.

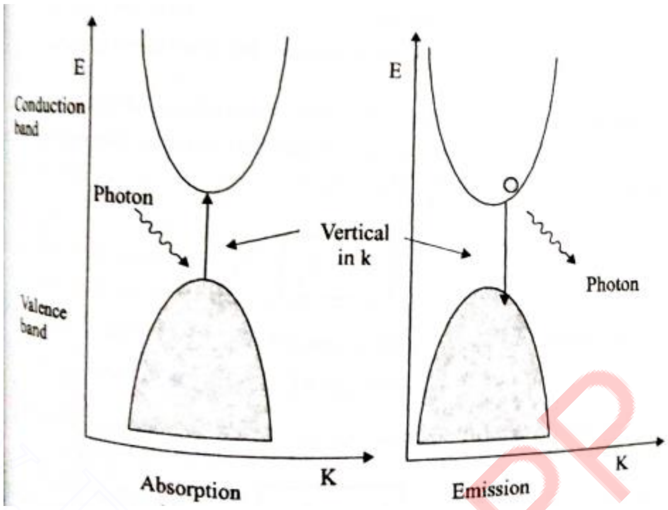
(3) **Opaque Materials:** Those materials that are impervious to the transmission of visible light are termed as opaque materials. These materials absorb all the energy from the light photons.

Examples: Metals, wood, brick stone, etc.

OPTICAL PROCESSES IN SEMICONDUCTORS

When light is incident on a semiconductor, an electron in the valence band goes to the conduction band. This process generates electron-hole pairs. It is also possible for an electron and a hole to recombine and emit light.

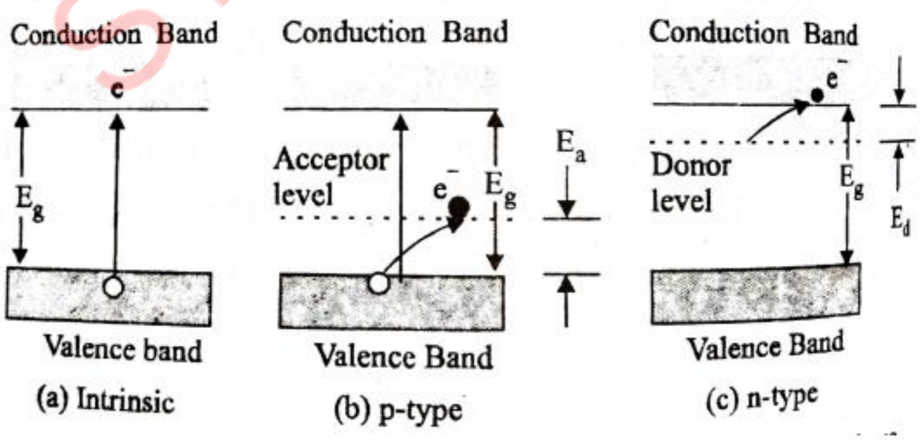
The interaction between light and electron in the semiconductor provides a variety of phenomena. These are used in the field of optoelectronics. The important optoelectronic interaction in semiconductors is the band-to-band transition. In the photon absorption process, a photon scatters an electron in the valence band.



Thus, electron jumps to the conduction band and leaving a hole in the valence band. In the reverse process the electrons in the conduction band recombines with a hole in the valence band to generate a photon. These two processes are importance for light detection and light emission devices. The rate of the light emission and absorption processes are determined by quantum mechanism.

OPTICAL ABSORPTION AND EMISSION OF LIGHT IN SEMICONDUCTORS

In semiconductors, light photons is absorbed in several ways. In intrinsic semiconductors such as Si, Ge and GaAs, light photons is absorbed to create electron-hole pairs. This absorption causes electrons to jump across the energy band gap from the valence band to the conduction band.



Absorption of Photons in Semiconductors

This transition occurs i.e., the excitation of electron due to absorption can take place if the photon energy is greater than that of the band gap E_g, that is if $h\upsilon > E_g$

Where h – Planck's constant

υ – Frequency of the light photon

In terms of wavelength λ $\frac{hc}{\lambda} > E_g$

The maximum wavelength for visible light λ_{max} is about 0.7 µm. therefore, the minimum band gap energy $E_{g(\min)}$ for which there is absorption of visible light is given by

$$E_{g(\min)} = \frac{hc}{\lambda_{max}}$$

Substituting the corresponding values, we have

$$E_{g(\min)} = \frac{(6.62 \text{ x } 10^{-34})\,(3 \text{ x } 10^{8})}{0.7\, x\, 10^{-6}}$$

$$E_{g(\min)} = 2.84\, x\, 10^{-19}\ \text{J}$$

$$E_{g(\min)} = \frac{2.84\, x\, 10^{-19}}{1.6\, x\, 10^{-19}}$$

$$E_{g(\min)} = 1.8\ eV$$

The result indicates that all visible light is absorbed by those semiconductors having band gap energies less than about 1.8 eV. Thus, these semiconductors are opaque.

In extrinsic semiconductors, the presence of acceptor and donor impurities creates new energy levels namely acceptor level (p-type semiconductor) and donor level (n-type semiconductor). These impurity levels lie within the band gap of the material.

Light radiation of specific wavelength may be absorbed as a result of electron transitions from or to these impurity levels within the band gap.

CHARGE INJECTION AND RADIATIVE RECOMBINATION

Electrons and holes can be injected into the conduction and valence band in a number of way. The light incident on the material and the absorption of photons creates electron-hole pairs. We also use an external battery bias in a p-n diode also inject electrons and holes. The electrons and holes will recombine with each other and the electron in the conduction band will return to the valence band.

This recombination process can be made in two processes. They are (i) radiative processes and (ii) non-radiative processes. In the radiative process the electron-hole pair recombines and a photon is emitted. This is the inverse of the photon absorption process.

Electron-hole pairs can also recombine without emitting light. Instead, they may emit (i) heat or (ii) a phonon or (iii) a long-wavelength photon together with a phonon. Such processes are non-radiative processes. As the electrons and holes are pumped into the semiconductor they recombine through the process of spontaneous emission. This process does not require photons to be present for the photon emission process to occur.

Types of carrier injections

(i) Minority Carrier Injection: If n >> p and the sample is heavily doped n-type, recombination rate is proportional to hole density. Thus the recombination rate is proportional to the minority carrier density.

(ii) Strong injection: this case is important when a high density of both electrons and holes is injected. The rate of recombination rate is proportional to the majority charge carrier.

(iii) Weak injection: in this case, the rate of recombination is low.

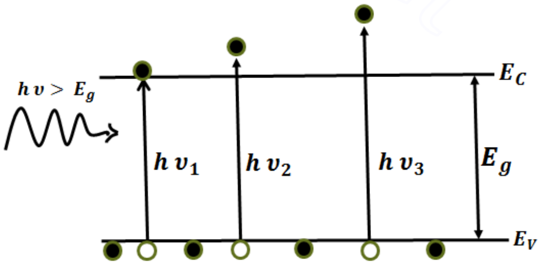
(iv) At low injection, the electrons have a low probability to find a hole with which to recombine.

CARRIER GENERATION AND RECOMBINATION PROCESSES

Carrier generation: The process by which free electrons and holes are generated in pair is called generation of carriers. When electrons in a valence band get enough energy, then they will absorb this energy and jumps into the conduction band. The electron which is jumped into a conduction band is called free electron and the place from where electron left is called hole.

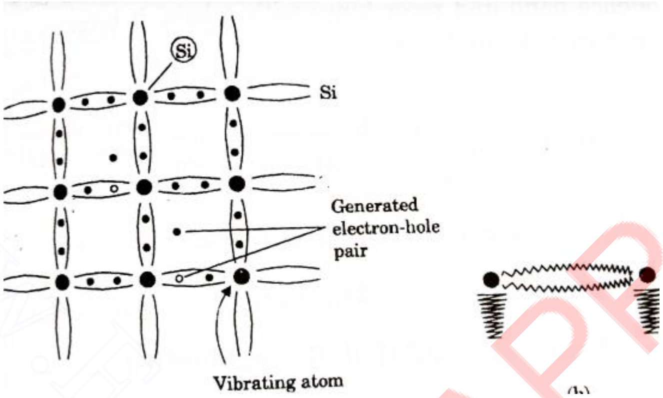
Types:

1. **Photo generation:** The generation of an electron-hole pair, is triggered by a sufficiently energetic photon which transfers its energy to a

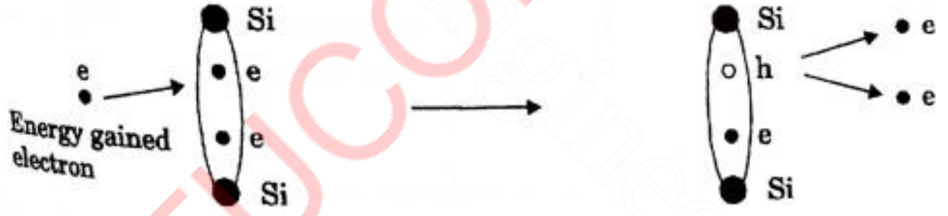


valence band electron which is excited to the conduction band leaving a hole behind.

2. **Phonon generation**: This occurs when a semiconductor is under thermal excitation. Due to increase in temperature the lattice vibrations increases which causes the covalent bonds to break and electron hole pairs are generated.

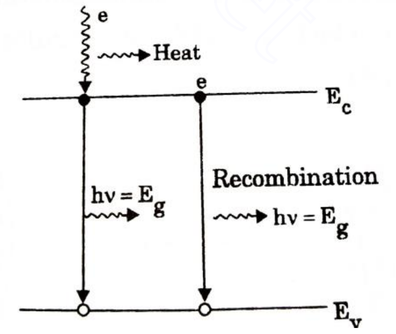


3. **Impact ionization**: a highly energetic carrier moves to the conduction or valence band, depending on the carrier type, and the excess energy is used to excite an electron from the valence band to the conduction band generating another electron hole pair



Carrier recombination: The process by which free electrons and the holes annihilate each other is called recombination of carriers. When free electron in the conduction band falls in to a hole in the valence band, then the free electron and hole gets recombined with the release of energy.

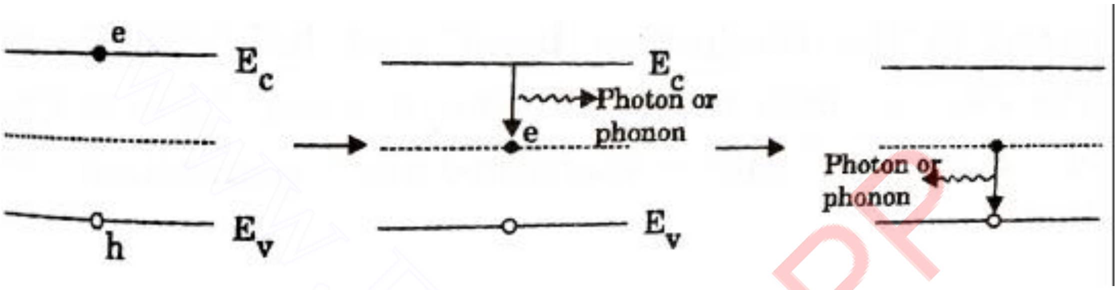
Types:



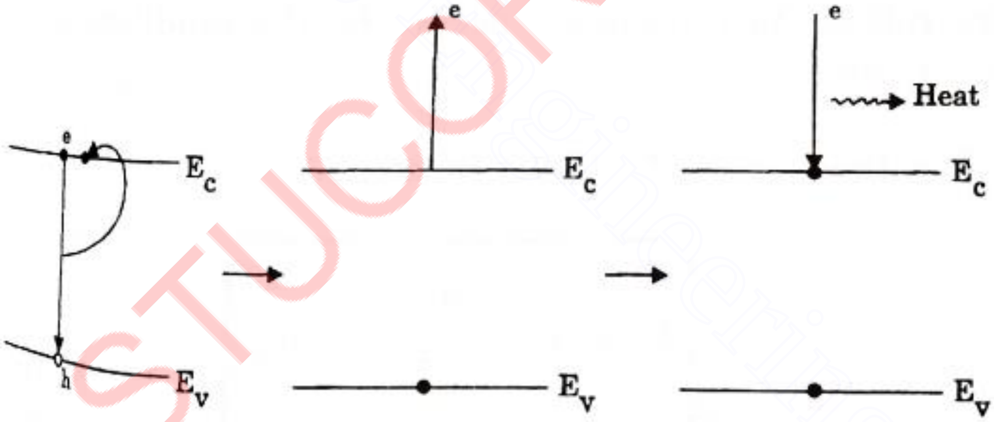
1. **Radiative recombination**: the process of electrons jumping down from the conduction band to the valence band in a radiative manner. During this recombination, the energy absorbed by a material is released in the form of photons. Generally these

photons contain the same or less energy than those initially absorbed.

2. **Shockley-Read-hall recombination**: the electron in transition between bands passes through a new energy state (localized state) created within the band gap by a dopant or a defect in the crystal lattice; such energy states are called traps. Non-radiative recombination occurs primarily at such sites. The energy is exchanged in the form of lattice vibration, a phonon exchanging thermal energy with the material.



3. **Auger Recombination**: In Auger recombination the energy is given to a third carrier which is excited to a higher energy level without moving to another energy band. After the interaction, the third carrier normally loses its excess energy to thermal vibrations.



OPTICAL ABSORPTION LOSS AND GAIN

Optical Gain

Optical gain in semiconductor lasers describes the optical amplification of the semiconductor material which is due to the stimulate emission associated light emission created by recombination of electrons and holes.

From the figure, we can see that due to recombination of electrons and holes, we get photons. Here, we get two photons due to stimulate emission process. Hence there is increase in intensity. Since there is increase in intensity it is called optical amplification (or) OPTICAL GAIN.

