

## COURSE INFORMATION SHEET

PROGRAMME: <b>B.TECH COMPUTER SCIENCE ENGINEERING</b>	
COURSE: <b>ENGINEERING PHYSICS</b>	Semester : <b>I</b> CREDITS: <b>3</b>
COURSE CODE: <b>R231101</b> REGULATION: <b>R23</b>	COURSE TYPE (CORE /ELECTIVE / BREADTH/ S&H): <b>CORE</b>
COURSE AREA/DOMAIN: <b>DESIGN</b>	PERIODS: <b>5</b> Per Week.

### COURSE PRE-REQUISITES:

C.CODE	COURSE NAME	DESCRIPTION	SEM
<b>R231101</b>	<b>ENGINEERING PHYSICS</b>	Knowledge of Light,sound,Electricity,and Magnetism	<b>I</b>

### COURSE OUTCOMES:

S.NO	COURSE OUTCOME STATEMENT
CO1	<b>Analyze:</b> the intensity variation of light due to polarization, interference and diffraction.
CO2	<b>Design,</b> : Familiarize with the basics of crystals and their structures.
CO3	<b>Develop</b> : Explain fundamentals of quantum mechanics and apply it to one dimensional motion of particles.
CO4	<b>Apply</b> : Summarize various types of polarization of dielectrics and classify the magnetic materials.
CO5	<b>Recognize</b> : Explain the basic concepts of Quantum Mechanics and the band theory of solids. Identify the type of semiconductor using Hall effect.

### SYLLABUS:

UNIT	DETAILS
<b>I</b>	Wave Optics Interference: Introduction - Principle of superposition –Interference of light - Interference in thin films (Reflection Geometry) & applications - Colours in thin films- Newton’s Rings, Determination of wavelength and refractive index. Diffraction: Introduction - Fresnel and Fraunhofer diffractions - Fraunhofer diffraction due to single slit, double slit & N-slits (Qualitative) – Diffraction Grating - Dispersive power and resolving power of Grating (Qualitative). Polarization: Introduction -Types of polarization - Polarization by reflection, refraction and Double refraction - Nicol’s Prism - Half wave and Quarter wave plates.
<b>II</b>	<b>Crystallography and X-ray diffraction</b> Crystallography: Space lattice, Basis, Unit Cell and lattice parameters – Bravais Lattices – crystal systems (3D) – coordination number - packing fraction of SC, BCC & FCC - Miller indices – separation between successive (hkl) planes. X-ray diffraction: Bragg’s law - X-ray Diffractometer – crystal structure determination by

	Laue's and powder methods polarizations (Qualitative)
<b>III</b>	<p><b>Dielectric and Magnetic Materials</b>  Dielectric Materials: Introduction - Dielectric polarization - Dielectric polarizability, Susceptibility, Dielectric constant and Displacement Vector – Relation between the electric vectors - Types of polarizations- Electronic (Quantitative), Ionic (Quantitative) and Orientation - Lorentz internal field - Clausius- Mossotti equation - complex dielectric constant – Frequency dependence of polarization – dielectric loss</p> <p>Magnetic Materials: Introduction - Magnetic dipole moment - Magnetization-Magnetic susceptibility and permeability – Atomic origin of magnetism - Classification of magnetic materials: Dia, para, Ferro, anti-ferro &amp; Ferri magnetic materials - Domain concept for Ferromagnetism &amp; Domain walls (Qualitative) - Hysteresis - soft and hard magnetic materials.</p>
<b>IV</b>	<p><b>Quantum Mechanics and Free electron Theory</b>  Quantum Mechanics: Dual nature of matter – Heisenberg's Uncertainty Principle – Significance and properties of wave function – Schrodinger's time independent and dependent wave equations– Particle in a one-dimensional infinite potential well.</p> <p>Free Electron Theory: Classical free electron theory (Qualitative with discussion of merits and demerits) – Quantum free electron theory – electrical conductivity based on quantum free electron theory - Fermi-Dirac distribution - Density of states - Fermi energy</p>
<b>V</b>	<p><b>Semiconductors</b>  Semiconductors: Formation of energy bands – classification of crystalline solids - Intrinsic semiconductors: Density of charge carriers – Electrical conductivity – Fermi level – Extrinsic semiconductors: density of charge carriers – dependence of Fermi energy on carrier concentration and temperature - Drift and diffusion currents – Einstein's equation – Hall effect and its applications.</p>

<b>TEXT BOOKS</b>	
<b>T</b>	<b>BOOK TITLE/AUTHORS/PUBLISHER</b>
T1	A Text book of Engineering Physics, M. N. Avadhanulu, P.G.Kshirsagar & TVS Arun Murthy, S. Chand Publications, 11th Edition 2019.
T2	Engineering Physics - D.K.Bhattacharya and Poonam Tandon, Oxford press (2015)
<b>REFERENCE BOOKS</b>	
<b>R</b>	<b>BOOK TITLE/AUTHORS/PUBLISHER</b>
R1	Engineering Physics - B.K. Pandey and S. Chaturvedi, Cengage Learning 2021.
R2	Engineering Physics - Shatendra Sharma, Jyotsna Sharma, Pearson Education, 2018.
R3	Engineering Physics" - Sanjay D. Jain, D. Sahasrabudhe and Girish, University Press. 2010
R4	Engineering Physics - M.R. Srinivasan, New Age international publishers (2009).

**TOPICS BEYOND SYLLABUS/ADVANCED TOPICS:**

<b>S.NO</b>	<b>DESCRIPTION</b>	<b>Associated PO &amp; PSO</b>
1	Lasers and its applications	PO1,PO2, PO4, PSO1

**WEB SOURCE REFERENCES:**

1	<b>UNIT I</b> <a href="https://www.loc.gov/rr/scitech/selected-internet/physics.html">https://www.loc.gov/rr/scitech/selected-internet/physics.html</a>
2	<b>UNIT II :</b> <a href="https://www.loc.gov/rr/scitech/selected-internet/physics.html">https://www.loc.gov/rr/scitech/selected-internet/physics.html</a>
3	<b>UNIT III :</b> <a href="https://www.loc.gov/rr/scitech/selected-internet/physics.html">https://www.loc.gov/rr/scitech/selected-internet/physics.html</a>
4	<b>UNIT IV :</b> <a href="https://www.loc.gov/rr/scitech/selected-internet/physics.html">https://www.loc.gov/rr/scitech/selected-internet/physics.html</a>
5	<b>UNIT V :</b> <a href="https://www.loc.gov/rr/scitech/selected-internet/physics.html">https://www.loc.gov/rr/scitech/selected-internet/physics.html</a> .

# UNIT-1

## INTERFERENCE

### PRINCIPLE OF SUPERPOSITION:

“This principle states that the resultant displacement of a particle of the medium acted upon by two or more waves simultaneously is the algebraic sum of the displacements of the same particle due to the individual waves in the absence of the others”.

Suppose due to a single wavetrain the displacement of the particle at a certain point at any instant is  $Y_1$  in a given direction and that due to another wavetrain, the displacement is  $Y_2$  in the absence of the first.

According to the principle of superposition, the instantaneous resultant displacement  $R$  of the particle due to two waves acting together is expressed by,

$$R = Y_1 + Y_2$$

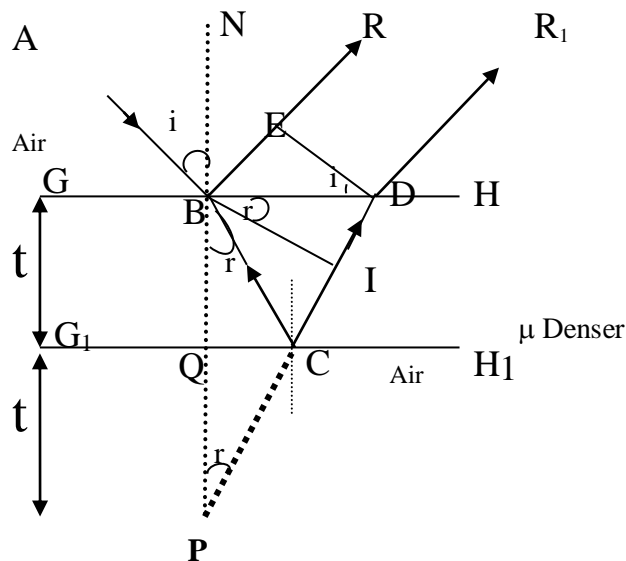
If the two displacements are in opposite directions, the instantaneous resultant displacement due to two waves acting together is expressed by,

$$R = Y_1 - Y_2$$

### INTERFERENCE OF LIGHT:

The modification in the distribution of intensity of light in the region of superposition is called interference.

### INTERFERENCE IN THIN FILMS BY REFLECTION:



Let  $GH$  &  $G_1H_1$  be the two surfaces of a transparent film of uniform thickness  $t$  and refractive index  $\mu$ . Suppose a ray  $AB$  of monochromatic light be incident on its upper surface. This ray is partly reflected along  $BR$  and refracted along  $BC$ . After one internal reflection at  $C$ , we obtain the

ray CD. After refraction at D, the ray finally emerges out along DR<sub>1</sub> in air. Obviously, DR<sub>1</sub> is parallel to BR. Draw a normal DE on BR and normal BI on DC. We also produce DC in the backward direction which meets the BQ produced at P.

In figure,  $\angle ABN = i$  the angle of incidence

$\angle QBC = r$  angle of refraction

from the geometry of figure  $\angle BDE = i$ ,  $\angle QPC = r$

the optical path difference between the two reflected light rays (BR<sub>1</sub> & DR<sub>2</sub>) is given by

$\Delta = \text{path } (BC+CD) \text{ in film} - \text{path } BE \text{ in air}$

$$= \mu (BC+CD) - BE \longrightarrow (1)$$

we know that  $\mu = \sin i / \sin r = (BE/BD) / (ID/BD) = BE/ID$

$$BE = \mu ID \longrightarrow (2)$$

from eqs (1) & (2)

$$\Delta = \mu (BC+CD) - \mu (ID)$$

$$= \mu (BC+CI+ID) - \mu (IFD)$$

$$= \mu (BC+CI)$$

$$= \mu (PI) \quad (BC=PC) \longrightarrow (3)$$

$$\Delta^{\text{le}} BPI, \cos r = PI/BP$$

$$PI = BP \cos r = 2t \cos r \longrightarrow (4)$$

substituting the value of PI from eq (4) in eq(3) we have

$$\Delta = 2\mu t \cos r \longrightarrow (5)$$

the optical path difference given by eq (5) is usually called as **Cosine law**.

**Note: cosine law** : It should be remembered that a ray reflected at a surface backed by a denser medium suffers an abrupt phase change of  $\pi$  which is equivalent to a path difference  $\lambda/2$ .

Thus the effective path difference between the two rays is  $(2\mu t \cos r \pm \lambda/2)$  we know that maxima occurs when the effective path difference  $\Delta = n\lambda$

$$\text{i.e } 2\mu t \cos r \pm \lambda/2 = n\lambda$$

$$2\mu t \cos r = (2n \pm 1)\lambda/2$$

if this condition is fulfilled, the film will appear bright in the reflected light. The minima occurs when the effective path difference is  $(2n \pm 1)\lambda/2$

$$\text{i.e } 2\mu t \cos r \pm \lambda/2 = (2n \pm 1)\lambda/2$$

$$2\mu t \cos r = (2n \pm 1)\lambda/2 \pm \lambda/2 = n\lambda$$

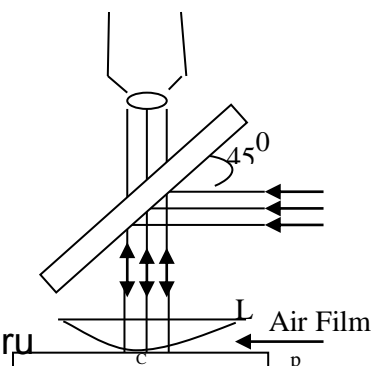
### NEWTON'S RINGS :

when a plano-convex lens with its convex surface is placed on a plane glass plate, an air film of gradually increasing thickness is formed between the two. If monochromatic light is allowed to fall normally then alternate dark and bright rings concentric around the point of contact between the lens and glass plate are seen. Since the phenomenon was first described by Newton that is why the rings are known as Newton's Rings after his name.

Microscope

### **Experimental arrangement**

The experimental arrangement of obtaining Newton's rings is shown. L is a plano convex lens of radius of large curvature. This lens with its convex surface is placed on a plane glass P. The lens makes contact with the plate at C. Light from



an extended monochromatic source such as sodium lamp falls on a glass plate G held at an angle of  $45^\circ$  with the vertical. The glass plate G reflects normally a part of the incident light towards the air film enclosed by the lens L and the glass plate p

A part of the incident light is reflected by the curved surface of the lens L and a part is transmitted which is reflected back from the plane surface of the plate. These two reflected rays interfere and give rise to an interference pattern in the form of circular rings. These rings are localised in the air film and can be seen with a microscope focussed on the film.

### Explanation of the formation of Newton's Rings

AB is monochromatic ray of light which falls on the system part is reflected at C, which goes out in the form of rays 1 without any phase reversal. The other part is refracted along CD. At point D, it is again reflected and goes out in the form of ray 2 with a phase reversal of  $\pi$ . The reflected rays 1 & 2 are in a position to produce interference. The path difference between them is  $(2\mu t \cos r + \lambda/2)$  for air film  $\mu = 1$  and for normal incidence  $r = 0$ , the path difference is  $(2t + \lambda/2)$ . At the point of contact  $t=0$ , and the path difference is  $\lambda/2$ , which is the condition of minimum intensity. Thus the central spot is dark. For  $n^{\text{th}}$  maximum, we have

$$(2t + \lambda/2) = n\lambda$$

This expression shows that a maximum of a particular order  $n$  will occur for a constant value of  $t$ . In this case  $t$  remains constant along a circle, the maximum in the form of a circle. For different values of  $t$ , different maxima will occur.

### Newton's Rings by reflected light :

Now we shall calculate the diameters of dark and bright rings. Let  $L O L^1$  be the lens placed on a glass plate AB. The curved surface  $L O L^1$  is the part of spherical surface with centre at C. Let  $R$  be the radius of curvature and  $r$  be the radius of Newton's ring corresponding to the constant film thickness  $t$ . As discussed above

$$2t + \lambda/2 = n\lambda$$

$$2t = (2n-1)\lambda/2 \quad \text{for bright ring, where } n=1,2,3,\dots\text{etc}$$

$$2t = n\lambda \quad \text{for dark ring, where } n=0,1,2,3,\dots\text{etc}$$

from the **property of the circle**,

$$NP \times NQ = NO \times ND$$

substituting the values

$$r * r = t(2R-t)$$

$$= 2Rt - t^2$$

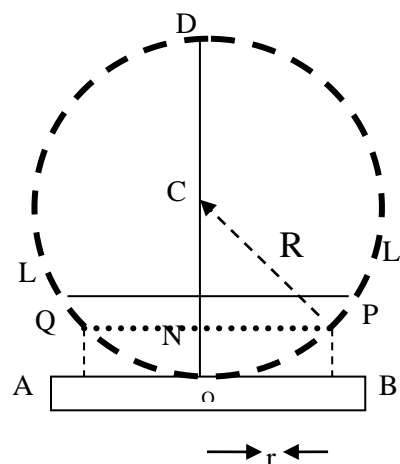
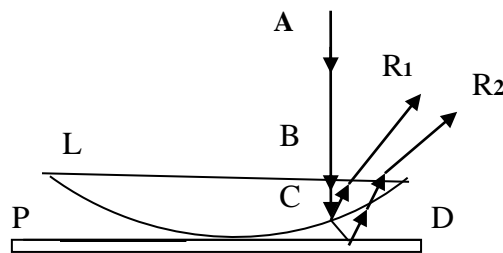
$$= 2Rt$$

$$\therefore r^2 = 2Rt \quad (\text{or}) \quad t = r^2/2R$$

thus for a **bright ring**

$$2 \frac{r^2}{2R} = (2n-1) \lambda / 2$$

$$r^2 = R(2n-1) \lambda / 2$$



Replacing  $r$  by  $D/2$ , we get the diameter of  $n^{\text{th}}$  bright ring as

$$D^2/4 = \frac{(2n-1)\lambda R}{2}$$

$$D = \sqrt{2\lambda R} \sqrt{2n-1}$$

$$D \propto \sqrt{2n-1}$$

Thus the diameters of the bright rings are proportional to the square roots of odd natural numbers as  $(2n-1)$  is an odd number.

similarly for a **dark ring**

$$2 \frac{r^2}{2R} = n\lambda$$

$$\text{or } r^2 = n\lambda R \Rightarrow D^2 = 4n\lambda R$$

$$D = 2\sqrt{n\lambda R} \Rightarrow D \propto \sqrt{n}$$

Thus the diameters of dark rings are proportional to the square roots of natural numbers. It can be shown that fringe width decreases with the order of the fringe and fringes get closer with increase in their order

### Newton's rings by transmitted light:-

In case of transmitted light

$$2t = n\lambda \text{ for bright rings.}$$

$$2t = (2n-1)\lambda/2 \text{ for dark rings.}$$

for **bright rings**

$$2 * r^2/2R = n\lambda \text{ or } r^2 = n\lambda R$$

$$D = \sqrt{n\lambda R} \Rightarrow D \propto \sqrt{n}$$

For **dark rings**

$$2 * r^2/2R = (2n-1)\lambda/2$$

$$r^2 = \frac{(2n-1)\lambda R}{2}$$

$$D = \sqrt{2\lambda R} * \sqrt{2n-1}$$

$$D \propto \sqrt{2n-1}$$

Thus in the case of transmitted light, the central ring is bright. The rings are just opposite to the rings in reflected light.

### Applications of Newton's rings:

#### 1. Determination of wavelength of sodium light using Newton's rings :

Let  $R$  be the radius of curvature of the surface in contact with the plate,  $\lambda$  is the wavelength of light used and  $D_n$  &  $D_m$  the diameters of  $n^{\text{th}}$  and  $m^{\text{th}}$  dark rings respectively, then

$$D_n^2 = 4n\lambda R \quad D_m^2 = 4m\lambda R$$

$$D_m^2 - D_n^2 = 4(m-n)\lambda R \quad \therefore \lambda = (D_m^2 - D_n^2) / 4(m-n)R$$

Using this formula  $\lambda$  can be calculated.

## 2.Determination of refractive index of a liquid :

when there is an air film between glassplate & plano convex lens,

$$D_n^2 = 4n\lambda R \quad D_m^2 = 4m\lambda R$$
$$\therefore D_m^2 - D_n^2 = 4(m-n)\lambda R \quad \longrightarrow \quad (1)$$

Now the liquid whose refractive index is to be determined is poured in the container without disturbing the whole arrangement, again the diameters of  $n^{\text{th}}$  and  $m^{\text{th}}$  ring are determined. when there is a liquid film between glassplate and plano convex lens, we have

$$D_n^{1\ 2} = \frac{4n\lambda R}{\mu} \quad D_m^{1\ 2} = \frac{4m\lambda R}{\mu}$$
$$D_m^{1\ 2} - D_n^{1\ 2} = \frac{4(m-n)\lambda R}{\mu} \quad \longrightarrow \quad (2)$$

From eqs(1) &(2) 
$$\mu = \frac{D_m^2 - D_n^2}{D_m^{1\ 2} - D_n^{1\ 2}}$$

### **Conditions for Interference of light :-**

To obtain a permanent or stationary interference pattern, the conditions are classified into the following three parts.

conditions for sustained interference

1. conditions for observation of the fringes
2. conditions for good contrast between maxima and minima.

#### **1. conditions for sustained interference:-**

- (i) The two sources should be coherent, i.e., they should vibrate in the same phase or there should be a constant phase difference between them.
- (ii). The two sources must emit continuous waves of the same wavelength and time period.

#### **2. Conditions for observation:-**

- (i). The separation between the two sources  $2d$  should be small.
- (ii). The distance  $D$  between the two sources and screen should be large.
- (iii). The background should be dark.

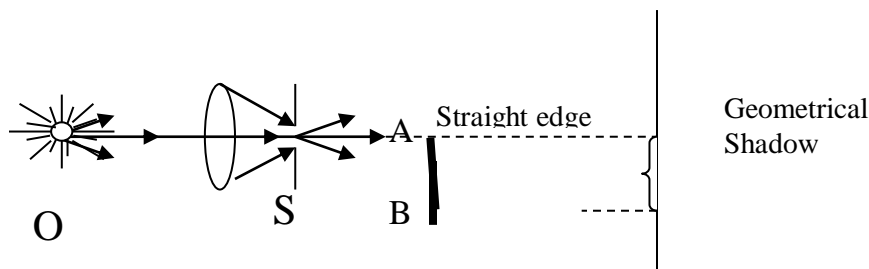
#### **3. conditions for good contrast:-**

- (i). The amplitudes of the interfering waves should be equal or nearly
- (ii). The sources must be narrow i.e., they must be extremely small.
- (iii). The sources should be monochromatic.



## DIFFRACTION

Light suffers some deviation from its straight path in passing close to the edges of opaque obstacles and narrow slits the amount of bending, however, depends upon the size of the obstacle and the wavelength of the wave. The deviation is extremely small when the wavelength of light waves is small in comparison to the dimensions of the obstacles or aperture. But when the size of the aperture is comparable with the wavelength of light, this deviation becomes much pronounced.



Thus “when light falls on obstacles or small apertures whose size is comparable with the wavelength of light, there is a departure from straight line propagation & the light bends round the corners of the obstacles or apertures and enters in the geometrical shadow. This bending of light is called diffraction.”

It was found that diffraction produces bright and dark fringes known as diffraction bands or fringes.

The correct interpretation of diffraction phenomenon was provided by Fresnel. According to Fresnel, the diffraction phenomenon is due to mutual interference of secondary wavelets originating from various points of the wavefront which are not blocked off by the obstacle. Fresnel, thus, applied Huygen's principle of secondary wavelets in conjunction with the principle of interference and calculated the position of fringes. It was observed that the calculated results were in good agreement with the observed diffraction pattern. The diffraction effects are observed only when a portion of the wavefront is cut off by the obstacle.

### Two kinds of diffraction:

diffraction phenomenon can be divided into following two general classes

#### 1. Fraunhofer's diffraction:

In this class of diffraction source and the screen or telescope (through which the image is viewed) are placed at infinity or effectively at infinity. In this case the wavefront which is incident on the aperture or obstacle is plane.

#### 2. Fresnel's diffraction:

In this class of diffraction, source and screen are placed at finite distances from the aperture of obstacle having sharp edges. In this case no lenses are used for making the rays parallel or convergent. This incident wavefront are either spherical or cylindrical.

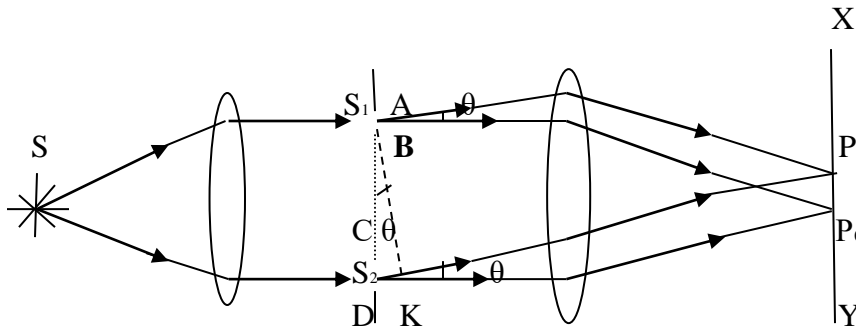
### Difference between Interference & Diffraction:

Following are the differences between Interference and Diffraction

1. In the phenomenon of Interference, the interaction takes place between two separate wavefronts originating from the two coherent sources. While in the phenomenon of diffraction, the interaction takes place between the secondary wavelets originating from different points of the exposed parts of the same wavefront.
2. In the interference pattern the regions of minimum intensity are usually almost perfectly dark. While it is not so in diffraction pattern.
3. The width of the fringes in interference may or may not be equal or uniform while in diffraction pattern fringe width of various fringes are never equal.
4. In an interference pattern all the maxima are of same intensity but in diffraction pattern they are of varying intensity.

### Fraunhofer Diffraction by a Double slit (Normal incidence):-

Let AB & CD be two parallel slits of equal width  $e$  and separated by an opaque distance  $d$ . The distance between the corresponding middle points of the two slits is  $e(d)$



Let a parallel beam of monochromatic light of wavelength  $\lambda$  be incident normally upon the two slits. The light diffracted from these slits is focussed by a lens on the screen XY placed in the focal plane of lens. The diffraction at two slits is the combination of diffraction as well as interference. i.e. the pattern on the screen is the diffraction pattern due to a single slit, on which a system of interference fringes is superposed.

### Explanation:

When a plane wave front is incident normally on both slits, all points within the slits become the sources of secondary wavelets which travel in all directions. The secondary waves travelling in the direction of incident light come to a focus  $P_0$ . While the secondary wavelets travelling in a direction making an angle  $\theta$  with the incident direction come to a focus  $P_1$ .

According to the theory of diffraction at a single slit, the resultant amplitude  $R$  due to all wavelets diffracted from each slit in a direction  $\theta$  is given by

$$R = \frac{A \sin \alpha}{\alpha}$$

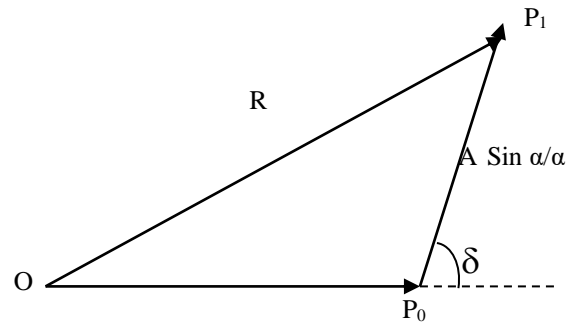
where  $A$  is a constant equal to the amplitude due to a single slit when  $\theta=0$  and  $\alpha=(\pi e \sin \theta / \lambda)$  we can consider the two slits as equivalent to two coherent sources  $S_1$  &  $S_2$  arranged at midpoints of the slits, and each source sending a wavelet of amplitude  $(A \sin \alpha / \alpha)$  in a direction  $\theta$ . The resultant amplitude at a point  $P_1$  on the screen will be a resultant of interference between two waves of amplitude  $(A \sin \alpha / \alpha)$  & having a phase difference  $\delta$ , we draw a perpendicular  $S_1k$  &  $S_2k$ . The path difference between the wavelets from  $S_1$  &  $S_2$  in the direction  $\theta$ .

$$= S_2k$$

$$= (e+d) \sin \theta.$$

$\therefore$  phase difference  $\delta = \frac{2\pi}{\lambda}$  (path difference)

$$\delta = \frac{2\pi}{\lambda} (e+d) \sin \theta$$



the resultant amplitude  $R$  at  $P_1$  can be obtained with the help of  $\delta$ . From fig

$$(OP_1)^2 = (OP_0)^2 + (P_1P_0)^2 + 2 (OP_0)(P_0P_1) \cos \delta$$

$\therefore R^2 = \left[ \frac{A \sin \alpha}{\alpha} \right]^2 + \left[ \frac{A \sin \alpha}{\alpha} \right]^2 + 2 \left[ \frac{A \sin \alpha}{\alpha} \right] \left[ \frac{A \sin \alpha}{\alpha} \right] \cos \delta$

$$R^2 = \left[ \frac{A \sin \alpha}{\alpha} \right]^2 [1+1+2\cos \delta]$$

$$R^2 = \left[ \frac{A \sin \alpha}{\alpha} \right]^2 [2+2\cos \delta]$$

$$R^2 = \left[ \frac{A \sin \alpha}{\alpha} \right]^2 2[1+\cos \delta]$$

$$R^2 = \left[ \frac{A \sin \alpha}{\alpha} \right]^2 2[1+2 \cos^2 \delta/2-1]$$

$$R^2 = 4 \left[ \frac{A \sin \alpha}{\alpha} \right]^2 \cos^2 \delta/2$$

### Discussion on intensity distribution:

The intensity in the resultant pattern depends upon the following two factors:

1.  $(A^2 \sin^2 \alpha / \alpha^2)$  which is the same as derives for a single Fraunhofer diffraction. This gives the intensity distribution in the diffraction pattern due to any individual slit.
2.  $\cos^2 \beta$  which gives the interference pattern due to waves starting from two parallel slits.