Optical Absorption and Loss

Optical loss is due to light which could have generated an electron-hole pair but due to absorption of light there is loss in intensity of light.

From the figure, we can see that a photon is absorbed by the electron in the valence band and hence the electron goes to conduction band. Here, a photon is lost in the absorption process and hence the intensity decreases. Since there is decrease in intensity of light, this phenomenon is known as OPTICAL LOSS.

OPTICAL PROCESSES IN QUANTUM WELLS

The term "well" refers to a semiconductor region that is grown to possess a lower energy, so that it acts as a trap for electrons and holes. These are called quantum wells because these semiconductor regions are only a few atomic layers thick. Quantum wells are real-world implementation of the "particle in one-dimensional box" problem.

Quantum sized effects

While dealing the electronic properties of bulk materials, the electron mean free path due to the application of external field (or) de Broglie wavelength is much smaller than the sample dimensions. Suppose the mean free path of the carriers are most comparable with the dimensions of the material, quantum sized effects becomes important, which dominates the electronic properties of material.

Quantum well structures are made by fusing the two semiconductors (of different band gap energies and of thickness comparable to the electron mean free path) together.

The basic properties of a quantum well is understood from the simple 'particle in a box' model. In quantum well an isolated thin semiconductor sheet of thickness L is considered as length of the box. Solving the Schrodinger equation and applying boundary conditions result in the following quantized energies for charge carrier.

$$E_n = \frac{n^2h^2}{8mL^2} \qquad \psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\,\pi\,x}{L}\right)$$

Where

n = 1,2,…… quantum numbers

h – Planck's constant

m – Mass of charge carrier (electron or hole)

OPTOELECTRONIC DEVICES

LIGHT DETECTORS

Light detectors are the devices which convert the light signal into electrical signals. The two important types of light detectors used in optical communication system are

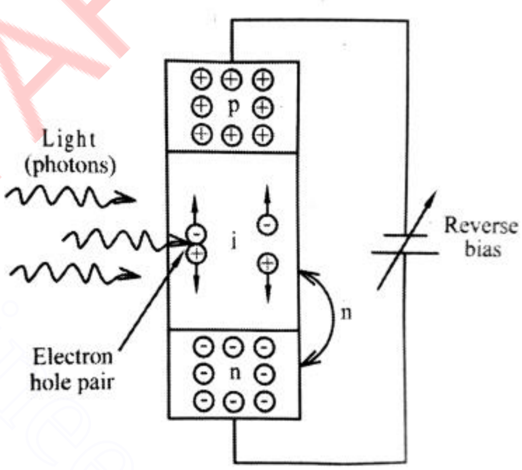
- p-i-n Photo diode
- Avalanche Photo diode

PIN PHOTODIODE

Principle: Under reverse bias when light is made to fall on the neutral (or) intrinsic region electron hole pairs are generated. These electrons and holes are generated by the external electric field which results in photocurrent. Thus light is converted into electrical signal.

Construction

It consist of 3 regions – p type, intrinsic and n type. The p and n regions are made up of Si, Ge and their alloys and are heavily doped. The intrinsic layer is a neutral layer and it is lightly doped with p or n- type material. The intrinsic layer is made as large as possible in order to have large light absorption. Since the p-n region is separated by an intrinsic region it is called as positive – intrinsic-negative (p-i-n) photo diode.



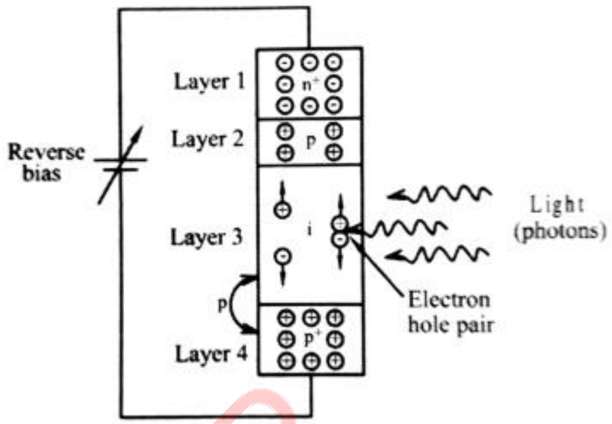
Working

The pin photo diode is applied with high reverse bias voltage. Since the intrinsic region contains very less mobile charge carriers, the width of the depletion region is increased. When photon of energy equal to or greater than the bandgap of the material is incident on the intrinsic region, the electron hole pairs are created due to photon absorption. The mobile charge carriers are accelerated to high voltages, which gives rise to photo current in the photo diode. This photodiode acts as a linear device since the photocurrent is directly proportional to the optical power incident on it.

AVALANCHE PHOTODIODE

This works under avalanche mechanism. The creation of shower of electron hole pairs from a single electron hole pair by collision process.

Principle: Under reverse bias when light is made to fall on the neutral (or) intrinsic region electron hole pairs are generated. By avalanche effect more amount of electron hole pairs are created which results in large photo current than that of PIN photodiode. Thus light is converted into electrical signal.



Construction

It consists of 4 layers. The Layer 1 consists of a heavily doped n-region, denoted by n+. The Layer 2 is made up of P-region and Layer 4 is heavily doped p-region denoted by p+. Layer 3 is intrinsic region lightly doped with p-material.

Working

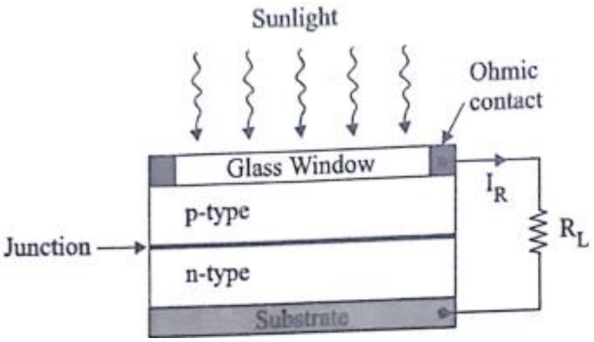
Before light is incident on the diode, a reverse bias voltage is applied. At a certain voltage the depletion region widens. Since both i and p are lightly doped the intrinsic region widen up – depleted mode. When light is allowed to fall on the diode light is absorbed by the intrinsic region and hence called as collection region. This creates the electron hole pairs in the intrinsic region.

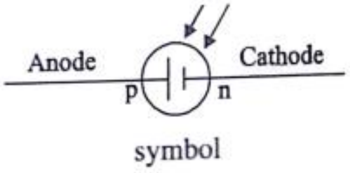
When the biasing voltage is increased the electrons moves from the intrinsic region to p layer and then to n layer. Here the electrons collide with the valence electrons and releases more number of free (or) conduction electrons and hence avalanche effect is produced.

Therefore, one generated photoelectron releases / liberates 1000's of free electrons by avalanche effect and in turn increases the output current enormously. Since large current is produced even when a single photon incidents on the diode, these diodes are termed as highly sensitive detectors.

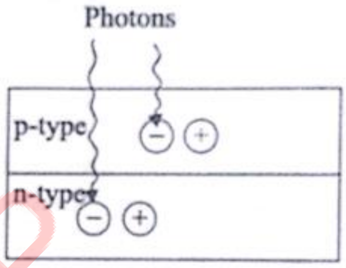
SOLAR CELL

Principle: A solar cell is a basically a large area photo-diode which converts sunlight (solar energy) directly into electricity (electrical energy), with larger efficiency, of photon absorption.





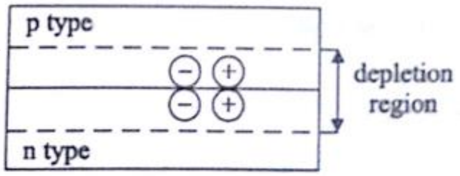
Construction: A solar cell is made up of a heavily doped ‘p’ and ‘n’ type materials grown over the substrate with larger exposure area for the sunlight to pass through it. The upper surface of the cell is made of the thin layer of the p-type material so that the light can easily enter into the material. The metal rings are placed around p-type and n-type material which acts as their positive and negative output terminals respectively. The ‘p’ and ‘n’ type material is connected to the load resistance R_L through the Ohmic contacts.



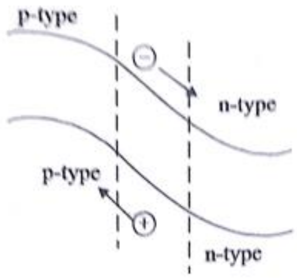
Working:

1. The solar cell is exposed to the light without load resistance (R_L) and the photons are allowed to fall on the ‘p’ and ‘n’ type materials.

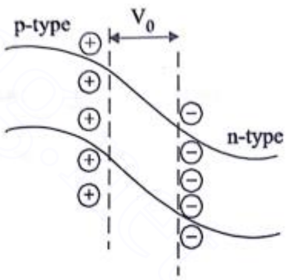
   The photons collide with the valence electrons and eject it out from the parent atoms, thus electron-hole pairs are generated.



2. The electrons and holes are quickly diffuses and reaches the depeletion region.
3. Now, due to strong barrier field, the electrons (minority charge carrier) from ‘p’ type moves towards the ‘n’ side and similarly holes from ‘n’ type moves towards the ‘p’ side.



4. As the p-n junction diode is open circuited, the electrons and holes are accumulated on either side of the junction, which gives rise to a open-circuit voltage(V_0).
5. Now if a load resistance R_L is connected across the diode, then a reverse current I_R flows through the circuit.



6. Here the magnitude of the current generated in the solar cell is proportional to the intensity of light falling on it.

Merits:

- The energy used by the solar cell is a renewable energy source.
- The cells are eco-friendly and saves electricity charges.
- Pollution free device.
- High efficiency.
- Long life time and durability.

Demerits:

- Investment / installation cost is high.
- Device s cannot work under winter / rainy seasons.
- Solar panels occupy more space during installation.
- The electrical energy generated should always be converted from DC to AC which is practically difficult.

Applications

- Solar cells are used in the production of electricity to our daily needs.
- Solar cells also provide electricity which may be used for commercial purposes.
- They are used in artificial satellites and in space probes.
- Solar panels are used in calculators, watches, street lights, toys, etc.

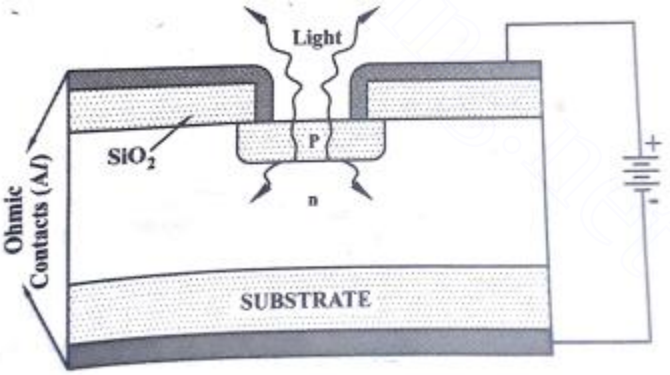
LIGHT EMITTING DIODE (LED)

A light Emitting Diode (LED) is an optical semiconductor device that emits light when voltage is applied. In other words, LED is an optical semiconductor device that converts electrical energy into light energy.

Principle: A light Emitting Diode (LED) is an optical semiconductor device that emits light when voltage is applied. In other words, LED is an optical semiconductor device that converts electrical energy into light energy.

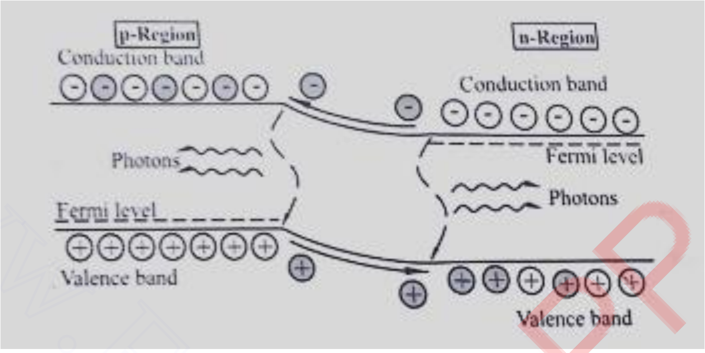
Construction:

The p-n junction is formed by diffusion or epitaxial techniques. The pn junction is made by doping silicon with GaAs crystal. Since silicon can act both as donor (when it replaces Gallium) and acceptor (when it replaces arsenide) if it is used as the impurity atom or dopant. Therefore a shallow p-n junction is formed on Ga As substrate such that p-layer is formed by diffusion on n-layer.



In order to increase the probability of radiative recombination, the thickness of the 'n' layer is taken higher than that of the thickness of the ‘p’ layer.

Ohmic contacts are made with the help of aluminium in such a way that top layer of the ‘p’ material is left uncovered, for the emission of light. Proper biasing can be applied at the Ohmic contacts. The whole p-n junction is surrounded by plastic material so that the losses due to reflection can be minimized.



Working: Light Emitting Diode (LED) works only in forward bias condition. When Light Emitting Diode (LED) is forward biased, the free electrons from n-side and the holes from p-side are pushed towards the junction. When free electrons reach the junction or depletion region, some of the free electrons recombine with the holes in the positive ions. Thus, free electrons recombine with holes in the depletion region. In the similar way, holes from p-side recombine with electrons in the depletion region. Because of the recombination of free electrons and holes in the depletion region, the width of depletion region decreases. As a result, more charge carriers will cross the p-n junction. Some of the charge carriers from p-side and n-side will cross the p-n junction before they recombine in the depletion region. Thus, recombination takes place in depletion region as well as in p-type and n-type semiconductor. The free electrons in the conduction band releases energy in the form of light before they recombine with holes in the valence band.