The resultant intensity at any point on the screen is given by the product of these two factors. Let us now examine each factor separately.

The diffraction term  $\left\{ \frac{\sin^2 \alpha}{\alpha^2} \right\}$  gives the central maximum in the direction  $\theta=0$  having alternate maxima and secondary maxima of decreasing intensity on either side as shown in fig. The maxima are obtained in the direction given by.

$$\sin \alpha = 0 \text{ but } \alpha \neq 0$$

$$\alpha = \pm m\pi, m=1,2,3,\dots$$

$$\pi e \sin \theta / \lambda = \pm m\pi$$

$$e \sin \theta = \pm m\lambda$$

the positions of secondary maxima approaches to  $\alpha = \frac{\pm 3\pi}{2}, \frac{\pm 5\pi}{2}, \frac{\pm 7\pi}{2}, \dots$

the interference term  $\cos^2 \beta$  gives a set of equidistant dark & bright fringes as shown. The maxima are obtained in the direction given by

$$\cos^2 \beta = 1 \quad \beta = \pm n\pi$$

$$\frac{\pi}{\lambda} (e+d) \sin \theta = \pm n\pi$$

$$(e+d) \sin \theta = \pm n\lambda$$

where  $n = 0, 1, 2, 3, \dots$

the intensity distribution is the resultant diffraction pattern is a plot of the product of constant

term  $4A^2$ , diffraction term  $\frac{\sin^2 \alpha}{\alpha^2}$  & interference term  $\cos^2 \beta$

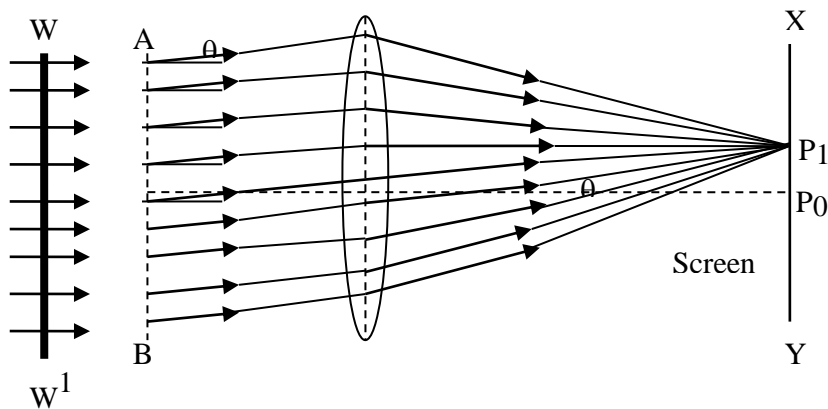
### **DIFFRACTION GRATING:**

An arrangement consists of large number of parallel slits of same width and separated by equal opaque spaces is known as diffraction grating

Fraunhofer used the first grating placed very closely side by side at regular intervals. When the spacing between the lines is of the order of wavelength of the light, then an appreciable deviation of the light is produced.

#### **Plane diffraction grating: (diffraction at N parallel slits)**

Figure represents the section of a plane transmission grating placed perpendicular to the plane of the paper.



Let  $e$  be the width of the each slit and  $d$  be the width of each opaque part. Then  $(e+d)$  is known as grating element.  $XY$  is the screen placed perpendicular to the plane of paper.

suppose a parallel beam of monochromatic light of wavelength  $\lambda$ . be incident normally on the grating. By Huygen's principle, each of the infinite points in the slits sends secondary wavelets in all directions. The secondary wavelets travelling in same direction of incident light will focus at  $P_0$ . As the screen is placed at focal plane of convex lens  $P_0$  will be central maximum.

Now consider the secondary waves travelling in a direction inclined at an angle  $\theta$  with the direction of incident light. These waves reach  $P_1$  on passing through convex lens in different phases. As a result, dark and bright bands on both sides of central maximum are obtained.

The intensity at  $P_1$  may be considered by applying the theory of Frounhofer diffraction at a single slit

The wavelets proceeding from all points in a slit along the direction  $\theta$  are equivalent to a single wave of amplitude  $\frac{A \sin \alpha}{\alpha}$  starting from the middle point of the slit, where  $\alpha = \frac{\pi e \sin \theta}{\lambda}$

If there are  $N$  slits, then we have diffracted waves, one each from the midpoints of the slits. the potential difference between two consecutive slits is  $(e+d)\sin \theta$  between two consecutive waves. this phase difference is constant and is  $2\beta$ .

Hence the problem of determining the intensity in a direction  $\theta$  reduces to finding the resultant amplitude of  $N$  vibrations each of amplitude  $\frac{A \sin \alpha}{\alpha}$  and having a common phase

difference  $\frac{2\pi}{\lambda} (e+d)\sin \theta = 2\beta$ .

by the method of vector addition of amplitudes

$$R = a \frac{\sin nd/2}{\sin d/2} \quad \text{here } a = \frac{A \sin \alpha}{\alpha}, n = N \text{ and } d = 2\beta$$

$$R = \frac{A \sin \alpha}{\alpha}$$

$\therefore$  the resultant amplitude in direction of  $\theta$  will be

$$R = \frac{A \sin \alpha}{\alpha} \frac{\sin N\beta}{\sin \beta} \longrightarrow (1)$$

$$\text{and } I = R^2 = \left( \frac{A \sin \alpha}{\alpha} \right)^2 \left( \frac{\sin N\beta}{\sin \beta} \right)^2 \longrightarrow (2)$$

$\frac{A \sin \alpha}{\alpha}$  gives the distribution of intensity due to a single slit while  $\frac{\sin N\beta}{\sin \beta}$  gives the distribution of intensity as combined effect of all the slits.

**Principle maxima:**

The intensity would be maximum when  $\sin \beta = 0$  or  $\beta = \pm n\pi \quad n = 0, 1, 2, 3, \dots$

but at some time  $\sin N\beta = 0$  so that  $\frac{\sin N\beta}{\sin \beta}$  becomes indeterminate using Hospital's

rule.  $\lim_{\beta \pm n\pi} \frac{\sin N\beta}{\sin \beta} = \frac{d/d\beta(\sin N\beta)}{d/d\beta \sin \beta} = \frac{N \cos N\beta}{\cos \beta} = \pm N$

the resultant intensity is  $\left(\frac{A \sin \alpha}{\alpha}\right)^2 N^2$  the maxima are most intense and are called principal maxima

the maxima are obtained for  $\beta = \pm n\pi$

$$\frac{2\pi}{\lambda} (e+d)\sin \theta = \pm n\pi \quad \text{or} \quad (e+d)\sin \theta = \pm n\lambda \quad \longrightarrow (3) \quad n = 0, 1, 2, 3, \dots$$

$n = 0$  corresponds to zero order maximum for  $n = 1, 2, 3, \dots$  we obtain first, second, third etc. principal maxima respectively. The  $\pm$  sign shows that there are two principal maxima of same order lying on either side of zero order maximum.

**Minima:**

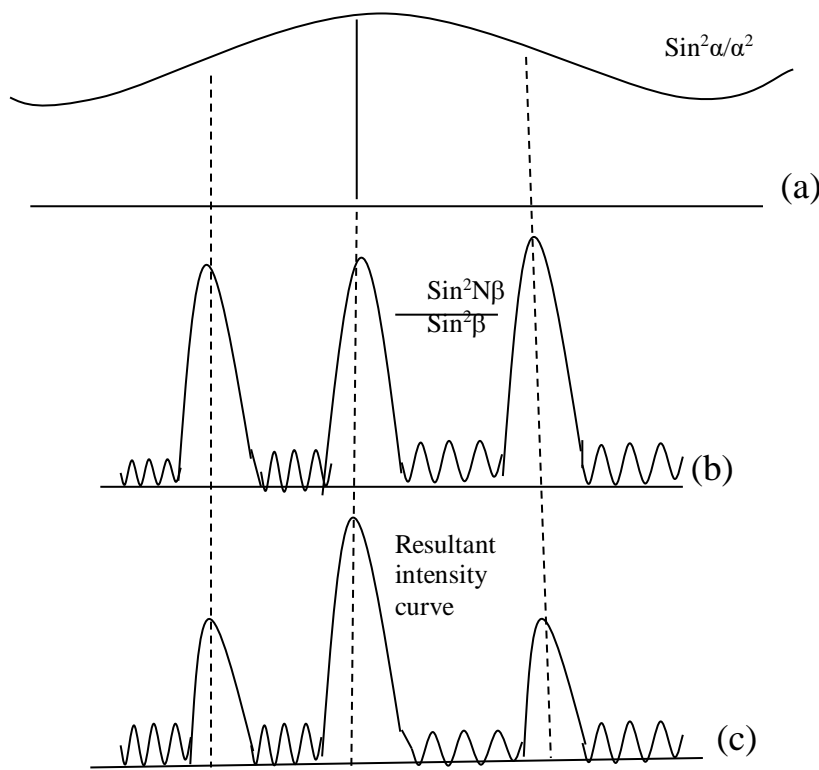
A series of minima occurs, when  $\sin N\beta = 0$  but  $\sin \beta \neq 0$   
for minima  $\sin N\beta = 0, N\beta = \pm m\pi$

$$\frac{2\pi}{\lambda} (e+d)\sin \theta = \pm m\pi \quad \text{or} \quad N(e+d)\sin \theta = \pm m\lambda \quad \longrightarrow (4)$$

$m$  has all integral values except  $0, N, 2N, \dots, nN$  because for these values,  $\sin \beta$  becomes zero and we get principal maxima. Thus  $m = 1, 2, 3, \dots, (N-1)$ . Hence there are adjacent principal maxima.

Fig (a) & (b) shows variation of intensity due to  $\frac{\sin^2 \alpha}{\alpha^2}$  and  $\frac{\sin^2 n\beta}{\sin^2 \beta}$  respectively.

The resultant intensity shown in fig.(c)



**RESOLVING POWER OF A GRATING:-**The capacity to form separate diffraction maxima of two wavelengths which are very close to each other.

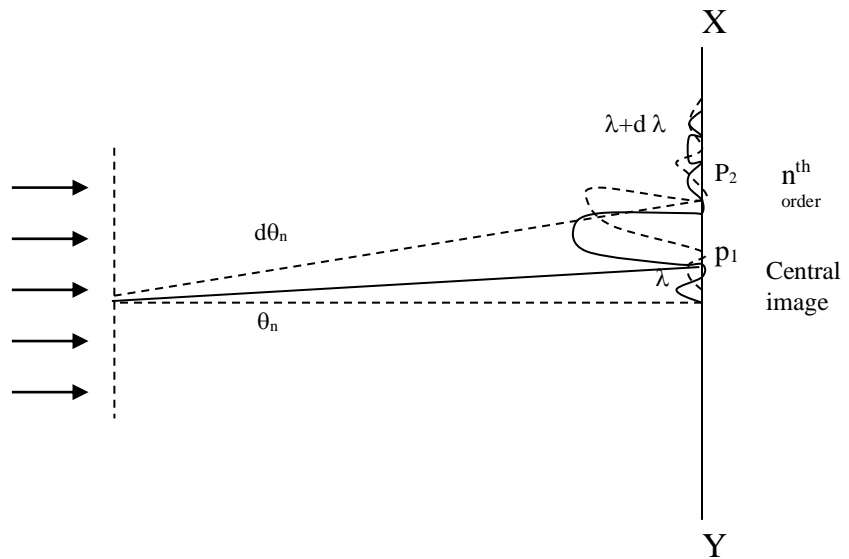
This is measured by  $\lambda/d\lambda$ .

Where  $d$  is the smallest difference in two wavelengths and  $\lambda$  is the mean wavelength.

**Expression for Resolving power:-**

Let  $AB$  represents the surface of plane transmission grating having grating element  $(e+d)$  and  $N$  total number of slits.

Let a beam of light having two wavelengths  $\lambda$  and  $\lambda + d\lambda$  is normally incident on the grating.