Advantages of LED

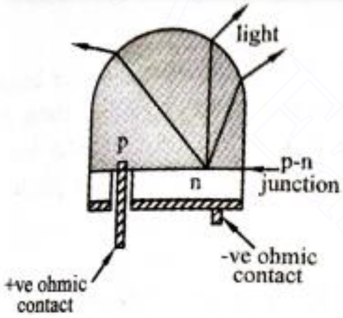
- Light emitting diodes consume low energy.
- LEDs are very cheap and readily available.
- LEDs are light in weight.
- Smaller size.
- LEDs have longer lifetime.
- LEDs operates very fast. They can be turned on and off in very less time.

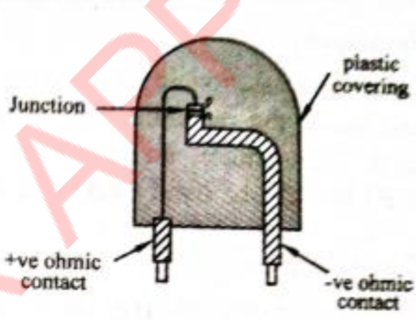
Disadvantages of LED

- LEDs need more power to operate than normal p-n junction diodes.
- Luminous efficiency of LEDs is low.

DOME SHAPED LED

In the planar LED, the reflection loss is more because most of the emitted light strikes the material interface at an angle greater than the critical angle. Therefore they are totally internally reflected and will not come out of the interface. Thus the light is lost. This loss of light due to internal reflection can be minimized by two ways.





(i) By making the ‘p’ material in the shape of a hemispherical dome. The angle at which the light strikes the interface can be made less than the critical angle and hence the light will not be lost by total internal reflection.

(ii) By covering the p-n junction by a plastic medium of higher refractive index in the shape of hemispherical dome. The total internal reflection can be reduced. This LED is used for commercial purpose. Hence, usually the dome shaped hemispherical LED is preferred than planar LED

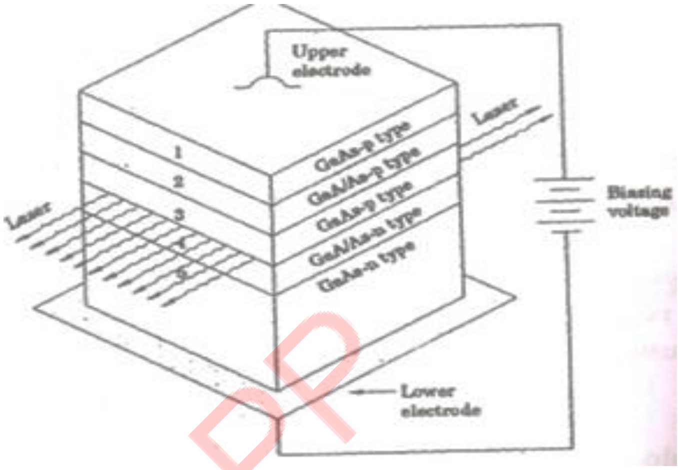
LASER DIODE

Definition: If the p-n junction is formed with different semiconducting materials, then it is called as hetero-junction laser. Ex: hetero-junction laser can be formed between **GaAs** and **GaAlAs**.

Principle: When the p-n junction diode is forward biased, the electrons from n-region and the holes from p-region cross the junction and recombine with each other. During the recombination process, the light radiation (photons) is released. This light radiation is known as recombination radiation. The photons emitted during recombination stimulate other electrons and holes to recombine. As a result, stimulated emission takes place which produces laser.

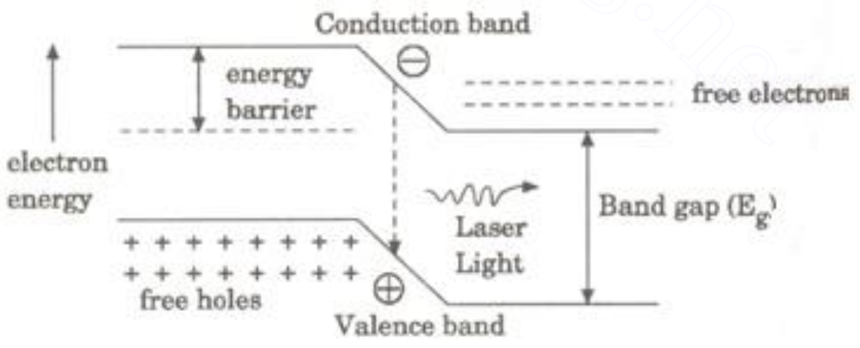
Construction:

This laser consists of five layers as shown in figure. A layer of Ga-As P-type (3rd layer) will act as the active region. This layer is sandwiched between the two layers having wider band gap. i.e., GaAlAs p-type (2nd layer) and GaAlAs n-type (4th layer). Electric current applied to the crystal through the electrodes which are fixed on the top and bottom layer. The end faces of the 3rd and 4th layers are well polished and made parallel to each other. They act as an optical resonator.



Working: Figure shows the energy level diagram of hetero-junction semiconductor laser. When the p-n junction is forward biased, the electrons and holes are injected towards the junction region. So, the size of junction region decreases. Also, the region around the junction contains large number of electrons in the n-region and large number of holes in the p-region. So, population inversion is achieved because, n-region has large number of electrons.

When the forward bias is increased, the electrons and holes will cross the junction and they recombine with each other. i.e., if one electron meets a hole, they will recombine with each other and due to this recombination one photon is emitted. The emitted photon will stimulate other electrons and holes to recombine. Hence, large number of recombination takes place. Thus, we get large number of photons and they travel back and forth between end faces and reflected. So, the photons grow in strength. After enough strength is attained the device emits laser beam of wavelength 8000 A^0.



Advantages

1. It produces continuous wave output.
2. The Power output is very high.
3. It has high directionality and high coherence.
4. It has low threshold current density compared to homojunction laser.
5. These diodes are highly stable and has longer lifetime.

Disadvantages

1. It is very difficult to from different layers of p-n junction.
2. The cost of this laser is very high.

Applications

1. This type of laser mostly used in optical communications.
2. It is widely used in computers, especially on CD-ROMs.

OPTICAL PROCESS IN ORGANIC SEMICONDUCTOR DEVICES – ORGANIC LED [OLED]

Organic light-emitting diode (OLED) is a new type of electronic device which emits light, consuming very less energy. It overcome the drawback of LCD, in which we suffer from poor viewing angle. Organic LED are generally made up of many layers with organic molecules of different conductivity levels, ranging from insulators to conductors.

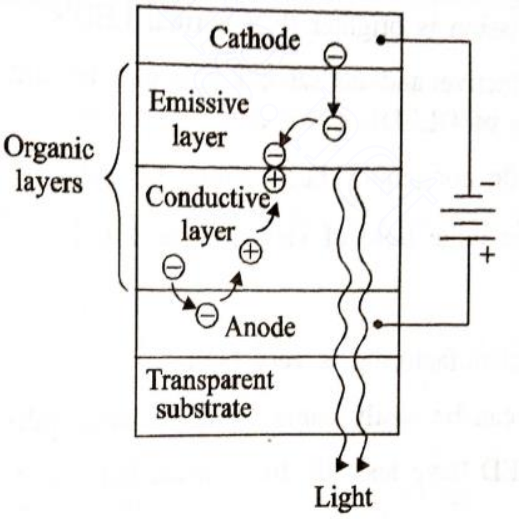
Principle: An electron moves from the cathode to emissive layer and the holes moves from the anode to the conductive layer and they recombine to produce photons. This is the principle used to emit light in OLED.

Construction

The 2-layer OLED consists of a cathode and an anode, in between which we have two organic layers.

1. Emissive layer
2. Conductive layer, made up of different conductivities.

All the layers are grown over a transparent substrate, through which the light has to be emitted. Necessary



biasing is given for the OLED, in such a way that the anode is given positive and the cathode is given negative.

Working

- ✓ Voltage is applied across the OLED.
- ✓ Due to applied voltage, the cathode gives electrons to the emissive layer.
- ✓ The anode withdraws an electron from the conductive layer and produces a hole in the conductive layer.
- ✓ Soon the emissive layer is rich in negatively charged electrons and conductive layer is rich in positively charged holes.
- ✓ Now due to the electrostatic forces these electrons and holes, they come closer and recombine with each other.
- ✓ The recombination of electrons and holes occurs in the emissive layer and this produces light and it is emitted through the transparent substrate.

Advantages of LED

- ➢ OLED is very thin and more flexible.
- ➢ They are light in weight and small in size.
- ➢ Light emission is brighter than normal LED's
- ➢ The conductive and emissive layers can be increased to increase the efficiency of OLED.
- ➢ OLEd's don't require backlighting like LCD's.
- ➢ They have large field of view[about 170°]

Disadvantages of LED

- ➢ Cost of manufacturing is very high.
- ➢ OLED's can be easily damaged when water falls on it.
- ➢ Blue OLED have less life time, when compared to red OLED.
- ➢ Maintenance cost also increases due to different life time.

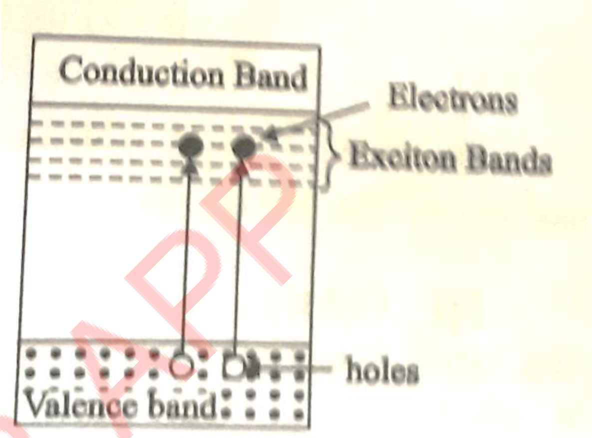
Applications

1. OLEd's are widely used in cell phones, digital cameras, etc.
2. They are also used in TV screens, computer monitors.
3. They are nowadays used in automotive dash boards and backlight in cars.

4. OLED's are used in flexible display boards, for displaying video's in real time.
5. In future, newspapers also may have OLED displays to refresh us with the latest or breaking news.

EXCITONIC STATE

When photons of energy less than the energy gap is made to fall on some crystals the electrons from valence band will not go to conduction band exactly, instead they will go to a level below the conduction band level called excitons bands.



The bound electron-hole pairs are called excitons, normally these exciton energy levels lies in the bandgap, very near to the conduction band. The excitons arise due to the pair formed by the electrons in the exciton energy level and associated holes in the valence band.

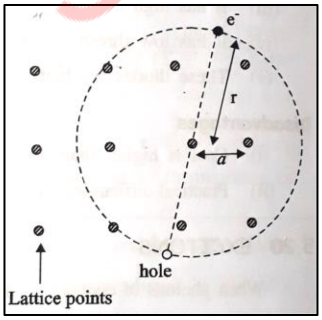
Types:

i) Weakly bound excitons

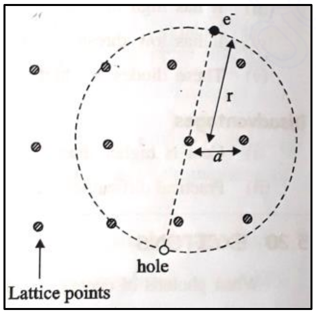
ii) Tightly bound excitons

Weakly bound exciton: In this exciton the electron hole interparticle distance is larger than lattice constant [r > a].

Example: Cu_2O has weakly bound excitons.



Weakly bound Exciton



Tightly bound Exciton

Tightly bound exciton: In this exciton the electron hole interparticle distance is less than the atomic radius [a > r]. This type of exciton, is localized on (or) near a single atom, i.e., the hole will also exist in the same atom as that of an electron, although the pair may be anywhere in the crystal.

Example: Alkali halide crystals such as NaCl, KBr etc. has tightly bound excitons.

NON LINEAR OPTICS

Optical properties of the materials are unaffected when an ordinary light is propagated through it. But it has to be noted that the optical properties of the materials (such as refractive index) may be affected when light of high intensity (laser beam) is allowed to pass through it.

The change in optical properties due to electric and magnetic field associated with light is called nonlinear effects and those materials which possess these effects are called non-linear materials. This phenomenon is termed as non-linear optics.

Examples:

(i) Ammonium- dihydrophosphate (ADO)
(ii) Potassium – dyhydrophosphate (KDP)
(iii) Lithium iodate (LiO_3)
(iv) Lithium tantalite
(v) Barium sodium niobate

In ordinary light the electric and magnetic field associated with it is so weak and hence we could not identify non – linear effects in it. But in LASER beam we can easily identify non- linear effects, because of the strong electric and magnetic field associated with it.

When magnetic field is applied along the axis of propagation of light beam to a glass medium, the plane of polarization of light beam is rotated. This is called **Faraday Effect.** Similarly, when electric field is applied along the direction of propagation of light, then the light will undergo double refraction, this is called **Kerr Effect**. Faraday and Kerr effect confirmed that both electrical and magnetic field will change the optical properties of a medium.

SECOND HARMONIC GENERATION

Definition: *Second harmonic generation represents the generation of new frequencies with the help of the crystals such as quartz, potassium- dihydrophosphate (KDP), etc.*

Explanation

Let us consider a material media in which the light is passed through it. We know that light consists of both electric and magnetic fields associated with it. These electric field associated with the light will distort the atoms and molecules in the material to form oscillating dipoles.

The induced electric dipole is due to the displacement of electron cloud with respect to the centre of the positive nucleus of an atom. This phenomenon is called electric polarization (P).

Relation between P and E for ordinary light (linear medium)

When light of low intensity (i.e. ., ordinary light) is passed through dielectric medium (i.e., glass), the electric field has smaller amplitude and the oscillation of dipoles can follow the field exactly.