In fig  $XY$  is the field of view of the telescope,  $P_1$  is  $n^{\text{th}}$  primary maximum of a spectral line of wavelength  $\lambda$  at an angle of diffraction  $\theta_n$  and  $p_2$  is the  $n^{\text{th}}$  primary maximum of wavelength  $(\lambda + d\lambda)$  at diffracting angle  $(\theta_n + d\theta_n)$ .

According to Rayleigh criterion, the two wavelengths will be resolved if the position of  $p_2$  corresponds to the first minimum of  $P_1$  i.e., the two lines will be resolved if the principal maximum of  $(\lambda + d\lambda)$  in a direction  $(\theta_n + d\theta_n)$  falls over the first minimum of  $\lambda$  in the same direction  $(\theta_n + d\theta_n)$ . Now we shall consider the first minimum of  $\lambda$  in the direction  $(\theta_n + d\theta_n)$ .

The principal maximum of  $\lambda$  in the direction  $\theta_n$  is given by

$$(e+d) \sin \theta_n = n \lambda \text{-----(1)}$$

the equation of minima is

$$N (e+d) \sin \theta = m \lambda$$

Where  $m$  has all integral values except  $0, N, 2N, \dots, nN$ , because for these values of  $m$ , the condition for maxima is satisfied and we obtain different maxima.

Thus the first minimum adjacent to  $n^{\text{th}}$  principal maximum in the direction  $(\theta_n + d\theta_n)$  can be obtained by substituting the value of  $m$  as  $(nN + 1)$ .  $\therefore$  The first minimum in the direction  $(\theta_n + d\theta_n)$  is given by

$$N (e+d) \sin (\theta_n + d\theta_n) = (nN + 1) \lambda \text{----- (2)}$$

The principal maximum of  $(\lambda + d\lambda)$  in a direction  $(\theta_n + d\theta_n)$  is given by

$$(e+d) \sin (\theta_n + d\theta_n) = n (\lambda + d\lambda) \text{-----(3)}$$

multiplying eq (3) by  $N$ , we have

$$N (e+d) \sin(\theta_n + d\theta_n) = nN (\lambda + d\lambda) \text{-----(4)}$$

from eqs (2) and (4) we get

$$(nN + 1) \lambda = nN (\lambda + d\lambda)$$

$$nN \lambda + \lambda = nN \lambda + nN d\lambda$$

$$\lambda = nN d\lambda$$

$$\lambda/d \lambda = nN \text{-----}(5)$$

this is the required expression.

The resolving power is directly proportional to (i) the order of the spectrum and (ii) the total number of lines on the grating surface. From equation (1)

$$n = (e+d) / \lambda \sin \theta_n$$

$$\lambda/d \lambda = N(e+d) \sin \theta_n / \lambda$$

**Rayleigh's criterion for resolving power:-**

According to Rayleigh criterion, two sources are resolvable by an optical instrument when the central maximum in the diffraction pattern of one falls over the first minimum in the diffraction of the other and vice versa..

In order to illustrate the criterion. Let us consider the resolution of two wavelengths  $\lambda_1 + \lambda_2$  by a grating fig (a) shows the intensity curves of the diffraction patterns of two wavelengths. The difference in wavelengths is such that their principal maxima are separately visible. There is a distinct point of zero intensity in between the two. Hence the two wavelengths are resolved.

Now consider the case when the difference in wavelengths is smaller and such that the central maximum of wave lengths coincides with the first minimum of the other as shown in fig (b). The curve shows a distinct dip in the middle of two central maxima indicating the presence of two different wavelengths. Thus the two wavelengths can be distinguished from one another and according to Rayleigh they are said to be just resolved.

when difference in wavelengths is so small that the central maxima corresponding to two wavelengths come still closer as shown in fig (c).The resultant intensity curve in this case is quite smooth without any dip thus giving the impression as if there is only one wavelength although some what bigger and stronger.Hence the two wavelengths are not resolved.

Thus the two lines can be resolved to a certain limit by Rayleigh criterion.

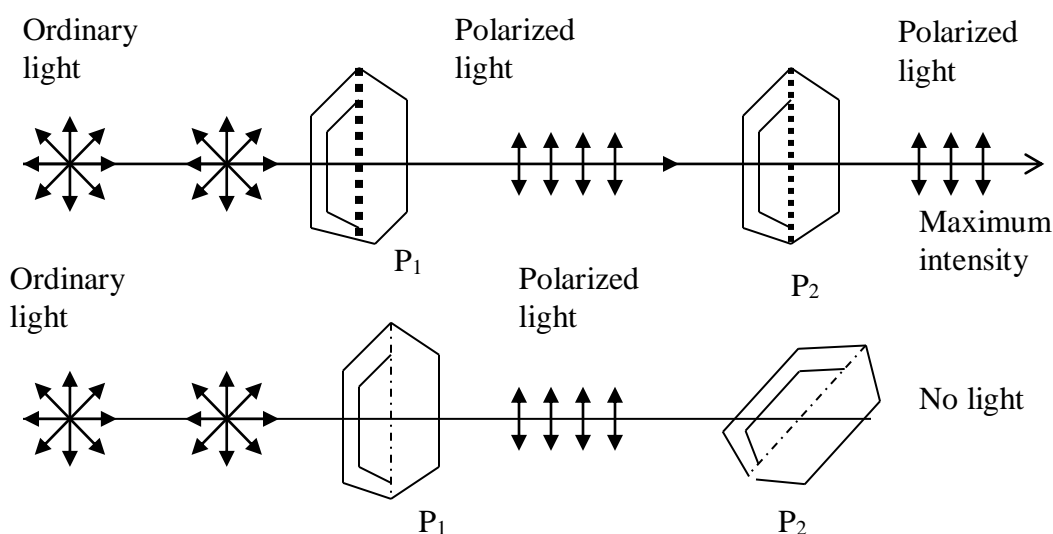


**Polarization:**

The process of transforming unpolarized light into polarized light is known as polarization or the oneness of a light is called polarization.

**Polarization of light waves:**

When ordinary light is passed through a pair of tourmaline crystal plates  $P_1$  &  $P_2$  with their planes at right angles to the direction of propagation of light, the intensity is maximum in this position. But when the plane  $P_2$  is rotated through  $90^\circ$  i.e. the plane  $P_2$  is perpendicular to  $P_1$  the intensity is minimum in this case. Light is transverse wave motion. After passing through the crystal  $P_1$ , the light vibrates only in one direction.

**Polarized light:**

**The light which has acquired the property of one sidedness is called polarized light.**

When the vibrations are confined along a single direction at right angles to the direction of propagation, the light is said as plane polarized. If the vibrations are along a circle or an ellipse lying in a plane normal to the direction of propagation, the line is said to be circularly or elliptically polarized respectively.

**Types of Polarization:**

There are three types of polarized light.

1. linearly polarized light.
2. Circularly polarized light
3. Elliptically polarized light

**linearly polarized light:**

When the amplitude of the electric vector of light changes but the orientation remains constant, the path traced by electric vector is a straight line and the light is said to be linearly polarized.

### **Circularly polarized light:**

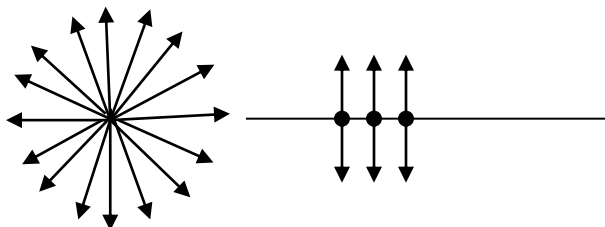
When the amplitude of the electric vector of light remain constant but the orientation changes, the path traced by electric vector is a circle and the light is said to be circularly polarized.

### **Elliptically polarized light:**

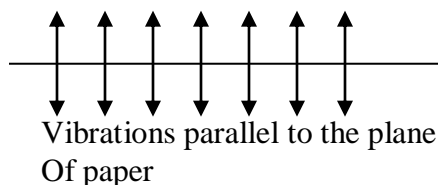
When the amplitude of the electric vector of light and its orientation are changing, the path traced by electric vector is a ellipse and the light is said to be elliptically polarized.

### **Representation of various type of light:**

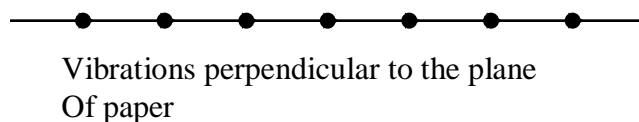
Un polarized  
light



Plane polarized  
light



Plane polarized  
light



### **Unpolarized light:**

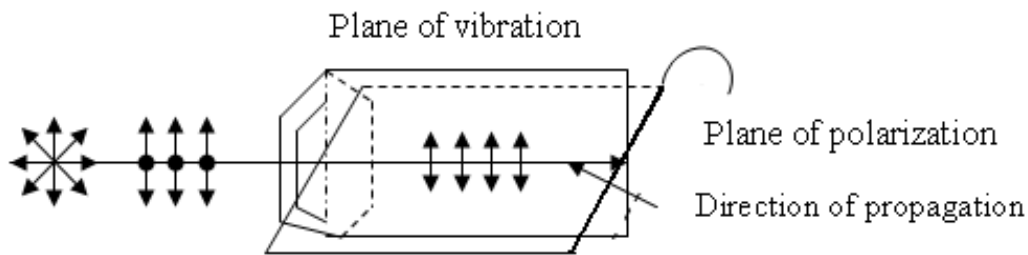
The ordinary light is also called as unpolarized light, consists of a very large number of vibrations in all planes with equal probability at right angles to the direction of propagation. Hence the unpolarized light is represented by a star.

### **Plane polarized light:**

In plane polarized light the vibrations are along a straight line. If the direction of propagation is parallel to the plane of paper, it is represented by a straight line arrow. If the direction of vibration is perpendicular to the plane of the paper, it is represented by dot.

### **Plane of polarization:**

When ordinary light is passed through a tourmaline crystal the light is polarized and the vibrations are confined only in one direction which is perpendicular to the direction of propagation of light. Now we consider the case of two planes, firstly in which the vibration of polarized are confirmed. This plane is known as **plane of vibration**. This plane contains the direction of vibration as well as the **direction of propagation**.

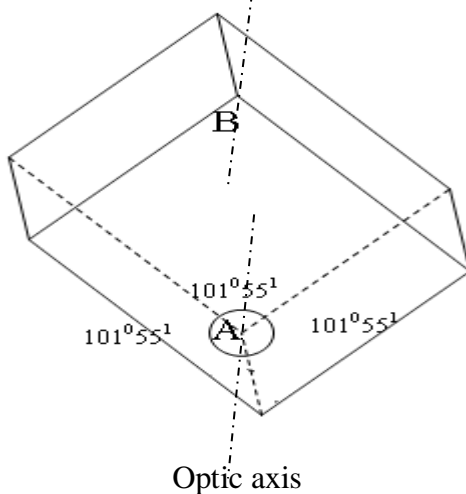


Secondly, the plane which has no vibrations this plane is known as **plane of polarization**. Thus a plane passing through the direction of propagation and perpendicular to the plane of vibration is known as plane of polarization.

**Optic axis:**

“A line passing through any one of the blunt corners (A or B) and making equal angles with the three faces which meet, at this corner, locate the direction of the optic axis of the crystal.” optic axis is a direction and not a particular plane.

Crystals having one optic axis are called uniaxial crystals (like quartz & calcite) and those having two optic axes are called biaxial crystals (like mica)



**Principal section:**

“Any plane which contains the optic axis and is Perpendicular to two opposite faces is called a principal section”.

As a crystal has six faces, so far every point inside the crystal there are three principal sections, one for each pair of opposite crystal faces. A principal section cuts the crystal surfaces in a parallelogram having angle  $71^\circ$  &  $109^\circ$

**Optic axis and its characteristics:**

The direction along which refracted, ordinary and extra ordinary rays travel together with the same velocity is called optic axis of the crystal.

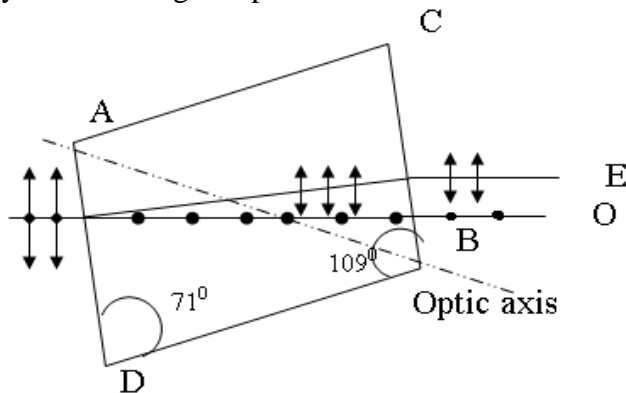
### Characteristics:

1. A beam of unpolarized light incident along the optic axis or in the direction parallel to the optic axis does not split up into ordinary and extra ordinary rays.
2. Optic axis is not obtained by joining the two blunt corners. Except in a special situation of rhombohedra.
3. When the light travel in a direction perpendicular to the optic axis, then both e-ray and o-ray travel in the same direction but with different speeds.

### Double refraction:

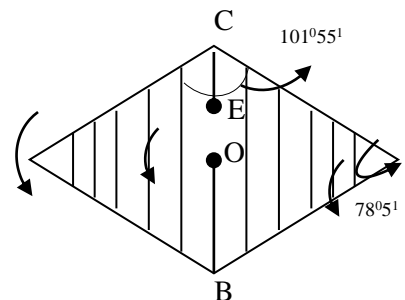
when a beam of ordinary unpolarised light is passed through a calcite crystal, the refracted light is split up into two refracted rays. The one which always obeys the ordinary laws of refraction and having vibrations perpendicular to the principal section is known as **ordinary ray**. The other, does not obey the laws of refraction and having vibrations in the principal section is called as **extra-ordinary ray**.