Hence the relation between the electric field E and polarization vector P can be written as,

$$P = \varepsilon_0 \chi_0 E$$

Where,

χ_0 – Electric field susceptibility

ε_0- Permittivity of the medium

Relation between P and E for LASER beam (Non –Linear Medium)

When light of higher intensity (i.e. laser) is passed through dielectric medium, the electric field has larger amplitude and the oscillation of dipoles are distorted. Therefore, some nonlinear is observed between P and E and hence the second harmonic generator is observed.

Thus, the polarization vector can be written as,

$$P = \varepsilon_0 (\chi_0 E + \chi_1 E^2 + \chi_2 E^3 + \chi_3 E^4 + \ldots\ldots) \qquad \ldots\ldots\ldots\ldots \; (1)$$

Where,

χ_0 – Linear susceptibility

χ_1, χ_2, χ_3 - Non linear (higher order) susceptibility

The higher order nonlinear susceptibility are very small when compared to linear susceptibilities. But the higher order susceptibility produces so many new optical phenomena.

We know the oscillating electric field on a medium is,

$$E = E_0 \cos \omega t \qquad \ldots\ldots\ldots\ldots\ldots\ldots (2)$$

Substituting equation (2) in equation (1), we get

$$P = \varepsilon_0\ \chi_0\ E_0 \cos \omega t + \varepsilon_0\ \chi_1\ E^2 \cos^2 \omega t + \varepsilon_0\ \chi_2\ E^3 \cos^3 \omega t + \ldots\ldots$$

We know $\cos^2\omega t = \dfrac{1+\cos 2\omega t}{2}$, $\cos^3 \omega t = \dfrac{\cos 3\omega t + 3\cos\omega t}{4}$

$$\therefore P = \varepsilon_0 \chi_0 E_0 \cos \omega t + \varepsilon_0\ \chi_1 E^2 \left[\frac{1+\cos 2\omega t}{2}\right] + \varepsilon_0 \chi_2 E^3 \left[\frac{\cos 3\omega t + 3\cos\omega t}{4}\right]$$

$$P = \varepsilon_0 \chi_0 E_0 \cos \omega t + \frac{\varepsilon_0\ \chi_1 E^2}{2} + \frac{\varepsilon_0\ \chi_1 E^2 \cos 2\omega t}{2} + \frac{\varepsilon_0\ \chi_2 E^3 \cos 3\omega t}{4} + \frac{3}{4}\ \varepsilon_0\ \chi_2 E^3 \cos 3\omega t$$

Rearranging we get,

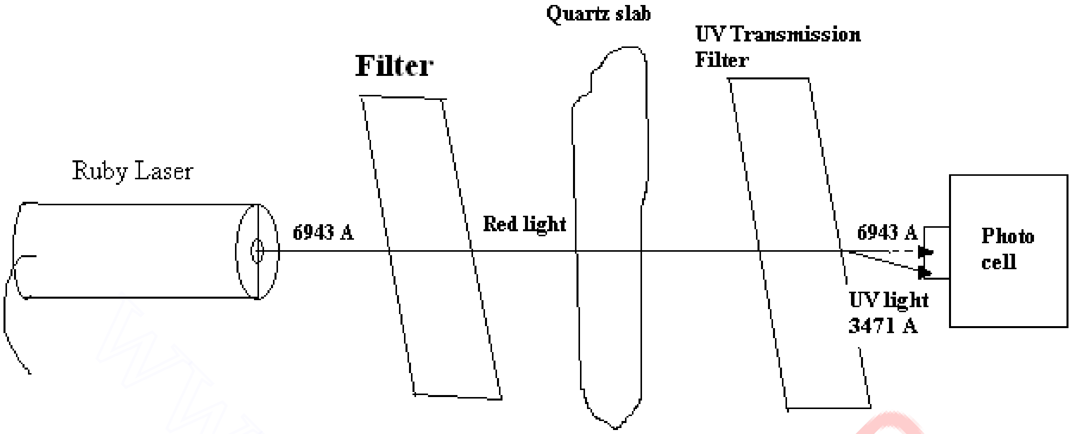
$$P = \underbrace{\tfrac{1}{2}\ \varepsilon_0\ \chi_1 E^2}_{\text{I}} + \underbrace{\varepsilon_0\ E_0 \cos \omega t \left[\chi_0 + \tfrac{3}{4}\chi_2 E^2\right]}_{\text{II}}$$

$$+ \underbrace{\tfrac{1}{2}\ \varepsilon_0\ \chi_1 E^2 \cos 2\omega t}_{\text{III}} + \tfrac{1}{4}\ \varepsilon_0\ \chi_2 E^3 \cos 3\omega t \quad \ldots\ldots\ldots(3)$$

Referring equation (3), the first term represents the dc field across the medium which has less importance (since it doesn't have cos ωt term). The second term represent the external polarization which is called as first (or) fundamental harmonic susceptibility (since it has cos ωt), third term represents the oscillation dipoles, which oscillates at a frequency 2ω and hence called second harmonic of polarization. The forth term which has cos 3ωt is called the third harmonic of polarization etc.

When the first term and the third term is added we can get the term called optical rectification.

Experimental evidence



The observation of second harmonic generation by quartz slab is illustrated in fig.

A high power ruby laser (of wavelength 6943 Å) is passed through a filter, which filters the red light and allows the ultraviolet light to the quartz slab. The emerging light from the quartz slab is made to pass through a **UV transmission filter**, which filters unwanted light and allows the ultraviolet light alone to pass through the photo cell. In this experiment, due to second harmonic generation, the wavelength of the incident beam is made half and hence the wave length of emerging beam is recorded as 3471 Å.

IMPORTANT NONLINEAR MATERIALS AND THEIR PROPERTIES

Important non-linear optical materials are,

1. Lithium niobate
2. Lithium tantalite
3. Barium sodium niobate

Lithium niobate ($LiNbO_3$)

1. It is a synthetic ferroelectric material.
2. It has highest Curie temperature i.e., 1210 ^{0}C.
3. It has high electric polarizability and low loss optical transmission.
4. It exhibits linear electro-optic effect due to the lack of an inversion centre in the structure.
5. At high temperatures it becomes electrically conductive.
6. It has multi domain structures.

7. Polarization is inversely proportional to the temperature.
8. Refractive index of this material may be changed by passing laser beam of even short wavelength. This property is called optical damage (or) photo refractive effect.

Lithium Tanalate ($LiTaO_3$)

1. It is a synthetic ferroelectric material.
2. Its curie temperature is 660^0C and melting point is 1650^0 C.
3. It has low temperature coefficient of resistance.
4. The domain size is much smaller than lithium niobate domains. Also, the domains are antiparallel polar domains.
5. $LiTaO_3$ and $LiNbO_3$ has applications of combining higher coupling factors and lower mechanical impedance values.

Barium sodium Niobate ($Ba_2NaNb_50_{15}$)

1. It is a synthetic ferroelectric material.
2. Its curie temperature is 560^0C and melting point is 1500ºC.
3. Phase transition takes place between the room temperature and Curie temperature.

APPLICATIONS OF NON – LINEAR MATERIALS

1. **Optical grating:** $LiNbO_3$ acts as an optical grating and second harmonic generator. Optical grating impose a periodic variation in the amplitude so that refractive index varies periodically and hence acts as a grating. The second harmonic generation is achieved in uniaxial crystal (like calcite and quartz)
2. **Optical amplifier:** Fiber losses can be completely eliminated by erbium doped silica fiber. Erbium doped silica fiber acts as laser amplifier or optical amplifier.
3. **Optical modulation and switching:** Electro-optic wave guide switching fabricated by $LiNbO_3$ is used for direct switching of the optical signals. The electro – optic coefficient of $LiNbO_3$ is very high and hence the crystals can be grown with good optical quality. Therefore, wave guides can be fabricated by titanium diffusion into the $LiNbO_3$ substrate. The refractive index of $LiNbO_3$ is increased by the addition of titanium. Hence light is guided in the diffused region.
4. **Optical frequency doublers:** Due to high electric polarizability and low loss optical transmission, lithium niobate, lithium tantalite and Barium sodium niobate are used in electro-optic modulators and optical frequency doublers.

5. **Delay lines and memories:** Delay line is a device which can delay the signals by converting electrical signals into slowly moving surface acoustic wave by means of a transducer. This may be reconverted into electrical signals by means of other transducer.

6. **Frequency filters:** These materials are used in signal processors, which prevent the unwanted signals from the base signal entering into the signal processor.

PLASMONICS

Plasmonics (or) nano plasmonics is a very dynamic field, which refers to the generation, detection and manipulation of signals at the range of optical frequencies along a metal-dielectric interfaces in a nano-metre scale.

Principle: the principle used in plasmonics is "Surface Plasmon Polaritons". The study of plasmons is called plasmonics. Here plasmons refer to the quantum of collective oscillations of metal's free electrons (or plasma) in response to the electric field component of electro-magnetic wave excitation.

Explanation: in metals, there are discrete number of oscillating electrons. Just like optical and phonon oscillations that include photons and mechanical vibrations respectively, here we can see quantum of plasma oscillations.

Plasma is a matter full of positive and negative charges that is almost neutral. In the case of plasmonics in which metal structures are used, we encounter with a sea of negative mobile charges inside fixed positive ions. Here, energy loss in some kind of Ohmic loss or electron-core interactions (due to resistance or damping) is inevitable.

Therefore, when an excitation occurs, the electrons will move (oscillate) due to the implemented electric field, until the total field would be cancelled. Definitely, inside metal there are infinite free electrons so we can expect the decreasing of oscillation as depth increases.

On metal's surface the neighboring electrons will make each other to oscillate; therefore, after excitation some waves will appear that are longitudinal and damping, so called **Surface Polariton Plasmons (SPPs)**. These waves are characterized by excitation's frequency and metal's structure and hence these waves are termal as plasmonics waves.

PLASMONIC MATERIALS

1. Metals (or) metal-like materials that exhibit negative real permittivity are used as plasmonic materials.
2. Plasmonics gold and silver nano-particles which have unique optical, electrical and thermal properties are termed as plasmonic materials.

APPLICATIONS

1. Plasmonic materials are used in antimicrobial coatings.
2. They are also used in molecular diagnostics.
3. Plasmonic techniques are widely used in color engineering.
4. Plasmonics are used in research areas such as food sciences, environmental sciences, biological sciences, physical sciences, etc.

PROBLEMS

1. **Calculate the wavelength of radiation emitted by an LED made up of a semiconducting material with band gap energy 2.8 eV.**

$$E_g = \frac{hc}{\lambda} \qquad \lambda = \frac{hc}{E_g}$$

$$\lambda = \frac{6.625 \, x \, 10^{-34} \, x \, 3 \, x 10^{8}}{2.8 \, x \, 1.6 \, x \, 10^{-19}}$$

$$\lambda = 4436 \text{ Å}$$

2. **For InP laser diode, the wavelength of light emission is 1.55 µm. what is its band gap in eV?**

$$E_g = \frac{hc}{\lambda}$$

$$E_g = \frac{6.625 \, x \, 10^{-34} \, x \, 3 \, x 10^{8}}{1.55 \, x \, 10^{-6}}$$

$$E_g = 1.28225 \, x \, 10^{-19} \text{ Joules}$$

$$E_g = \frac{1.28225 \, x \, 10^{-19}}{1.6 \, x \, 10^{-19}}$$

$$E_g = 0.8014 \;\; eV$$

3. **Calculate the long wavelength limit of an extrinsic semiconductor if the ionization energy is 0.02 eV.**

$$E = hv = \frac{hc}{\lambda}$$

$$\lambda_{long} = \frac{hc}{E} = \frac{6.625 \, x \, 10^{-34} \, x \, 3 \, x 10^{8}}{0.02 \, x \, 1.6 \, x \, 10^{-19}}$$

$$\lambda_{long} = 6.210 \, x \, 10^{-5} \, m$$

4. **Calculate the number of photons from green light of mercury (λ =4961 x 10^{-10}m) requires to do one joule of work.**

$$E = h\upsilon = \frac{hc}{\lambda}$$

$$E = \frac{6.625\ x\ 10^{-34}\ x\ 3\ x10^{8}}{4961\ x\ 10^{-10}}$$

$$E = 3.991\ x\ 10^{-19}\ \text{Joules}$$

Number of photons required to do one Joule of work

$$N = \frac{1\ Joules}{3.991\ x\ 10^{-19}\ \text{Joules}}$$

$$N = 2.5055\ x\ 10^{18}\ /\ m^{3}$$

UNIT 5 – NANODEVICES

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.

INTRODUCTION

Nanotechnology is a broad term used when referring to any science or technology which manipulates things in the atomic level, which is measured in nanometres. It is used in a number of fields, such as biology, medicine, computers, materials, manufacturing, physics and several others. Nanophase materials are materials with a grain size in the 1 to 100 nm range as shown in Fig5.7.A nanometre is one-billionth of a metre - approximately 100,000 times smaller than the diameter of a human hair. For example, the width of human hair is approximately 80,000 nanometres, and human fingernails grow roughly one nanometre per second. A nanometre-sized particle is also smaller than a living cell and can be seen only with the most powerful microscopes available today.

These materials have created a high interest in recent years by virtue of their unusual Mechanical, electrical, optical and magnetic properties. Some examples are given below:

I. Nanophase ceramics are of particular interest because they are more ductile at elevated temperatures as compared to the coarse-grained ceramics.
II. Nanostructured semiconductors are known to show various non-linear optical properties. They are used as window layers in solar cells.
III. Nanosized metallic powders have been used for the production of gas tight materials and porous coatings. Cold welding properties combined with the ductility make them suitable for metal-metal bonding especially in the electronic industry.
IV. Single nanosized magnetic particles have special atomic structures with discrete electronic states, which give rise to special properties in addition to the super paramagnetism behavior.
V. Nanostructured metal clusters have a special impact in catalytic applications.

Thus nanophase materials exhibit greatly altered mechanical, optical, electrical, magnetic, chemical and physical properties compared to their normal, large-grained counterparts with the same chemical composition.

SIZE DEPENDENCE OF FERMI ENERGY

In terms of distribution of energy, solids have thick energy bands, whereas atoms have thin, discrete energy states.

The electron density in a conductor at T = 0k is $n = \frac{\pi}{3}\left[\frac{8m}{h^2}\right]^{3/2} {E_{F}}_{0}^{3/2}$ ------------(1)

Fermi energy of a conductor at T = 0K is ${E_{F}}_{0} = \frac{h^2}{8m}\left[\frac{3n}{\pi}\right]^{2/3}$ ------------(2)

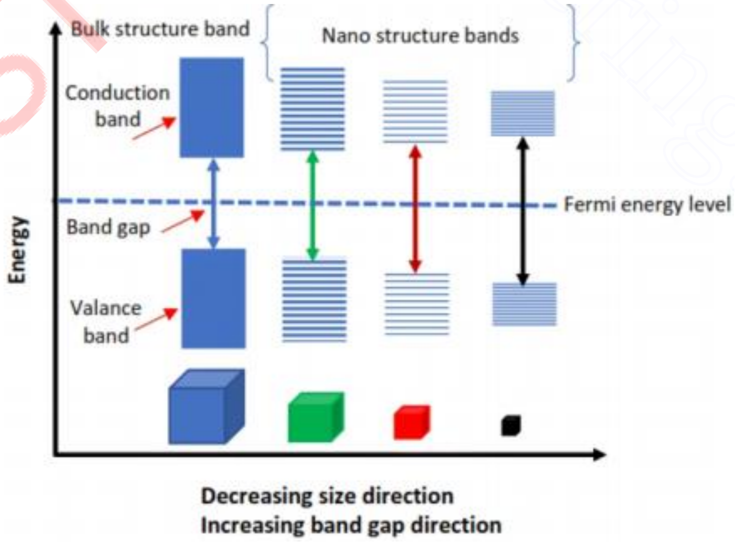
In the above equation 'n' is the only variable. The fermi energy depends on the number of free electrons 'n' per unit volume 'V'. ${E_{F}}_{0} \propto (n)^{2/3} \propto \left(\frac{N}{V}\right)^{2/3}$

Electron density is the property of the material, the fermi energy does not vary with material's size. Femi energy is same for a particle of copper as it is for a brick of copper.

Hence, we can say that the energy states will have same range for small volume and large volume of atoms. But for small volume of atoms we get larger spacing between the energy states.

The average spacing between the energy states is inversely proportional to the volume of the solid. $\Delta E \propto \frac{1}{V}$

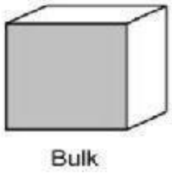
Thus the spacing between energy states is inversely proportional to the volume of the solid.



QUANTUM CONFINEMENT

The quantum confinement effect is observed when the size of the particle is too small to be comparable to the wavelength of the electron.

To understand this effect we break the words like quantum and confinement. The word confinement means to confine the motion of randomly moving electron to restrict its motion in specific energy levels (discreteness). Quantum reflects the atomic dimensions of particles. So as the size of a particle decrease till it reach a nano scale the decrease in confining dimension makes the energy levels discrete and this increases or widens up the band gap and ultimately the band gap energy also increases. Due to this, there is significant change in the electronic and optical materials of nano-dimensions as compared to the bulk materials.



QUANTUM STRUCTURES

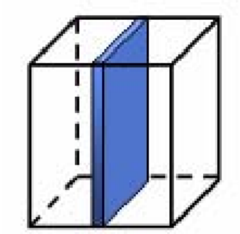
When a bulk material is reduced in its size, atleast one of its dimensions, in the order of few nanometers, then the structure is known as quantum structure. A quantum confined structure is one in which the motion of the electrons or holes are confined in one or more directions by an potential barrier.

Based on the confinement direction, a quantum confined structure will be classified into three categories as quantum well, quantum wire and quantum dot.

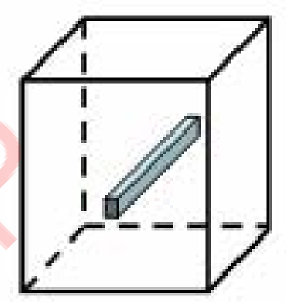
Structure	Quantum Confinement	Number of dimensions confined
Bulk	0	3
Quantum well	1	2
Quantum wire	2	1
Quantum dot	3	0

Three dimensional (3D) structure or bulk structure: No quantization of the particle motion occurs i.e., the particle is free. Electron in conduction band and holes in valence band are free to move in all three dimensions of space. E.g. cube

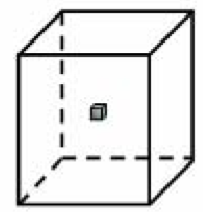
Two-dimensional (2D) structure or quantum well: Quantum confinement in nanostructure-If one dimension is confined or reduced to the nanometre ranges while other two dimensions remain large then we get a structure called quantum well. Electrons confined in one direction. Electrons can easily move in 2 dimensions E.g. nano wire s, nano rod, nanotube.



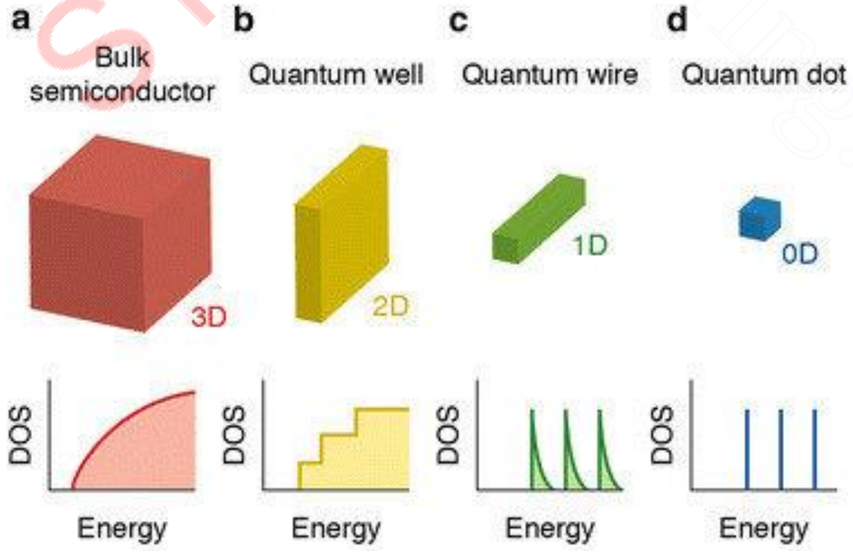
One-dimensional (1D) structure or quantum wire: If two dimensions are reduced in to the nanometre range and remain large the structure to as a quantum wire. Eg. nanoseed (Graphene). The semiconductor wires surrounded by a material with large band gap .Surrounding material confines electron and hole in two dimensions (carriers can only move in one dimensions) due its larger bandgap. Radius of quantum wires, nano rods and nano tube, nano pillars (1D structures) 1-100 nm range (Typical nano scale dimension)



Zero-dimensional (0D) structure or quantum dot: The extreme case of this process of size reduction in which all three dimensions reach the low nanometer range is called quantum dot. Eg. Nano dot. Electron confined in three dimensions Quantum dot: electron can easily moves in zero dimensions.

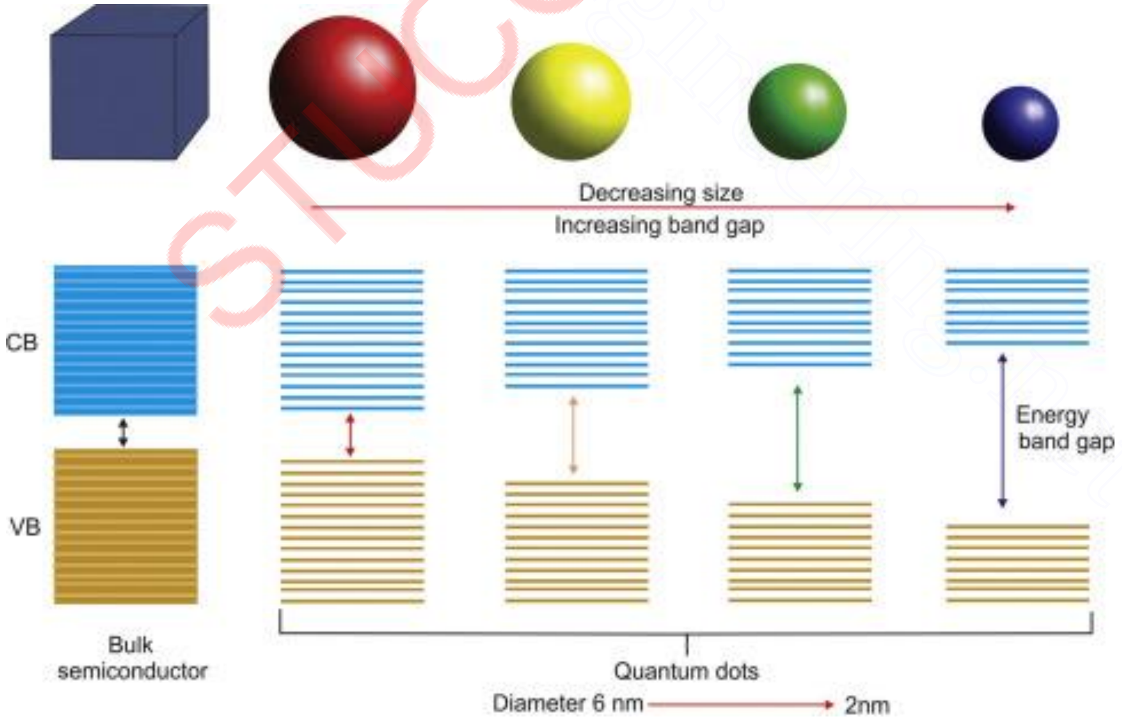


Electron and holes are confined in all the three dimensions of space by a surrounding material with a larger band gap. Discrete energy levels (artificial atoms) No quantum dots has a larger band gap like bulk semiconductor. Typical dimensions: 1-10 nm



BAND GAP ON NANOMATERIALS

- Very few atoms in a material not only causes the energy states to spread out but also widens the band gap for semiconductors and insulators.
- When energy stares are discrete, the addition or removal of just a few atoms adjust the boundaries of the band gap. This is because once two atoms are next to each other, the sublevels split and then begin to broaden into bands.
- The broader the bands get, the smaller the band gaps between them get. Finally, the bands reach a point where they will not get any wider no matter how many atoms are they in the solid.
- In case of quantum dots, the smaller the particle, and the bigger the band gap.
- Once the volume is reduced from that of a solid, which has bands for sublevels, to that of a nanomaterial, which has distict splits in each sublevel, the band gap will widen if only a few atoms are removed.
- Thus changes in band gap allows us to tune the electronic and optical characteristics of the material.
- Thus when material band gap energy changes there is a change in the electromagnetic radiation it emits. This phenomenon is especially used in optical applications.



ZENER BLOCH OSCILLATIONS

***Definition**: It denotes the oscillation of a particle confined in a periodic potential when a constant force is acting on it.*

This was pointed out by Zener and Bloch while studying the electrical properties of crystals. In particular, they predicted that the motion of electrons under the action of a constant electrical field is oscillatory instead of uniform. While in natural crystal this phenomenon is hard to observe due to scattering of electrons by the presence of lattice defects. Zener-Bloch oscillations is observed in semiconductor super lattices and in different physical systems such as cold atoms in an optical potential and ultrasmall Josephson junctions.

DERIVATION

Consider the 1-dimensional equation of motion for an electron in an constant electric field E.

$$F = \frac{dP}{dt} = -eE \qquad \text{--------(1)}$$

From de-Broglie concept the momentum is given by $p = \frac{h}{\lambda}$

$$p = \frac{h}{2\pi} x \frac{2\pi}{\lambda}$$

$$p = \hbar\, k \qquad \text{---------(2)}$$

Here, $k = \frac{2\pi}{\lambda}$ is a wave vector and $\hbar = \frac{h}{2\pi}$

Substituting eqn (2) in (1) $\quad \frac{d}{dt}(\hbar\, k) = -eE$

$$\hbar \frac{dk}{dt} = -eE$$

$$\frac{dk}{dt} = \frac{-eE}{\hbar} \qquad \text{---------(3)}$$

On integration of equation (3) with function of time is

$$k(t) = k(0) - \frac{eE}{\hbar}$$

The velocity v of an electron is given by $\quad v(k) = \frac{1}{\hbar}\frac{d\mathcal{E}}{dk}$

Where $\mathcal{E}(k)$ denotes the energy band. Suppose that the energy band has the tight-binding form

$$\mathcal{E}(k) = A\cos ak$$

Where a is lattice parameter and A is constant

Then $v(k)$ is given by $\quad v(k) = \frac{1}{\hbar}\frac{d\mathcal{E}}{dk} = -\frac{A\,a}{\hbar}\sin ak$

The electron position *x* is given by $x(t) = \int_0^t v\big(k(t)\big)dt$

$$x(t) = \int_0^t -\frac{A\,a}{\hbar}\sin ak\ \ dt$$

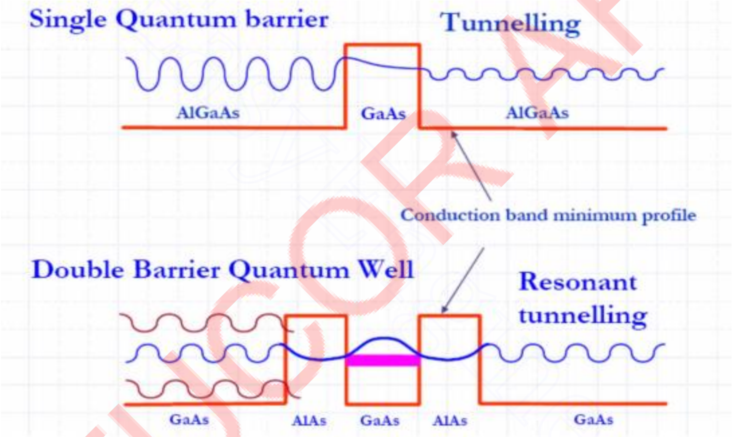
$$x(t) = \int_0^t -\frac{A\,a}{\hbar}\sin a\left[k(0) - \frac{eE}{\hbar}\right] dt$$

$$x(t) = x(0) - \frac{A}{eE}\ cos\left[\frac{a\,e\,E}{\hbar}\right]\ t$$

This shows that the electron oscillates in real space. The angular frequency of the oscillation is given by $\omega_B = \frac{a\,e\,E}{\hbar}$

<u>RESONANT TUNNELING</u>

An interesting phenomenon occurs when two barriers of width a separated by a potential well of small distance L. This leads to the concept of resonant tunneling.