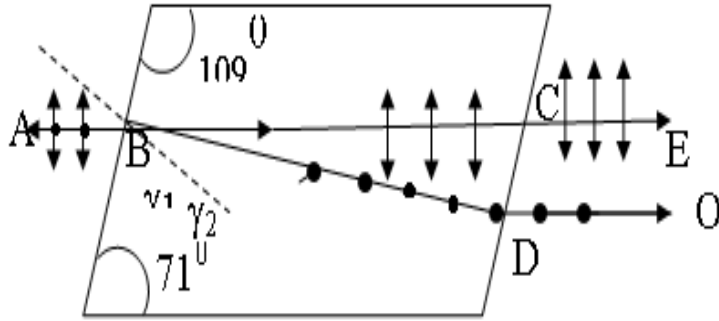
Both the rays are plane polarised. This phenomenon is known as double refraction. The crystals showing this phenomenon are known as doubly refracting crystals.



The phenomenon of double refraction can be illustrated with the following experiment. An ink dot is made on a white paper and a calcite crystal is placed over it. Now looking through the top face, two images are observed. If now the crystal is rotated slowly in the direction shown in fig, it is observed that one image remains stationary while the other rotates in the direction of rotation of crystal. The stationary image is known as ordinary image while the rotating one is known as ex-ordinary image.

Consider a beam AB of unpolarised light incident on the calcite crystal at an angle of incidence  $i$ .





Inside the crystal the ray breaks up into ordinary & extra-ordinary rays. The ordinary ray travelling along BD makes an angle of refraction  $r_1$  while the extra-ordinary travelling along BC makes an angle of refraction  $r_2$ . Since the two opposite faces of the crystal are always parallel, both the rays emerge parallel to the incident rays. The refractive indices of ordinary & extra-ordinary rays can be expressed as

$$\mu_o = \frac{\sin i}{\sin r_1} \quad \& \quad \mu_e = \frac{\sin i}{\sin r_2} \quad \text{respectively}$$

In case of calcite  $\mu_o > \mu_e$  because  $r_1 < r_2$ .

$\therefore$  the velocity of light for ordinary ray inside the crystal will be less than the extra-ordinary ray. It is observed that  $\mu_o$  is same for all the angles of incidence while  $\mu_e$  varies with angles of incidence. Therefore ordinary ray travels with the same speed in all directions while extra-ordinary has different speeds in different directions.

**Quarter wave plate:**

A Quarter wave plate is a thin plate of crystal having its refracting faces parallel to optic axis and its thickness adjusted such that it introduces a quarter wave ( $\lambda/4$ ) path difference between the e-ray and o-ray propagating through it.

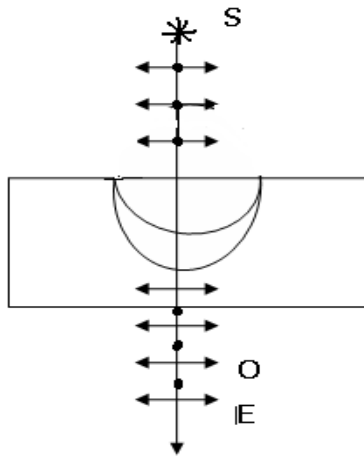
The path difference between e-ray and o-ray

$$\Delta = (\mu_o - \mu_e)d \quad \text{for -ve crystal}$$

For Quarter wave plate  $(\mu_o - \mu_e)d = \frac{\lambda}{4} \quad \therefore d = \frac{\lambda}{4(\mu_o - \mu_e)} \quad \text{for -ve crystal}$

Similarly  $d = \frac{\lambda}{4(\mu_e - \mu_o)} \quad \text{for +ve crystal}$

A quarter wave plate is therefor, used to produce elliptically or circularly polarized light since the e-ray and o-ray having the phase difference  $\frac{\pi}{2}$  or  $90^\circ$ .



**Half wave plate:**

A half wave plate is a thin plate of crystal having its refracting faces parallel to optic axis and its thickness adjusted such that it introduces a quarter wave ( $\lambda/2$ ) path difference between the e-ray and o-ray propagating through it.

The path difference between e-ray and o-ray

$$\Delta = (\mu_o - \mu_e)d \quad \text{for -ve crystal}$$

For Quarter wave plate

$$(\mu_o - \mu_e)d = \frac{\lambda}{2} \quad \therefore d = \frac{\lambda}{2(\mu_o - \mu_e)} \quad \text{for -ve crystal}$$

$$\text{Similarly} \quad d = \frac{\lambda}{2(\mu_e - \mu_o)} \quad \text{for +ve crystal}$$

A half wave plate is therefore, used to produce plane polarized light since the e-ray and o-ray having the phase difference  $\pi$  or  $180^\circ$ .

**Distinction between unpolarized light & polarized light:**

When ordinary light is passed through a single rotating tourmaline crystal it shows no variation in the intensity of light. This shows that ordinary light is symmetrical about its direction of propagation. So the “unpolarized light may be considered to consist of an infinite number of waves, each having its own direction of vibration.”

In polarized light, there is a lack of symmetry about the direction of propagation of the light. If the polarized light is rotating through a tourmaline crystal, it shows a change in the intensity of light. In one position the intensity maximum, while in another position, the intensity is minimum. This shows that the vibrations in polarized light are confined to one particular direction only.

### INTRODUCTION

A laser is a manifestation of a coherent optical process. It is the acronym for Light Amplification by Stimulated Emission of Radiation. Stimulated emission was first postulated by Einstein and first used by Townes and Schawlow in USA, Boso and Prokhorov in USSR.

Laser is an optical device which produces powerful monochromatic beam of radiation in which the waves are coherent. From Laser the light beam emerges as a narrow beam which can travel over a long distance without loss of energy. Laser is sometimes also referred as optical maser.

The development of laser is extremely rapid and laser action was demonstrated with gases, liquids, solids, semiconductors etc. This chapter deals with the unique characteristics, construction and working of few conventional lasers along with their applications.

### INTERACTION OF RADIATION WITH MATTER

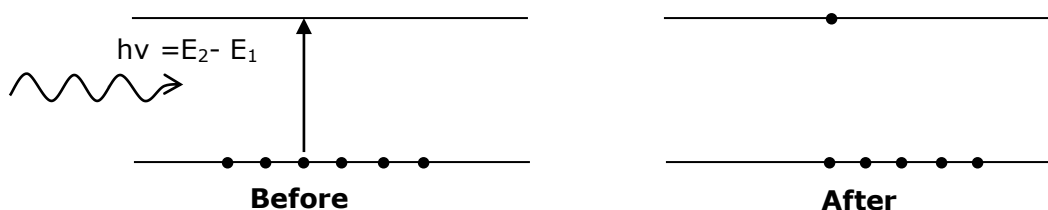
The understanding of the principle of a laser requires a superficial idea of quantum processes that take place in a material when exposed to radiation.

A material medium is composed of identical atoms or molecules, each of which is characterized by a set of discrete allowed energy states. **An atom can move from one energy state to another when it receives or releases an amount of energy equal to the energy difference between those two states. It is termed as a quantum jump or a transition.**

Let us consider two energy states  $E_1$  and  $E_2$  of an atom such that  $E_1$  is the lower energy state and  $E_2$  is the higher energy state. Let a monochromatic radiation of frequency  $\nu$  be incident on the medium. The radiation may be viewed as a stream of photons, each photon carrying an energy  $h\nu$ . If this energy  $h\nu = E_2 - E_1$ , then the interaction of the radiation with the atoms may be in three different ways;

#### Induced Absorption:

Usually atoms are in the ground state. When a photon of energy  $h\nu (=E_2 - E_1)$  is incident on the atom lying in ground state then it absorbs energy and gets excited to the higher energy state.



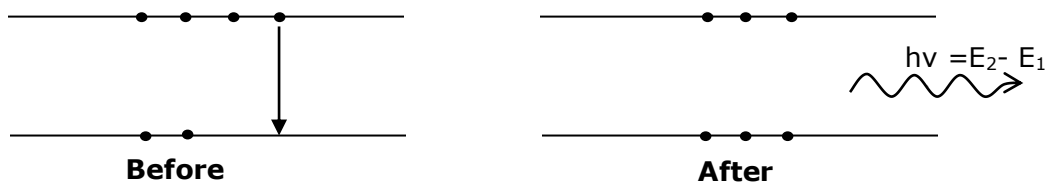
This process is called **induced absorption**. Corresponding to each transition made by an atom, one photon disappears from the incident beam.

### Spontaneous Emission:

Excited state with higher energy is highly unstable because of the natural tendency of the atoms to seek out the lowest energy configuration. Hence, the excited atoms do not stay in the higher energy state for a relatively longer time but tend to return to the lower state by giving up the excess energy.

So an atom can remain in an excited state only for a limited time. This **duration of time spent by an atom in an excited state is known as life time of a state**. For example the life time of hydrogen atom is  $10^{-8}$ sec.

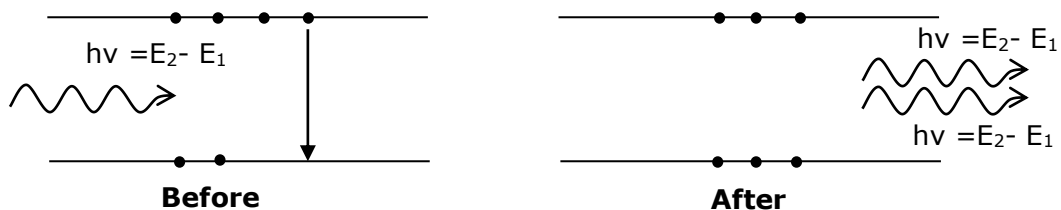
After this life time has been spent, the atom de-excites to the lower level spontaneously by emitting a photon of energy  $h\nu (=E_2 - E_1)$  as shown in Fig. **The process in which photon emission occurs without any external impetus is called spontaneous emission.**



This phenomenon depends on type of the particle and type of transition, but it is independent of external conditions. The photons in this case have various wavelengths and they are out of phase. Thus this radiation is **incoherent** and **non monochromatic**. This emission was postulated by **Bohr**.

### Stimulated Emission:

An atom in an excited state need not wait for spontaneous emission to occur. There exists an alternative mechanism by which an excited atom can make a downward transition.



Before the life time is completed, if an external photon of energy  $h\nu (=E_2 - E_1)$  strikes an excited atom, then it drops to the lower energy state giving up a photon with same frequency in same direction and same phase to that of the incident photon. These kind of forced emissions are called stimulated emissions.

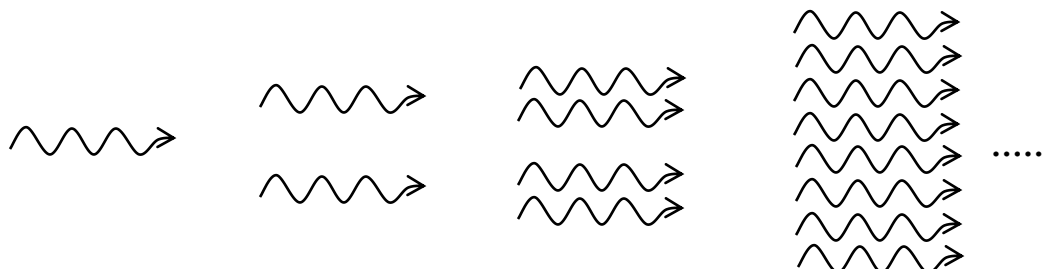
**This emission which takes place with the help of an external incitement is known as stimulated emission.** This radiation is **coherent** and **monochromatic**. This was postulated by **Einstein**.



## LASING ACTION

In stimulated emission, one photon induces an atom to emit a second photon, these two traveling along the same direction de-excite two atoms in their path producing a total of four photons which in turn stimulate four atoms generating eight atoms and so on.

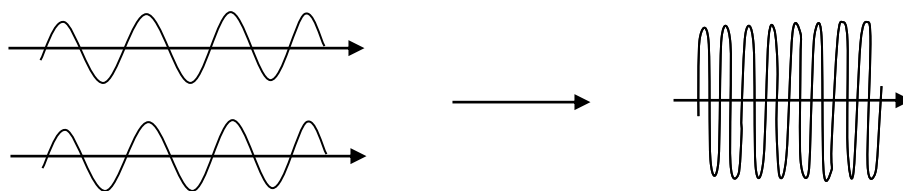
The number of photons builds up in an avalanche-like manner. This is called **lasing action**.



Hence, electromagnetic waves of extremely high amplitude could be generated, by the combined stimulated emissions from a large sample of atoms leading to the amplification of light.

The constructive interference of many waves traveling in the same direction with a common frequency and phase produces an intense coherent light beam. Since the number of atoms in light source is very large, coherent emission leads to enormously high intense light than incoherent emission.

Hence, **the stimulated emission is the key to the operation of a laser.**



Following are the conditions to be met to attain lasing action

- The system must be in a state of population inversion.
- The system must contain metastable states.
- In addition to these, there has to be a mechanism available, by which the long lived upper level can be preferentially populated.

## EINSTEIN'S COEFFICIENTS AND THEIR RELATIONS

In order to know these let us consider a material which consists of two non degenerate energy levels,  $E_1$  and  $E_2$  having population densities  $N_1$  and  $N_2$ . Further the total number of atoms in the two levels is assumed to be constant.