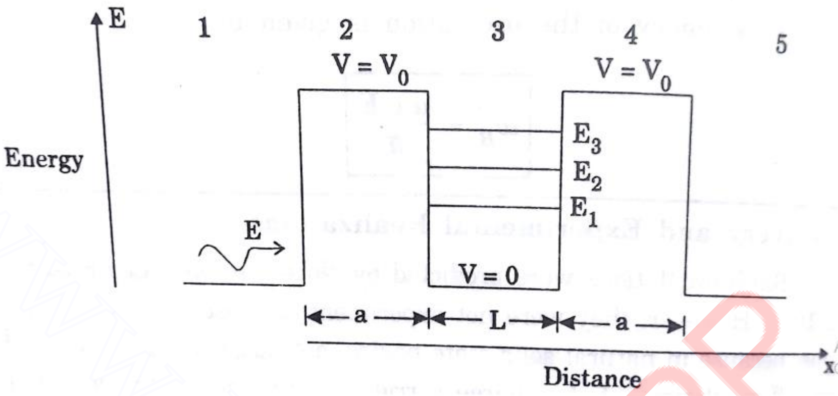
The barriers are sufficiently thin to allow tunneling and the well region between the two barriers is also sufficiently narrow to form discrete energy levels.

The analysis of the double barrier structure is essentially the same as considered as single barrier tunneling.

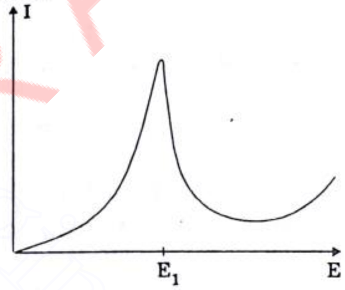
The transmission coefficient of the double symmetric barrier becomes unity, when the energy of the incoming electron wave (E) coincides with the energy of one of the discrete states formed by the well. $E = E_n = \frac{n^2h^2}{8mL^2}$

Thus, 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 quantized energy state of the well. This phenomenon is known as <u>resonance tunneling</u>.**

The double barrier tunnel junction has important applications to a device known as a resonant tunneling diode. The working of these diodes can be understood by considering the influence of bias on the energy band diagram for the double barrier system.



When incident electron of energy E is very different from the energy of a discrete state E$_n$, transmission is low. As E tends to E$_n$, transmission will increase, becoming a maximum when E = E$_n$. As E increases, tunnelling will increase, reaching a peak when E = E$_1$. After a point, a further increase in E will result in a decreasing current. This decrease in current with an increase of bias is called negative resistance. Further, peaks and valleys will occur as E approaches, and then moves across, other discrete energy states.



Current - Energy characteristic for a resonant tunneling junction

MESOSCOPIC STRUCTURES

The term ‘mesoscopic’ refers to ‘intermediate’ between long and short, and applies to microstructures to be seen in between the atomic and the macroscopic length scales.

Definition: ***The structure which have a size between the macroscopic world and the microscopic or atomic one are called mesoscopic structure.***

The electrons behave like a wave. Their behavior is dependent on the geometry of the sample. For the description of behavior of electrons it is convenient to define a series of characteristic length.

CHARACTERISTICS LENGTH IN MESOSCOPIC SYSTEMS

1. de-Broglie wavelength:

It is well known from quantum mechanics that for an electron of momentum p, there corresponds a wave of wavelength given by the de-Broglie wavelength.

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

It is relatively easy to construct semiconductor nanostructures with one or two of their dimensions of the order of, or smaller thanλ_B.

2. Mean free path:

As electron moves inside a solid, it is usually scattered by crystal imperfections like impurities, defects, lattice vibrations (phonons), etc.

In most cases, these scattering events or collisions are inelastic. The distance travelled by an electron between two inelastic collisions is usually called the mean free path of the electron in the solid. If v is the speed of the electron, then $l = v\,\tau$

Where τ is called relaxation time.

3. Diffusion Length:

In a mesoscopic system of length L, the electrons can move either in the ballistic regime or in the diffusive regime. If the mean free path *l* is much larger than L, the particle moves throughout the structure without scattering.

This is so called ballistic transport regime in which the surfaces are usually the scattering entities. If *l* << L, transport can be explained as diffusion process. The diffusion L_e is defined as

$$L_e = (D\,\tau_e)^{1/2}$$

SINGLE ELECTRON PHENOMENA AND SINGLE ELECTRON TRANSISTOR

A transistor is a fundamental building block of modern electronic devices. A semiconductor device (usually doped-Silicon or Germanium) used to amplify or switch electronic signals and electrical power. At least 3 terminals for connection to an external circuit. When a voltage or current applied to one pair of the terminals, control the current through another pair of terminals, and since the output power can be much higher than the input power, a transistor mainly acts as a signal amplifier (or as a switch).

SINGLE ELECTRON TRANSISTOR (SET)

The single electron transistor is a new type of switching device that uses controlled electron tunneling to amplify current. An electron tunnels in two steps: source - dot – drain. The gate voltage Vg is used to control the charge on the gate-dot capacitor. The idea of SET was given by D. Averin and Likharev in 1985. The first SET was realized by T. Fulton and G. Dolan at Bell Laboratories in 1987. It's based on the Quantum Tunneling phenomenon. The requirements for it to work is the Coulomb Blockade and the Heisenberg Uncertainty Principle.

THE COULOMB BLOCKADE

Definition: the resistance to electron transport caused by electrostatic coulomb forces in certain electronic structures, including quantum dots and single electron transistors is called coulomb blockade effect.

- This prevents constant tunneling to and from a quantum dot.
- Coulomb forces are electrostatic. If we put together 2 or more negative charges (electrons), these forces are repulsive.
- Capacitance of a quantum dot defines how much electric charge it can store.

$$C_{dot} = G\,\varepsilon\,d$$

Where

ε - Permittivity of the material surrounding the dot

d – Diameter of the dot

G – Geometrical term

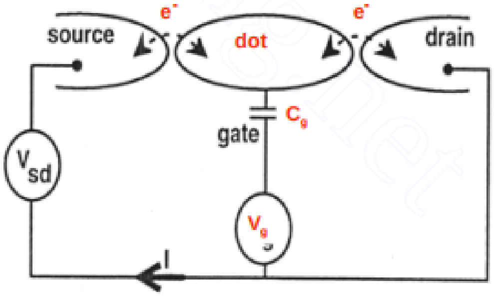
- Energy required to add negatively charged electron to the dot is known as charging energy E_c

$$E = \frac{1}{2}\,C\,V^2$$

$$Charge\ q = CV$$

$$V = \frac{e}{C}$$

$$E_c = \frac{e^2}{2C}$$



- The free electron in a solid has a certain amount of energy depending on the band it is.
- Due to thermal vibration of atoms in the lattice, these free electrons will get extra energy to go to higher bands. The extra energy is equal to K_BT

- With this extra energy an excited electron might br able to tunnel through a small barrier.
- QD's Capacitance depends on its size (d) →high E_C is required to store an additional electron
- But how high must E_C must be in order to block tunneling? $\boldsymbol{E_C \gg K_BT}$
- The smaller the quantum dot the easier the Coulomb blockade criterion is achieved.

OVERCOMING UNCERTAINTY

- According to Heisenberg's uncertainty principle: $\Delta E \approx \frac{h}{\Delta t}$
- Tiny capacitor → Δt is the time constant, therefore for a RC circuit:
- $\Delta t = R_t C_{dot}$
- How to make sure that no tunneling occurs?
- Uncertainty of charging energy must be less than the charging energy.

$$\Delta E < E_c \qquad \frac{h}{\Delta t} < \frac{e^2}{2C_{dot}} \qquad \frac{h}{R_t C_{dot}} < \frac{e^2}{2C_{dot}}$$

- Therefore, the second requirement for a SET to work is: $R_t \gg \frac{h}{e^2}$
- To meet this last criterion it is usually enough to make sure that the insulating layer is thick enough.

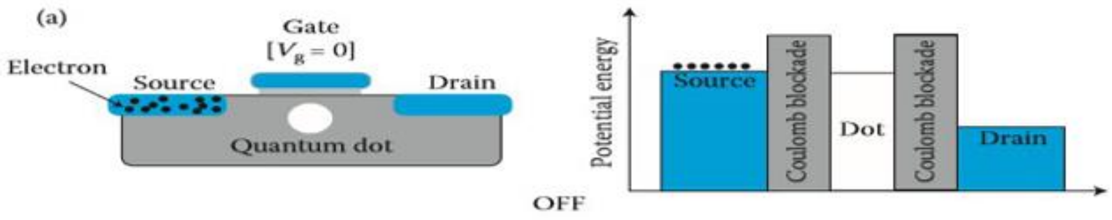
WORKING OF SET

In SET we can individually control the tunneling of electron into and out of quantum dot. In FET the gate voltage creates an electric field and changes the conductivity of semiconducting channel. Therefore the current flow from source to drain. In SET applying voltage to gate creates electric field which changes the potential energy of the dot. This gate voltage controlled Potential difference can make electron attracted from source to dot and then to drain. For current to flow this gate bias voltage must be larger than coulomb blockade.

Coulomb blockade: It prevents unwanted tunneling when charging energy is much higher than the thermal energy of electron.

A) OFF CONDITION

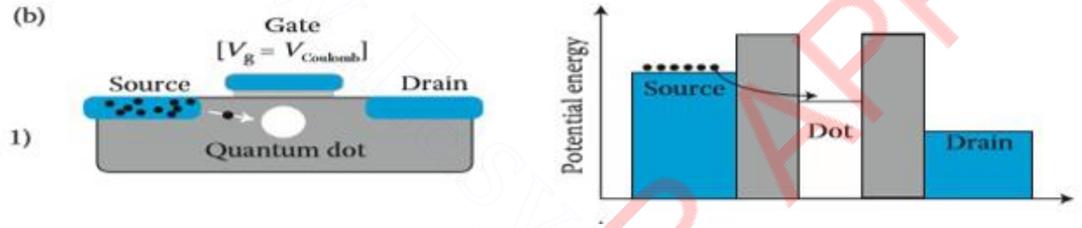
The corresponding potential energy shows it is not energetically favorable for electrons in source to tunnel to the dot.



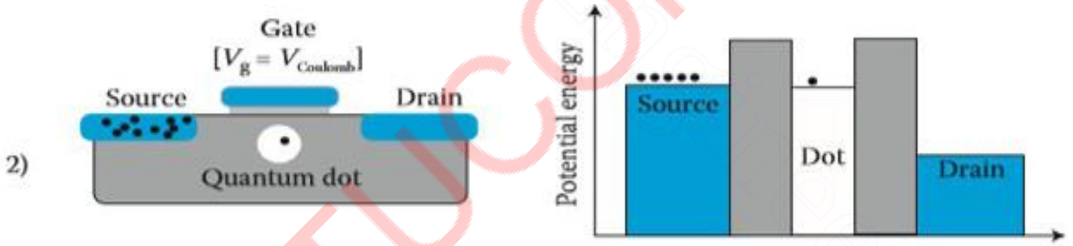
B) ON MODE

At lowest setting, electrons tunnel one at a time, source to tunnel through the dot.

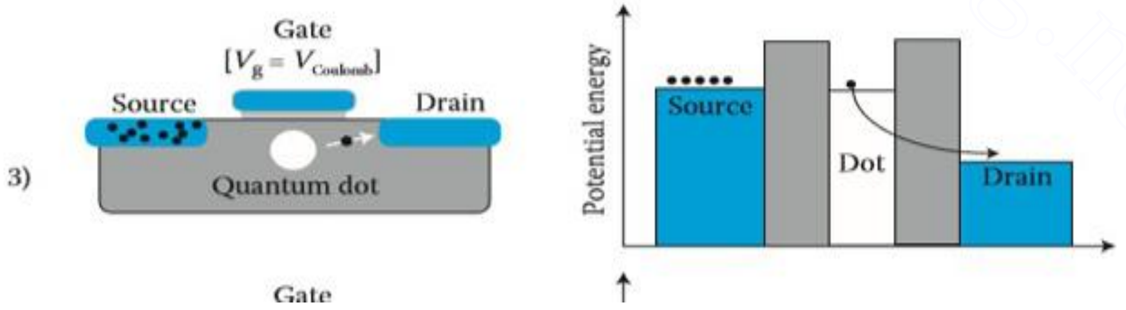
1) This is made possible by first applying proper gate voltage - Potential energy of the dot is made low so that electrons can tunnel through the energy barrier to Quantum dot.



2) Once Quantum dot gets an electron it potential energy rises.

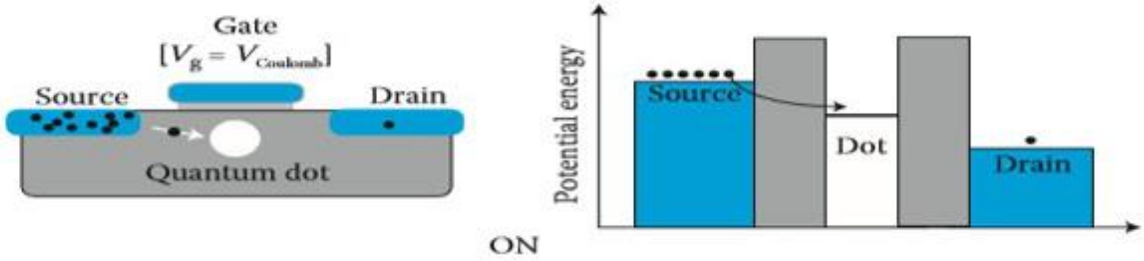


3) The electron then tunnels through the coulomb barrier on the other side to reach the lower potential energy at the drain.



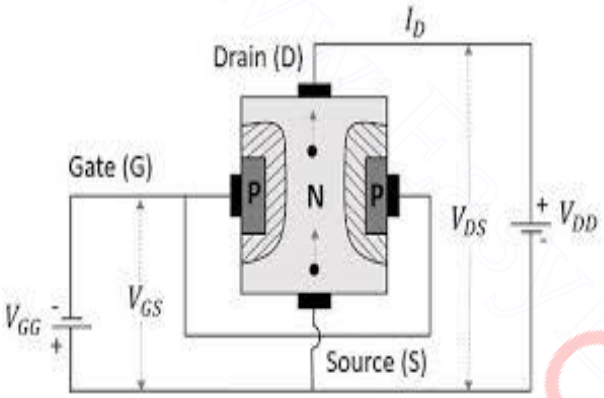
4) With the quantum dot empty the potential energy lowers again and the process repeats

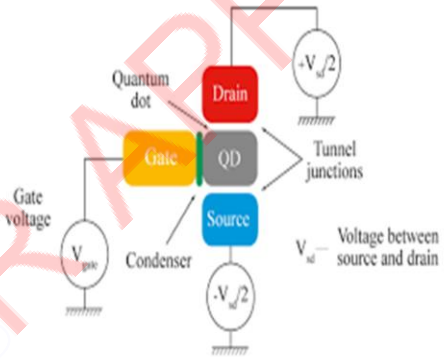
4)



Difference between ordinary transistor and single electron transistor

- ❖ In FET semiconductor diode is placed between source and drain
- ❖ In SET quantum dot is placed between source and drain.





LIMITATIONS

- ➢ In order to operate SET circuit at room temperature, the size of the quantum dot should be smaller than 10 nm.
- ➢ It is very hard to fabricate by traditional optical lithography and semiconductor process.
- ➢ The methods must be developed for connecting the individual structures into logic circuits and these circuits must be arranged into larger 2D patterns.

ADVANTAGES OF SET

- ❖ It consumes less power for operation.
- ❖ The coulomb blockade effect: an alternative operating principle for nanometre-scale devices.
- ❖ It reduces circuit power dissipation.
- ❖ It raises the possibility of even higher levels of circuit integration.

APPLICATIONS OF SET

- The main fields of application of the single electron transistor is used in sensor technology and digital electronic circuits.
- A variety of digital logic functions, including AND or NOR gates, is obtained based on SET operating at room temperature.
- It is used for mass data storage.
- It is used in highly sensitive electrometer.
- SET can be used as a temperature probe, particularly in the range of very low temperatures.
- SET is a suitable measurement set-up for single electron spectroscopy.
- It is used for the fabrication of a homo-dyn receiver operating at frequencies between 10 and 300 MHz.

SEMICONDUCTOR PHOTONIC STRUCTURES

Photonic crystals: Photonic crystals are spatially a periodic structures of dielectric materials with different refractive indices. It is a medium in which refractive index varies periodically on the order of wavelength of light. They can guide the motion of photons using the photonic bandgap. They are mode from periodic patterns of materials with different permittivities.

When a photon travels through an interface between two materials of different permittivity, the photon may be reflected. The reflection depends on the arrangement of atoms in a material's crystal lattice. The photons of certain wavelength pass through the material, while photons of a specific range of wavelengths will be reflected. This represents the photonic band gap that is a range of photon wavelengths (frequencies) are forbidden making them suitable for light harvesting applications.

Examples

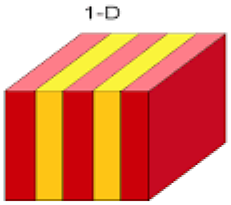
1. Photonic crystals usually occur in nature in the form of structural coloration and animal reflectors which are very useful in a wide range of applications.
2. Wings of some butterflies contain photonic crystals and hence they show different colors due to their structure, which can selectively reflect certain band of wavelength.
3. The opal in the bracelet contains a natural periodic microstructure responsible for its iridescent color. It is essentially a natural photonic crystal.

TYPES OF PHOTONIC CRYSTALS

There are 3 types of photonic crystals. They are

i. 1D Photonic crystal
ii. 2D Photonic crystal
iii. 3D photonic crystal

1D PHOTONIC CRYSTAL



A 1D Photonic crystal is a one-dimensional virtual medium, whose refractive index has periodic modulation in one dimension.

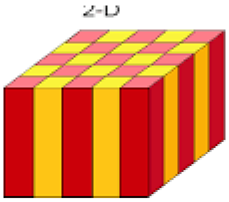
To produce a one-dimensional photonic crystal, thin film layers of different dielectric constant may be periodically deposited on a surface which leads to a band gap in a particular propagation direction (such as normal to the surface)

EXAMPLE: A Bragg grating is an example of this type of photonic crystal. One-dimensional photonic crystals can include layers of non-linear optical materials. The non-linear behavior is provides field enhancement at wavelengths near degenerate band edge.

APPLICATIONS

1. A graphene-based Bragg grating (one-dimensional photonic crystal) supports excitation of surface electromagnetic waves in the periodic structure by using 633 nm He-Ne laser as the light source.
2. A one-dimensional graphene-dielectric photonic crystal can act as a far-IR filter and can support low-loss surface plasmons for waveguide and sensing applications.
3. 1D photonic crystals doped with bio-active metals (i.e. silver) have been also proposed as sensing devices for bacterial contaminants.
4. A planar 1D photonic crystals made of polymers have been used to detect volatile organic compounds vapors in atmosphere.
5. 1D Photonic crystals are used in antireflection coatings by decreasing the reflectance and improving the quality of the lenses.

2D PHOTONIC CRYSTAL



A 2D Photonic crystal is a two-dimensional virtual medium, whose refractive index has periodic modulation in two dimension.

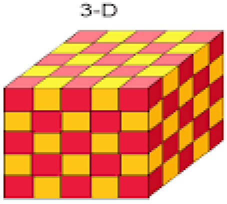
To produce a one-dimensional photonic crystal, holes may be drilled in a substrate that is transparent to the wavelength of radiation and the bandgap is designed to block the modes. Triangular and square lattices of holes have been successfully employed.

EXAMPLE: The **Holey fiber** or photonic crystal fiber can be made by taking cylindrical rods of glass in hexagonal lattice, and then heating and stretching them, the triangle-like air gaps between the glass rods become the holes that confine the modes.

APPLICATIONS

1. 2D photonic crystals show total internal reflection in the hollow core inorder to propagate light which you cannot see in normal fiber optics.
2. They are also used in non-linear devices and to guide exotic wavelengths.

3D PHOTONIC CRYSTAL



A 3D Photonic have periodic modulation along three different axes. They reflect light that incident from any direction and behave as a highly directional reflective. Further theses crystals will control and manipulate the light flow.

In a 3D photonic crystal, the dielectric constant is a tailor made to vary periodically in three dimensions, giving rise to the so called photonic bandgap which prohibits electromagnetic wave propagation and substantially modifies the dispersion around a specific wavelength region.

The woodpile structure – “rods” are repeatedly etched with the beam lithography, filled in, and covered with a layer of new material. As the process repeats, the channels etched in each layer are perpendicular to the layer below and parallel to and out phases with the channels two layers below.

The process repeats until the structure is of desired height. The fill-in material is then dissolved using an agent that dissolves the fill-in material but not the deposition material. It is generally hard to introduce defects into this structure.

EXAMPLE: The three dimensional woodpile structure and Spheres in a diamond lattice

APPLICATIONS

1. A 3D optical microchip can guide light through air regions in a 3D circuit such as the sunlight is trapped and absorbed as it flows indifferent patterns.
2. 3D metallic photonic crystals are used to investigate various photonic transport phenomenon and has a wide range of applications in thermophoto voltaics.

OPTOELECTRONIC DEVICES

Optics and electronics form a new branch of study called as optoelectronics, which includes the design and manufacture of a hardware device that converts electrical energy into light energy and vice-versa through semiconductors.

TYPES OF OPTOELECTRONICS DEVICES

There are two types of optoelectronic devices

(i) Active optoelectronic devices
(ii) Passive optoelectronic devices

ACTIVE OPTOELECTRONIC DEVICES

In active optoelectronic devices, the light intensity can be directly varied in accordance with applied input voltage source the external light is not needed for its working.

Example:

1. Light Emitting Diode (LED)
2. Laser Diode
3. Quantum well modulator
4. Self-electro optic effect switches

PASSIVE OPTOELECTRONIC DEVICES

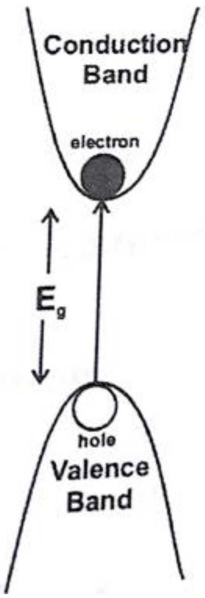
In passive optoelectronic devices, the light intensity is not changed by controlling voltage. On the other hand, the plane of polarization is turned by the application of control voltage. In passive optoelectronic devices, the external light source such as polarizer and analyzer are required.

Example:

1. Kerr cell
2. NLO crystals
3. Laser Doppler velocimetry
4. Displacement sensor

PHOTO PROCESSES

The operation of almost all optoelectronic devices is based on the creation or annihilation of electron – hole pairs so called photo process. Pair formation essentially involves raising an electron from the valence band to the conduction band thereby leaving a hole behind the valence band.



In principle, any energetic particle with energy equal to the band gap, when incident on a semiconductor, will make the valence electron to move to the conduction band, thereby creating electron-hole pairs. The simplest way to create electron-hole pair is to irradiate the semiconductor. Photons with sufficient energy are absorbed and these impart their energy to the valence band electrons and raise them to the conduction band. This process, is therefore called absorption.

The reverse process is electron-hole recombination, give up its excess energy. The recombination may be of two types. They are

(i) Non-radiative transition process

(ii) Radiative transition process

NON-RADIATIVE TRANSITION PROCESS: In a non-radiative transition process, the excess energy due to recombination is usually imparted to photons and dissipated in the form of heat.

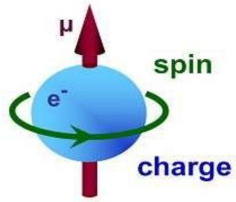
RADIATIVE TRANSITION PROCESS: In a radiative transition process, the excess energy is dissipated as photons usually having energy equal to bandgap energy. This is called as luminescent process and hence emits light.

Examples:

1. Photo-luminescence is the process in which electron-hole pairs are created by injection of photons.
2. Cathode-luminescence is the process in which electron-hole pairs are created by electron bombardment.
3. Electro-luminescence is the process in which electron-hole pairs are created in a p-n junction.

SPINTRONICS - SPIN-BASED ELECTRONICS

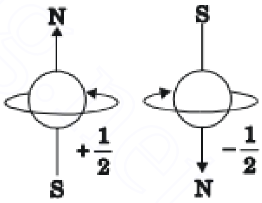
Spintronics is a NANO technology which deals with spin dependent properties of an electron instead of charge dependent properties



Spintronics uses electron spins in addition to or in place of the electron charge. The rotational moment creates a small magnetic field. Key concept is controlling the spin of electrons. Spintronics is intrinsic spin of the electron + its associated magnetic moment + its fundamental electronic charge.

PRINCIPLE:

- Origin of the spin is electron's intrinsic property "angular momentum"
- Every electron exists in one of the two sates – spin up and spin down, with spins either positive half or negative half.
- In other words, electrons can rotate either clock wise or anti-clockwise around its own axis with constant frequency.
- The two possible spin states represent '0'and'1' in logical operations.



EXPLANATION: Spin is a characteristic that makes an electron a tiny magnet with north and south poles. The orientation of north-south axis depends on the particle's axis of spin. Every electron exist in one of the two states spin- up and spin-down, with spins either positive half or negative half.

In ordinary materials, the up magnetic moments cancel the down magnetic moment so no surplus moment piles up. Ferro-magnetic materials like iron, cobalt and nickel is needed for designing of spin electronic devices.

These have tiny regions called domains in which an excess of electrons have spins with axis pointing either up or down. The domains are randomly scattered and evenly divided between majority-up and majority-down. But, an externally applied magnetic field will line up the domains in the direction of the field. This results in a permanent magnet.

WORKING

All Spintronics devices acts according to the simple scheme.