Hence, the total number of the atoms in the material is given as

$$N_1 + N_2 = N_{\text{total}} \longrightarrow (1)$$

Radiative transfer is allowed between the levels i.e. atoms can transfer from higher energy level to lower energy level and lower to higher by emitting and absorbing energy respectively.

### **Absorption:**

If an electromagnetic wave of frequency  $\nu_{21}$  passes the atomic system, the population  $N_1$  of lower level decreases at a rate which is proportional to  $U\nu$ , the radiation density and the population of that level.

$$\text{i.e. } \left( \frac{dN_1}{dt} \right)_{\text{abs}} = -B_{12}U\nu N_1 \longrightarrow (2)$$

Where  $B_{12}$  is proportionality constant called Einstein's coefficient of absorption and the product  $B_{12}U\nu$  can be interpreted as unit frequency that is induced by the effect of the field.

### **Spontaneous emission:**

After an atom has been raised to upper level by absorption, it spends its life time in the upper state. Then, the population of upper level decreases at rate which is proportional to the population of that level.

$$\text{i.e. } \left( \frac{dN_2}{dt} \right)_{\text{sp}} = -A_{21}N_2 \longrightarrow (3)$$

Where  $A_{21}$  is known as proportionality constant. This is known as Einstein's coefficient of spontaneous emission. This is also known as spontaneous transition probability of an atom.

### **Stimulated Emission:**

When there is an induced emission, the population of upper level decays at rate which is proportional to the population of that level and radiation density

$$\text{i.e. } \left( \frac{dN_2}{dt} \right)_{\text{stim}} = -B_{21}U\nu N_2 \longrightarrow (4)$$

Where  $B_{21}$  is a proportionality constant, which is known as Einstein's coefficient of stimulated emission.

Hence, the radiation emitted from an atomic system consists of two parts

- one due to the spontaneous emission
- The other due to the stimulated emission.

From equation (1) it follows that the total change in the population of the two levels should be zero.

At thermal equilibrium rate of transition from  $E_1$  to  $E_2$  is equal to rate of transition from  $E_2$  to  $E_1$  i.e. number of atoms absorbing radiation per unit time is equal to number of atoms emitting radiation per unit time.

$$\text{i.e. } B_{21}U\nu N_2 - B_{12}U\nu N_1 + N_2 A_{21} = 0$$

$$N_2 A_{21} + N_2 U \nu B_{21} = B_{12} U \nu N_1 \longrightarrow (5)$$

$$U \nu [B_{12}N_1 - B_{21}N_2] = A_{21}N_2$$

$$U \nu = \frac{A_{21} / B_{21}}{\left( \frac{B_{12}}{B_{21}} \right) \left( \frac{N_1}{N_2} \right) - 1} \longrightarrow (6)$$

But according to Boltzmann's distribution, at thermal equilibrium,

$$\frac{N_2}{N_1} = \exp\left[-\left(\frac{E_2 - E_1}{k_b T}\right)\right] \longrightarrow (7)$$

By substituting equation (7) in equation (6) we have

$$U_\nu = \frac{A_{21} / B_{21}}{\left(\frac{B_{12}}{B_{21}}\right) \exp\left[\left(\frac{E_2 - E_1}{k_b T}\right)\right] - 1}$$

$$U_\nu = \frac{A_{21} / B_{21}}{\left(\frac{B_{12}}{B_{21}}\right) \exp\left(\frac{h\nu_{21}}{k_b T}\right) - 1} \longrightarrow (8)$$

Where  $h\nu_{21} = E_2 - E_1$

But according to Planck's radiation law we have

$$U_\nu = \frac{8\pi\nu^2}{c^3} \frac{h\nu}{e^{\frac{h\nu}{k_b T}} - 1} \longrightarrow (9)$$

Where  $\nu = \nu_{12} = \nu_{21}$ . By comparing equations (9) and (8) we have

$$\frac{A_{21}}{B_{21}} = \frac{8\pi h\nu^3}{c^3} \text{ and } B_{21} = B_{12} \longrightarrow (10)$$

$$\frac{A}{B} = \frac{8\pi h\nu^3}{c^3} \longrightarrow (11)$$

The above equation is the relation between Einstein's A and B coefficients. From the above relations, we can arrive at the following conclusions:

- As  $B_{12} = B_{21}$ , the probability of the induced absorption is equal to the probability of the stimulated emission.
- $\frac{A}{B} \propto \nu^3$ , i.e. the ratio of the spontaneous emission to the stimulated emission is proportional to  $\nu^3$ . Thus, the probability of spontaneous emission increases rapidly with the increase in the energy difference between the two states.

### **PROPERTIES OF LASER BEAM**

- **Coherence**  
A conventional light source produces incoherent light since they emit random wavelengths with no common phase relationships. The waves emitted by a laser source will be in phase and are of same frequency. Hence, light generated by a laser is highly coherent.
- **Directionality**  
Conventional sources emit light in all the directions. Lasers emit light only in one direction as the photons traveling along the optical axis of the system are selected and augmented with the help of a resonator.
- **Divergence**

Conventional source produces light in the form of spherical wave fronts and hence, it is highly divergent. The divergence or angular spread of the laser beam is very small.

- **Monochromaticity**

Light from normal monochromatic source spreads over a wavelength range of order of 100 Å to 1000 Å. Laser light is highly monochromatic. The spread is of the order of a few angstroms (< 10 Å) only.

### POPULATION DENSITY

The number of atoms per unit volume in an energy level is known as population of that level. If  $N$  is the number of atoms per unit volume in an energy state  $E$  then the expression for population can be written as

$$N = N_0 \exp [E/k_b T]$$

Where  $N_0$  is the population in ground state,  $k_b$  is Boltzmann's constant and  $T$  is absolute temperature.

### POPULATION INVERSION

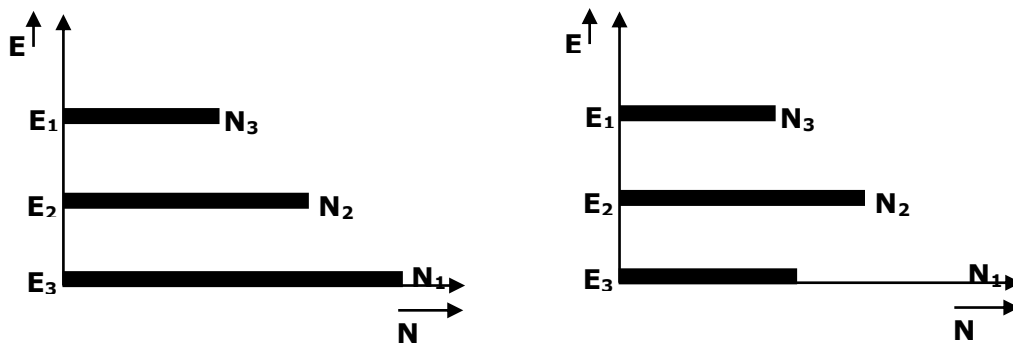
Consider a system which consists of three energy levels  $E_1$ ,  $E_2$  and  $E_3$  and population densities of those levels are  $N_1$ ,  $N_2$  and  $N_3$  respectively. In normal conditions,  $E_1 < E_2 < E_3$  and  $N_1 > N_2 > N_3$ .

Among the three states suppose  $E_2$  is metastable state, so its life time is more. When a suitable form of energy is supplied in suitable way, then the atoms excite from ground state ( $E_1$ ) to excite states  $E_2$  and  $E_3$ . If we supply energy continuously at a particular stage the population of level  $E_2$  i.e.  $N_2$  will be greater than that of the level  $E_1$  i.e.  $N_1$  as shown in fig.

This situation is known as **population inversion**. It can be defined as the process by which a large number of atoms are made available at a higher energy state relative to the lower energy state.

Following are the conditions to achieve population inversion

- The system should possess at least a pair of energy levels ( $E_2 > E_1$ ) separated by an energy equal to the energy of a photon ( $h\nu$ ).
- There should be continuous supply of energy to the system such that the atoms must be raised continuously to the excited state.



## **IMPORTANT COMPONENTS OF A LASER**

The three main important components of Laser are

- 1. Amplifying Medium,**
- 2. The Pumping source and**
- 3. Optical Resonator/cavity.**

### **1. Amplifying Medium or Active Medium**

A medium in which light gets amplified is called an **active medium**. The medium may be a solid or liquid or gas. Out of different number of atoms in a medium, only a small fraction of atoms of a particular species are responsible for stimulated emissions and consequent light amplification. They are called **active centers**. The remaining bulk of the medium plays the role of a host and supports the active centers.

### **2. Pumping Source**

For realizing and maintaining the condition of population inversion, the atoms have to be raised continuously to the excited state. This requires energy to be supplied to the system.

**The process of supplying energy to a system with a view to transfer it in to the state of population inversion is called pumping and the source which supplies the energy is called pumping source.**

Out of various pumping techniques, a few mechanisms are often employed. They are,

- Optical Pumping
- Electrical Pumping
- Inelastic atom-atom collision
- Direct Conversion
- Chemical Reaction

### **Optical Pumping**

In optical pumping, a coherent radiation can be use for exciting the laser medium. Generally arc lamps and tungsten lamps are used in continuous lasers. Flash lamps are used in pulsed lasers. In general, optical pumping is used in solid lasers and liquid lasers.

### **Electrical Pumping**

In electrical pumping, a discharge is created in the medium which excite the population inversion. This type of pumping is used in gas lasers.

### **Inelastic atom-atom collision**

Here, an indirect use of electric field is observed. Electric discharge first ionizes one type of atoms and excites them. These atoms collide in-elastically with other type of atoms and excite them. The second type of provide the population inversion needed for the lasing action.

### **Direct Conversion**

In some semiconductors, lasing action is produced by the conversion of electrical energy into light energy, in which recombination of electrons and holes occur.

### **Chemical Reaction**

In chemical lasers, the excitation energy comes from a chemical reaction without any need for the other source.

### 3.Optical Resonator or Resonant Cavity

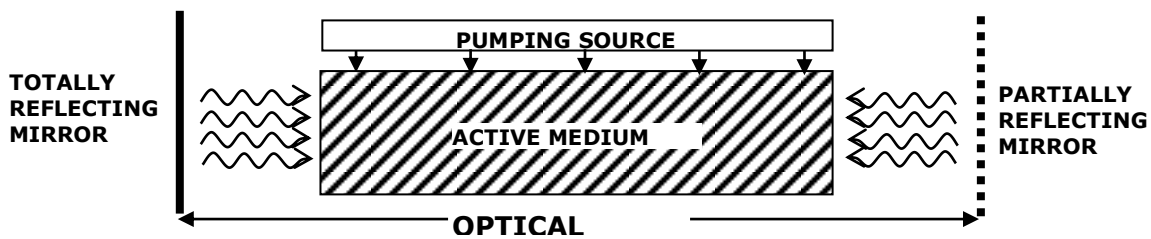
An optical cavity consists of an active medium enclosed between a pair of parallel mirrors facing each other. Among the two mirrors, one is completely reflecting and the other is partially reflecting.

Along with the stimulated emission components, we also get spontaneous emission components during the lasing process. But, we need only that beam which results from the stimulated emission.

Hence, **we need a mechanism to suppress spontaneously emitted light and allow stimulated emissions to grow in intensity and come out. Such an arrangement in the laser is called an optical cavity.**

The light which resulted from stimulated emissions to and fro between the mirrors along the direction of optic axis. Once the beam is sufficiently intense, some part of it escapes from the partially reflecting mirror, giving a laser output. The other radiations, if any, are absorbed by the cavity and are thus eliminated.

The block diagram of a laser is shown in the figure below.



### RUBY LASER

Ruby is basically  $\text{Al}_2\text{O}_3$  crystal containing about 0.05% of chromium atoms. The  $\text{Al}^{+3}$  ions in the crystal lattice are substituted by  $\text{Cr}^{+3}$  ions. These chromium ions constitute the active centers. Due to these chromium ions, crystal is pink in color.

Ruby laser was first fabricated in the year 1960 by Maiman.

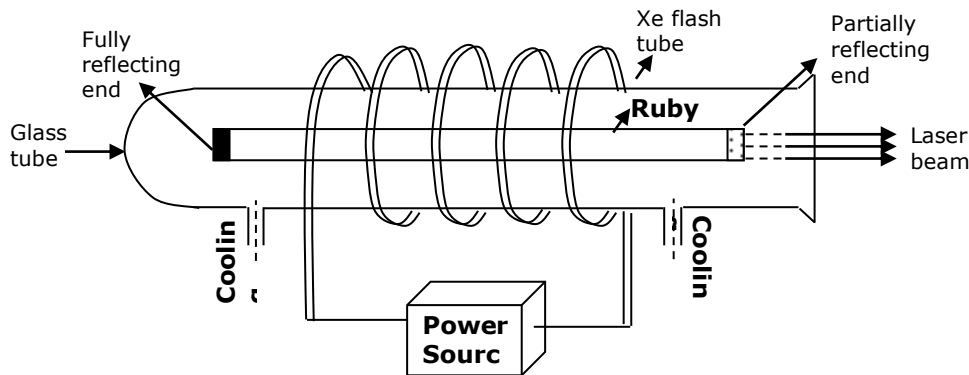
### Construction

**Active medium** is a rod of ruby crystal in the form of a cylinder which has 3 to 5 mm diameter and length of 5 to 30 cm.

**Pumping source** is a helical xenon flash lamp which is wound around the rod. This lamp is activated by a power supply.