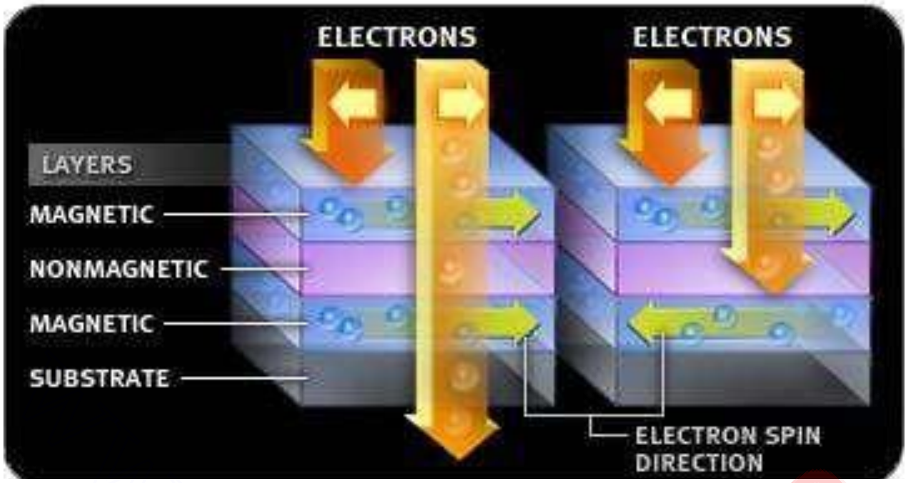
1. The information is stored into spins as a particular spin orientation (up or down).
2. The spins, being attached to mobile electrons, carry information along a wire and the information is read at the terminal.
3. Spin orientation of conduction electrons survives for relatively long time (nanoseconds, compared to tens of femto seconds during which electron moment decays) which makes spintronic device useful for memory storage and magnetic sensor applications.
4. They are used for quantum computing where electron spin will represent a bit of information. When electron spins are aligned, this creates a large scale net magnetic moment.

APPLICATIONS OF SPINTRONICS

GIANT MAGNETORESISTANCE

Definition: *Giant magnetoresistance is a quantum mechanical phenomenon in which electrons travelling in ultra-thin magnetic film multilayer structures experience large scattering according to their spin states which give rise to correspondingly large changes in electrical resistance.*

The basic GMR device consists of a layer of non -magnetic metal between two magnetic layers. A current consisting of spin-up and spin-down electrons is passed through the layers. Those oriented in the same direction as the electron spins in a magnetic layer pass through quite easily while those oriented in the opposite direction are scattered.



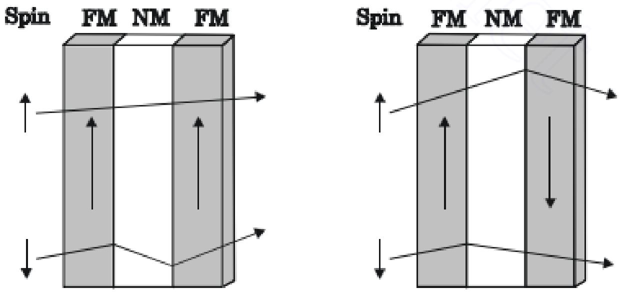
WORKING

Each ferromagnetic layer has a magnetization vector M, and when these vectors are parallel, an electric current can pass through the device. This is due to serval reasons.

1. First, since the spacer layer is thin, spin can be diffuse across the spacer to read, the other ferromagnetic layer.
2. Since that material’s magnetization is parallel to the magnetization of the first layer, the density of states for those spin electrons is relatively high, and so there is low scattering.
3. Thus, the flow of electrons can occur, resulting in a low electrical resistance. However, if the magnetization vector of the second ferromagnetic material is antiparallel with that of the first material, the majority spin electrons and spin scattering is high.
4. This is reflected by a much larger resistance to current flow.
5. The resistance to the current flow is magneto resistance, and the percentage ratio of the large and small resistance values is called GMR ratio.

SPIN VALVE

A spin valve is a device which provides the Giant Magneto resistive effect. The device can be made to be highly resistive or highly conductive depending on the direction of the applied magnetic fields in the conducting layers. This technology offers very fast switching speeds and reduced power consumption.



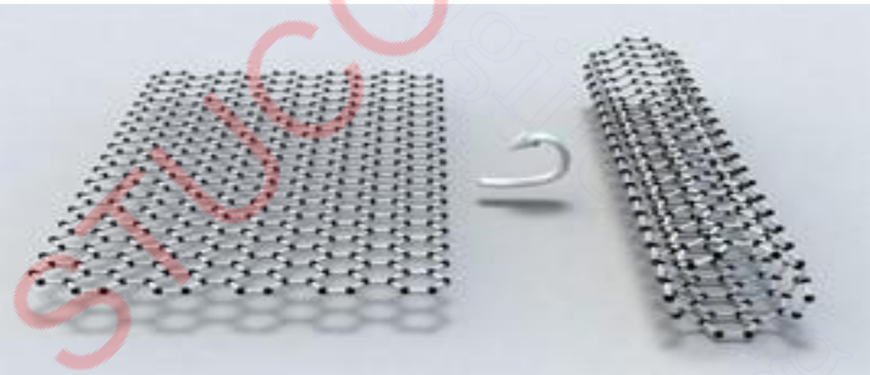
FM - Ferromagnetic; NM-Non-magnetic

ADVANTAGE OF SPINTRONICS

- Low power consumption.
- Less heat dissipation.
- Spintronic memory is non-volatile.
- Takes up lesser space on chip, thus more compact.
- Spin manipulation is faster, so greater read & write speed. Spintronics does not require unique and specialized semiconductors. Common metals such as Fe, Al, Ag, etc. can be used.

CARBON NANOTUBES (CNT)

CNTs are long, thin cylinders of carbon. They can be thought of as a sheet of graphite (a hexagonal lattice of carbon) rolled into a cylinder. Nanotubes have been constructed with length-to-diameter ratio of up to 132,000,000:1. CNTs were discovered in 1991 by Sumio Iijima. The structure of CNT is formd by a layer of carbon atoms that are bonded together in a hexagonal (honeycomb) mesh. This one-atom thick layer of carbon is called *graphene*, and it is wrapped in the shape of a cylinder and bonded together to form a carbon nanotube.

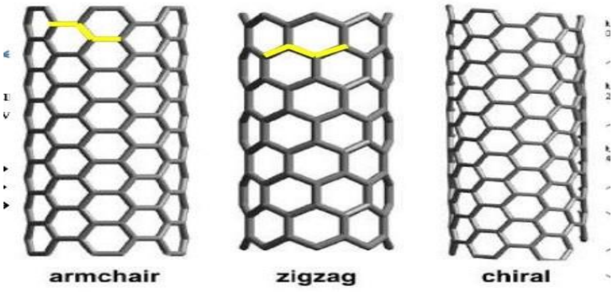


TYPES OF CARBON NANOTUBES

Nanotubes can have a *single outer wall* of carbon, or they can be made of *multiple walls* (cylinders inside other cylinders of carbon). Accordingly they are called:

- Single-walled carbon nanotube
- Multi-walled carbon nanotube

STRUCTURE OF CARBON NANOTUBES



The CNT's have many structures on the basis of their length, type of spiral and number of layers. Their electrical properties depends on their structure and they act as both a metal and a semiconductor. There a variety of structures of carbon nanotubes with different properties.

Three types of nanotube structures are considered by rolling a graphite sheet with different orientations about the axis. They are

- Armchair structure
- Zig-Zag structure
- Chiral structure

Armchair structure – when the axis of the tube parallel to C – C bonds of the carbon hexagons, it is referred to as "armchair" structure.

Zig-zag structure – when the axis of the tube is perpendicular to C – C bonds of the carbon hexagons, it is referred to as "Zig-zag" structure.

Chiral structure – when the axis of the tube is inclined towards C – C bond, it is referred to as "Chiral" structure.

PROPERTIES OF CNT'S

1. **Mechanical Properties**: The Carbon nanotubes are highly elastic. The Young's modulus is directly a measure of the elasticity. The Young's modulus of carbon nanotubes is about 1800 GPa whereas it is about 210 GPa for steel. CNT's exhibit large strength in tension. They are about twenty times stronger than steel. The yield strength is a measure of the strength. Carbon nanotubes can withstand larger strains than steel. They can be bent without breaking.
2. **Electrical Properties**: The electrical properties of CNT's depends on their diameter and chirality. They show electrical properties ranging from semiconductors to those of good conductors. The energy gap decreases as the diameter of the CNT is increased. Due to very low resistivity, the heat dissipation in the CNT is very small and hence they can carry very

larger current than metals. The conductivity of the CNT is maximum along its axis and very low in a perpendicular direction. Hence they are very equivalent to one dimensional conductors. At low temperatures, the resistance decreases with increasing magnetic field applied across the CNT. This effect is known as magnetoresistance.

3. **Thermal Properties**: Carbon nanotubes are very good conductors of heat. Their thermal conductivity is more than twice that of diamond. The thermal conductivity also varies with direction. The conductivity is very good along the axis of the tube and very low in a perpendicular direction.
4. **Physical Properties**: CNT's have very high strength to weight ratio. They have low density.
5. **Chemical Properties**: CNT's are more chemically inert compared to other forms of carbon.

APPLICATIONS OF CNT'S

1. Carbon nanotubes can store lithium due to which they can be used in batteries. CNT's also store hydrogen and find potential applications in fuel cells.
2. They are use in tips for atomic force microscope probes.
3. They are being used to develop flat panel displays for television and computer displays.
4. They are being used to develop light weight shield for electromagnetic radiation.
5. Field effect transistors are being developed using semiconductor CNT's which can be used to build faster processors for computers. It is estimated that these processors will be 10^4 times faster than the present processors.
6. CNT's are being used to produce lightweight materials with higher strength than steel. These can be used in automobile, aircraft and rocket parts.
7. They are used in chemical sensors to detect gases.

OPTICS IN QUANTUM STRUCTURES

Quantum Structures: Quantum structures are the structures in which the electrons are confined to move in one, two or three dimensions which led to new physical discoveries and technological applications.

Semiconductor quantum structure \s with their unique properties make it possible to observe many optical effects in low dimensional electron system and to discover their novel features.

Optics in quantum structures

Optical experiments are the powerful tools for the characterization of heterostructure. Further, heterostructure will enhance a set of new effects which do not occur in the bulk materials. The electronic properties, lattice parameters, surface quality, optical and electrical properties are most important in the field of modern solid-state devices. Many of these properties shall be microscopically analyzed with the help of modern optics as a tool in the study of quantum structures.

These specific features of optical processes originate from two basic physical peculiarities, viz.,

(i) The behavior of the electromagnetic waves in hetrostructures is different from bulk materials. The spatial non-uniformity affects the specific characterization of interaction of light with matter like light propagation, absorption etc.,

(ii) Electron in the quantum structure have energy spectra which are different from those of electrons in the bulk materials.

APPLICATIONS

1. Quantum optics is useful in quantum information processing and quantum communication.
2. It is also used to demonstrate quantum teleportation between atomic systems over longer distances.
3. Quantum optics is a key for all emerging technologies like sensing, imaging, simulation computation etc.,

QUANTUM WELL LASER

A quantum well laser is a laser diode in which the active region of the device is very narrow so that quantum confinement occurs. Laser diodes are formed in compound semiconductor materials and it can emit light efficiently. The wavelength of light emitted by quantum well laser depends on the width of the active region rather than the bandgap of the materials.

Types or Quantum Well Laser

There are two types of quantum well laser based on the number of active regions.

1. Single-quantum-well Laser (SQWL) – consists of one active region

2. Multi-quantum-well Laser (MQWL) - consists of multiple active region

A quantum well laser is shown in fig. The active laser (GaAs) is in between p-type AlGaAs and n-type AlGaAs. The metal contacts are provided to bias the QWL. In this laser the current is confined to narrow strip. It will limit the amount of current flowing in the laser, and thus prevent thermal damage to the semiconductor.

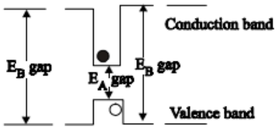


Fig. 5.29 Quantum well laser structure.

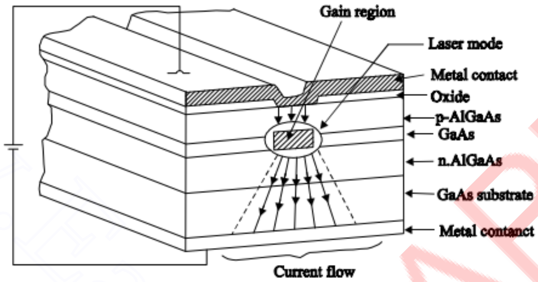


Fig. 5.30 Energy band in quantum well laser

This, also limit the laser gain region and in turn the dimension of the laser mode in the lateral direction. So, when the current flows through the layers of the semiconductor into the active region, it produces gain only in a narrow Gaussian-shaped stripe.

WORKING: In quantum-well lasers, the active layer is made thinner than 10 nm. Therefore, the electronic and the optical properties are drastically altered due to the reduced dimensionality. Thus, the motion of the free electrons are confined in one direction and free other two mutually perpendicular directions. The electron confinement results in a quantization in the permitted energy levels.

$$E_n = \frac{n^2 h^2}{8\,mL^2}$$

Here, h is Planck's constant, m the effective mass of the electrons, n an integer and L, the thickness of the quantum well. The valence band also can have discrete energy levels. The variation of spacing of the band-gap in semiconductor materials can vary the wavelength of laser emission. It can be made by using different bandgap semiconductor in active region.

The wavelength of the laser can be changed by:

(a) Varying the thickness of the quantum-well.

(b) Varying the composition of the quantum-well. This happens due to the .change in the energy band-gap.

ADVANTAGES OF QUANTUM WELL LASERS

Quantum well lasers have attracted a great deal of attention by their many advantages such as

- Higher efficiency
- Low threshold current density.
- Excellent temperature feature
- High modulation bandwidth and
- Wavelength adjustability etc.

APPLICATIONS OF QUANTUM WELL LASER

Quantum-well (QW) active semiconductor lasers enjoy widespread commercial use in

- Optoelectronic applications ranging from high-power sources for medical therapy
- Material processing
- Laser printing, and pumps for solid-state laser to lower output power single-mode
- Single-mode single-frequency sources for telecommunications.