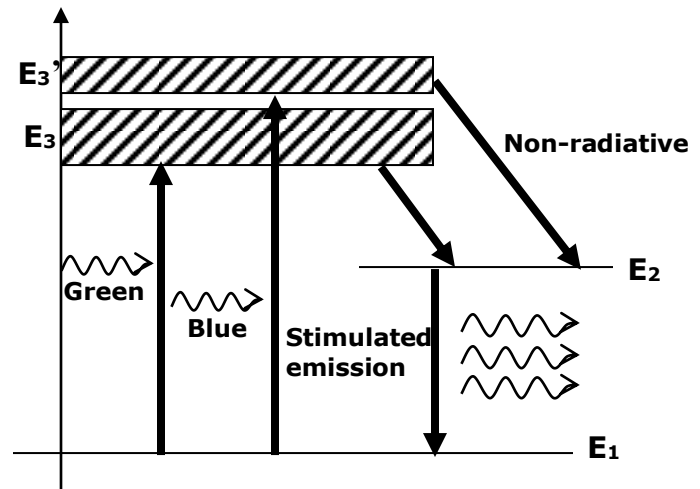
**Resonant cavity** made of fully reflecting end at the left and partially reflecting end at the right of the crystal. Both end faces of the rod are optically plane and exactly parallel to each other.

The flash of Xe tube consumes several thousand joules of energy. Only a part of this energy is used in pumping  $\text{Cr}^{+3}$  ions, while the rest heats up the apparatus. Hence, a coolant is used to cool the system.



### Working

- The energy levels of  $\text{Cr}^{+3}$  ions in the crystal lattice are shown in the fig. They form basically a three-level laser system.
- The Xe discharge generates an intense burst of white light lasting for a few milliseconds. The green component of the spectrum of wavelength centered on  $5500 \text{ \AA}$  is absorbed by  $\text{Cr}^{+3}$  ions.
- $\text{Cr}^{+3}$  ions rise to the band of levels  $E_3$  from  $E_1$ . These excited levels are highly unstable.

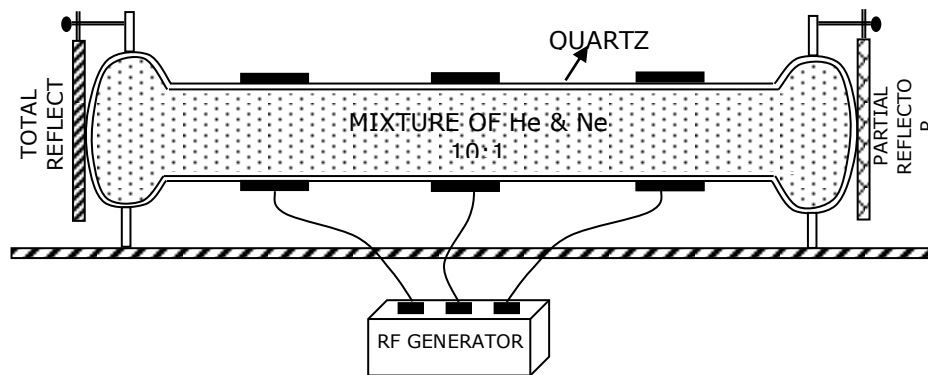


- The  $\text{Cr}^{+3}$  ions rapidly lose part of their energy  $E_3 - E_2$  to the crystal lattice and undergo non-radiative transitions to the state  $E_2$ .  $E_2$  is a meta stable state. Hence, chromium ions get accumulated there.
- If pumping occurs at a faster rate, the population at the level  $E_2$  exceeds that of  $E_1$  in a short time and population inversion is established between  $E_2$  and  $E_1$ .
- A spontaneous photon emitted by a  $\text{Cr}^{+3}$  ion at  $E_2$  level initiates the stimulated emission by other  $\text{Cr}^{+3}$  ions in the meta stable state.
- Photons traveling along the axial direction are repeatedly reflected and amplified and emerge out of the semi-transparent end in the form of a strong laser beam.
- The beam is red in color and corresponds to a wavelength of  $6943 \text{ \AA}$ .
- Green light plays the role of pumping. A random red photon radiated by one of the chromium spontaneously acts as an input and gets amplified.
- Once stimulated emissions commence,  $E_2$  level gets depopulated very rapidly and lasing occurs.

- The Xe lamp lasts only for a few milliseconds. Laser does not operate through out this period. Thus, the out put of the laser is in the form of pulses. This is considered to be a demerit of the ruby laser.

### He – Ne LASER

The main drawback of ruby laser is that the output beam is not continuous though very intense. For continuous beam, gas lasers are used. The first gas laser which was operated successfully was He-Ne laser in 1961 by Javan, Bennett and Harriot of Bell Telephone Labs.



### Construction

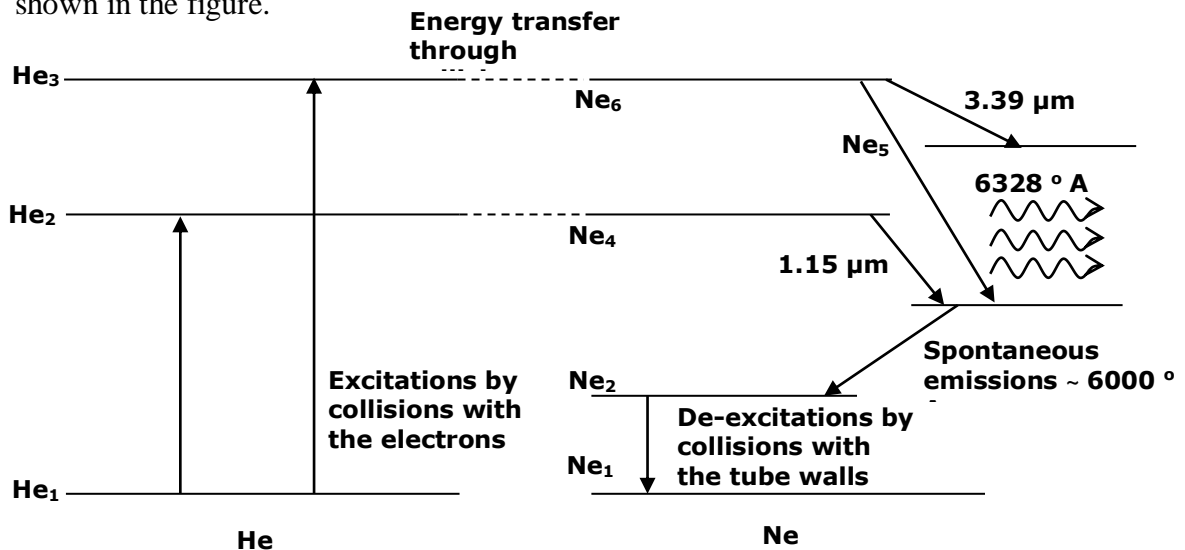
**Active medium** is a mixture of Neon under the pressure of 0.1mm of Hg and helium gas under the pressure of 1mm of Hg in the ratio 10:1. This mixture is placed in a long narrow discharge tube with a diameter of about 1.5cm and 10 to 100cm long

**Pumping source** is an electrical discharge produced by the electrodes connected to a high voltage power supply. In gas lasers since the atoms are characterized by sharp energy levels as compared to those in solids, the electric discharge method is used to pump the atoms to the higher energy levels.

**Optical cavity** constitutes two windows arranged at the ends of the glass tube. One window is completely polished and the other is partially polished.

### Working

- The He - Ne laser employs a four-level pumping scheme. The energy level diagram is shown in the figure.





- When the power is switched ON, the electric field ionizes some of the atoms in the gaseous mixture. The He atoms are more readily excitable than the Ne atoms because they are lighter.
- The energetic electrons excite the He atoms through collisions to the energy levels He<sub>2</sub> & He<sub>3</sub> (19.81 eV and 20.61 eV )
- These two states are meta stable states. With passage of current through the discharge tube more and more He atoms accumulate in the higher energy states.
- These He atoms return to the ground state by transferring their energy to Ne atoms through collisions. Such an identical energy transfer can take place when the colliding atoms have identical energy states.
- The Ne<sub>4</sub> and Ne<sub>6</sub> states of Ne atoms nearly coincide in energy with He<sub>2</sub> & He<sub>3</sub> (20.66 eV and 18.7 eV). Thus, Ne atoms move to these states on colliding with the He atoms.
- The kinetic energy of the He atoms provides the additional 0.05 eV for exciting the Ne atoms to Ne<sub>6</sub>.
- Thus, Ne atoms are active centers and the role of the He atoms is to excite them and cause population inversion.
- The probability of energy transfer from He atoms to Ne atoms is more as there are 10 He atoms to 1Ne atom in the mixture. For this reason the transfer of energy from Ne to He is extremely small.
- Ne<sub>4</sub> and Ne<sub>6</sub> states are meta stable. Successive collisions with the He atoms increase the population of these states.
- At ordinary temperature, Ne<sub>3</sub> and Ne<sub>5</sub> are sparsely populated and population inversion is achieved between Ne<sub>6</sub> – Ne<sub>5</sub>, Ne<sub>6</sub> – Ne<sub>3</sub> and Ne<sub>4</sub> - Ne<sub>3</sub>
- Random photons emitted spontaneously sets on stimulated emissions and coherent radiation is produced.
- Ne<sub>6</sub> – Ne<sub>5</sub> : a far infra-red beam of wavelength 3.39μm  
Ne<sub>6</sub> – Ne<sub>3</sub> : a red laser beam of wavelength 6328 °A  
Ne<sub>4</sub> - Ne<sub>3</sub>: infra red beam of wavelength 1.15 μm
- From the terminal levels Ne<sub>5</sub> & Ne<sub>3</sub> the atoms can make spontaneous transitions to the level Ne<sub>2</sub>. Incoherent light is emitted due to these. As lower lasing levels depopulate faster than the upper levels, it is easier to maintain the population inversion between the lasing levels through out the laser operation.
- Ne atoms accumulate at the Ne<sub>2</sub> level since it is a meta stable state. But, when they drift towards the tube wall and collide with it, they give out their energy quickly and fall to the ground state.
- Otherwise the number of atoms available in the ground state decreases and the laser output decreases.
- To increase the probability of the atomic collisions with the walls, the glass tube is made very narrow.

## **APPLICATIONS OF LASERS**

Due to the outstanding characteristics, laser has a remarkable importance in various fields. Some of them are listed below.

### **Communication**

- It is possible to transmit thousands of TV programs to the entire world simultaneously using lasers.
- Lasers make communication between moon and earth possible
- Extremely useful in optical fiber communication.

### **Computers**

- Using lasers, we can transmit an entire memory bank from one computer to another.
- Laser is used to read the data from CD-ROM as well as to print computer printouts

### **Chemistry**

- It is possible to investigate the structure of molecules.
- Some chemical reactions can be accelerated using lasers
- New chemical compounds can be created by breaking the bonds between atoms and molecules.

### **Industry**

- High power laser is used to weld or melt any material
- Using lasers, minute holes can be made in the crystals without any damage in crystal structure.

### **Medicine**

- For treatment of cancer tissues, skin tumors and to modify the detached retina.
- CO<sub>2</sub> laser is widely used in microsurgery and neurosurgery
- Used in endoscopy to scan inner parts of the stomach.

### **Military**

- Laser can be used for detection and ranging (LIDAR)
- A laser beam can be used to destroy objects like aircrafts, missiles etc.

**INTRODUCTION**

Solids are broadly classified as crystalline and non-crystalline. A crystal consists of a regular periodic arrangement of atoms in all directions, whereas a non-crystalline substance is marked by a random arrangement of atoms.

Crystalline substances can be further classified as

- **Single crystalline**, which has only one crystal as a whole
- **Poly crystalline**, which is an aggregate of many small crystals separated by well-defined boundaries.

Non-crystalline solids are also called amorphous solids. They have no directional properties and hence they are isotropic. These solids do not possess a regular shape and they have a wide range of melting point.

A crystal has a sharp melting point. Since the crystalline solids may have different periodic arrangements in all three directions, the physical properties of the crystal vary with the direction. Hence, these substances are anisotropic.

We shall study various crystal structures while running through this chapter.

**SPACE LATTICE**

The atomic arrangement in a crystal varies in its periodicity with the direction. It is easy to imagine points at which these points are located. Such points in the space are called **lattice points** and the totality of such points forms a space lattice or crystal lattice.

**A space lattice is defined as, an infinite array of points in three dimensions, in which every point has surroundings identical to that of every other point in the array.**

**Or**

**A space lattice is defined as, an infinite collection of points in space such that every point in the collection possess the same environment.**

We see that the distance between any two points in a particular direction is the same. This distance between the points may or may not vary from direction to direction. We refer this distance between the points to as the periodicity of the lattice. By the repeated translation of two vectors  $\bar{a}$  &  $\bar{b}$  on the plane of the paper, we get a 2D lattice. Here,  $\bar{a}$  is called the periodicity of the lattice in X-direction and  $\bar{b}$  is the periodicity of the lattice in Y-direction. These are also called the **lattice vectors**.

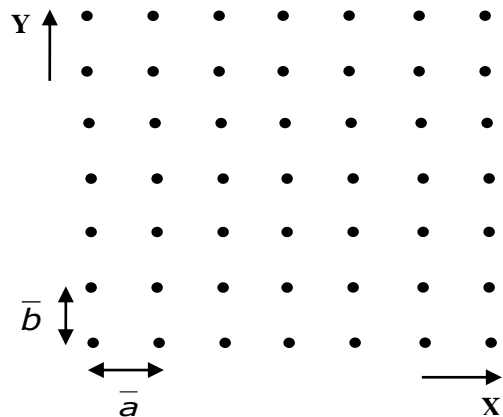
Let  $n_1$  be the number of translations along X-direction each of magnitude  $\bar{a}$ . Then its translation vector is given as,

$$\bar{T}_1 = n_1 \bar{a}$$

Let  $n_2$  be the number of translations along the Y-direction each of magnitude  $\bar{b}$ . Then its translation vector is given as,

$$\bar{T}_2 = n_2 \bar{b}$$

Let  $\bar{T}$  be the total translation vector so that,  $\bar{T} = \bar{T}_1 + \bar{T}_2$



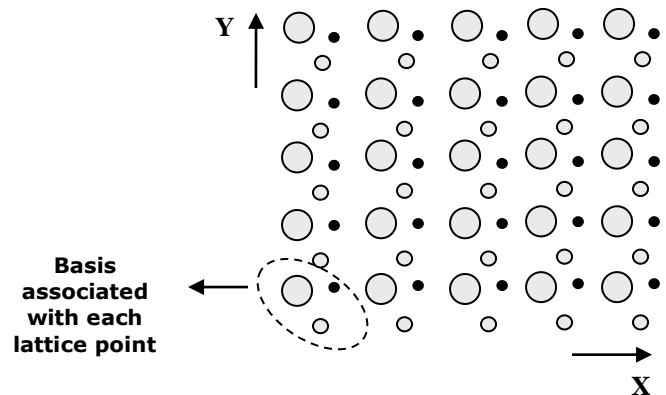
$\Rightarrow \vec{T} = n_1 \vec{a} + n_2 \vec{b}$ , where  $n_1$  and  $n_2$  are integers. In a 3D lattice,  $\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$  where  $\vec{c}$  is the periodicity of the lattice in Z-direction.

Space lattice is only a geometrical arrangement of lattice points in the space. It is purely imaginary concept. Each lattice point may be a collection of atoms or ions or molecules.

**BASIS:** Since a lattice point is an infinitesimal point in the space, it is an imaginary concept. When each atom of the crystal is replaced by a point, we are left with an infinite array of points in space.

Now the crystal structure is formed by associating with every lattice point, a set of atoms, or ions, or molecules identical in composition, arrangement and orientation. This set of atoms or ions or molecules is called the basis or motif.

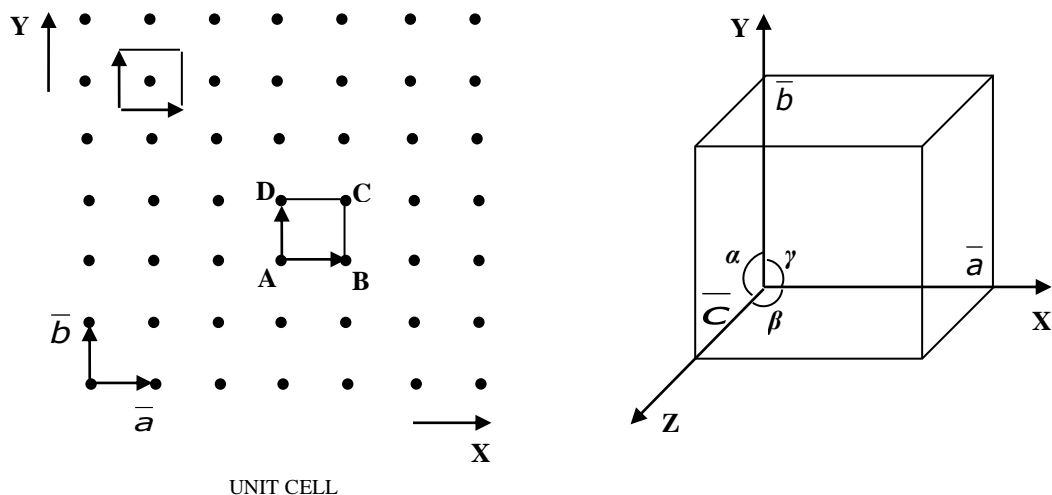
When this basis is repeated with periodicity  $(\vec{a}, \vec{b}, \vec{c})$  along X, Y, Z directions respectively, we get the crystal structure. Thus, lattice+Basis=Crystal Structure



### UNIT CELL AND LATTICE PARAMETERS

Consider a 2D lattice where  $\vec{a}$  &  $\vec{b}$  are the lattice parameters of two directions shown in figure. When a parallelogram such as ABCD is translated repeatedly by the vectors  $\vec{a}$  &  $\vec{b}$  corresponding to AB & AD, the whole array is obtained. This cell ABCD is called the unit cell.  $\vec{a}$  &  $\vec{b}$  are called the **basis vectors or lattice vectors**.

Thus, unit cell is the smallest geometric figure, the repetition of which in 3D will give the actual crystal structure. This cell is formed by the lattice vectors. Hence, it can be defined as, “**the smallest fundamental elementary pattern of minimum of atoms, which represents fully all the characteristics of the crystal**”(Or) “**the volume of a solid from which the entire crystal may be constructed by the translational repetition in three dimensions**”.



Unit cells are the building blocks that make up the crystal. A three-dimensional cell is shown in figure. It is a parallelepiped. This unit cell is described by the vectors  $\bar{a}, \bar{b}, \bar{c}$ . These three vectors form three angles between them, denoted by  $\alpha, \beta, \gamma$ . These angles are termed as **interfacial angles**. The three vectors  $\bar{a}, \bar{b}, \bar{c}$  and the three angles  $\alpha, \beta, \gamma$  constitute the **lattice parameters of a unit cell**.

### PRIMITIVE CELL

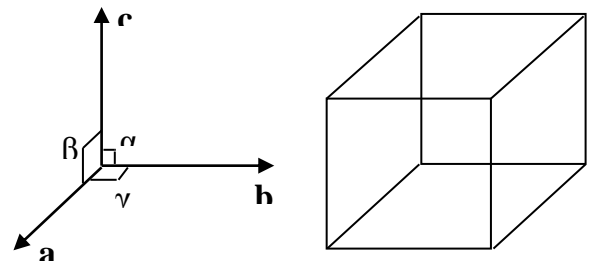
A parallelepiped, formed by lattice points only at their corners is called a primitive cell or simple cell. This is defined as, “**a geometrical shape which, when repeated infinitely in three dimensions, will fill all the space and is equivalent of one lattice point**”.

**CRYSTAL SYSTEMS:** There are 32 classes of crystals based on geometrical considerations. All these classes of crystals are classified into seven different systems based on the angles between the three axes,  $\alpha, \beta, \gamma$  and the intercepts of the faces along them  $\bar{a}, \bar{b}, \bar{c}$ . These crystal systems, in the order of symmetry, are discussed below:

**CUBIC:** This is the most symmetric system. In this system, all the lattice vectors are equal and the interfacial angles are mutually perpendicular to each other.

i.e.  $\bar{a} = \bar{b} = \bar{c}$ , and  $\alpha = \beta = \gamma = 90^\circ$

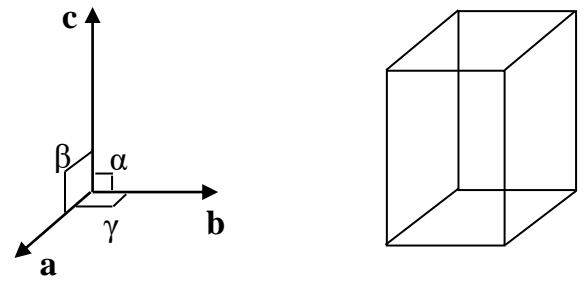
**Examples:** diamond, zinc sulphide (ZnS), anhydrous chlorides of alkali metals



**TETRAGONAL:** The symmetry decreases from cubic system. In this system, only two lattice vectors are equal and the angles are mutually perpendicular to each other.

i.e.  $\bar{a} = \bar{b} \neq \bar{c}$ , and  $\alpha = \beta = \gamma = 90^\circ$

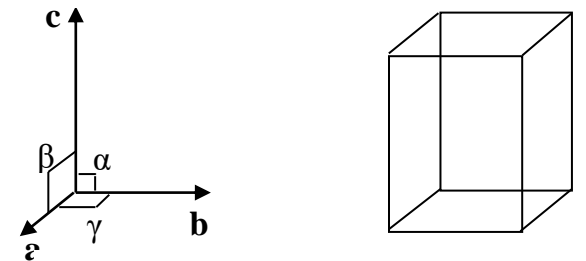
**Examples:** white tin SnO<sub>4</sub>, titanium oxide TiO<sub>2</sub>, etc.



**ORTHORHOMBIC:** The crystal axes are perpendicular to each other, but the lattice vectors are different along the three axes in the orthorhombic system.

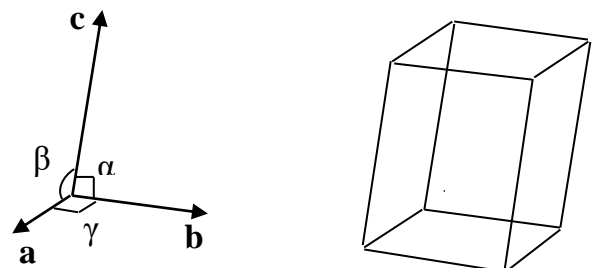
i.e.  $\bar{a} \neq \bar{b} \neq \bar{c}$ , and  $\alpha = \beta = \gamma = 90^\circ$

**Examples:** Celestine (SnSO<sub>4</sub>), olivine (Mg<sub>2</sub>SiO<sub>4</sub>), carnallite (KCl.MgCl<sub>2</sub>.5H<sub>2</sub>O)



**MONOCLINIC:** This system is also called monosymmetric system. In this system, all the lattice vectors are different and two angles are right angles.

The third angle is unequal to these two. i.e.  $\bar{a} \neq \bar{b} \neq \bar{c}$ , and  $\alpha = \beta = 90^\circ \neq \gamma$

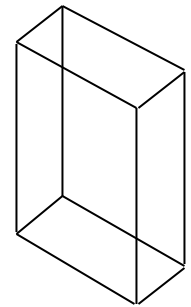
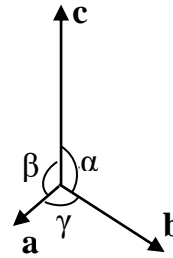


**Examples:** borax ( $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$ ), cryolite ( $\text{Na}_3\text{AlF}_6$ ) etc.

**TRICLINIC:** This is the most asymmetric crystal. In this system, neither of the three lattice vectors nor the angles are equal and none of these are right angles.

i.e.  $\bar{a} \neq \bar{b} \neq \bar{c}$ , and  $\alpha \neq \beta \neq \gamma \neq 90^\circ$

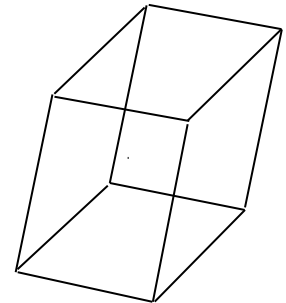
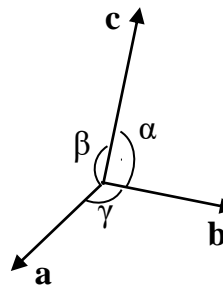
**Examples:** potassium dichromate ( $\text{K}_2\text{Cr}_2\text{O}_7$ ), sassolite ( $\text{H}_3\text{BO}_3$ ), albite ( $\text{NaAlSi}_3\text{O}_8$ ), etc.



**RHOMBOHEDRAL (TRIGONAL):** In this system, all the lattice vectors are equal and all the angles are equal. But, the angles are not right angles. This system is a three dimensional extension of a rhombus.

i.e.  $\bar{a} = \bar{b} = \bar{c}$ , and  $\alpha = \beta = \gamma \neq 90^\circ < 120^\circ$

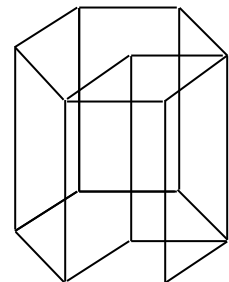
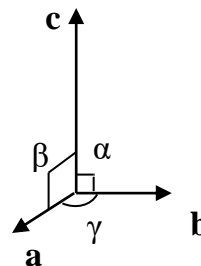
**Examples:** quartz, calcite ( $\text{CaCO}_3$ ), arsenic (As), antimony (Sb), bismuth (Bi) etc.



**HEXAGONAL:** The hexagonal system has eight faces. The two equilateral axes are equal and intersect at an angle of  $120^\circ$ .

i.e.  $\bar{a} = \bar{b} \neq \bar{c}$ , and  $\alpha = \beta = 90^\circ, \gamma = 120^\circ$

**Examples:** zincite ( $\text{ZnO}$ ), ice ( $\text{H}_2\text{O}$ ), apatite ( $\text{CaCl}_2 \cdot 3\text{Ca}_3(\text{PO}_4)_2$ ) etc.



## **BRAVAIS LATTICES**

There are many number of ways in which an actual crystal may be built up and atoms can be piled together resulting in many crystal structures. It was shown by Bravais in 1948 that there are only 14 different arrays or networks of lattices in which points can be arranged in the space so that each point has identical surroundings. These are known as Bravais lattices.

i.e. **the possible number of ways in which we can arrange atoms in a crystal system such that the arrangement becomes a space lattice, are said to be the Bravais lattices associated with that particular crystal system.**

**If all the atoms at a single lattice point are identical, then such a space lattice is called a Bravais lattice.**

There are four maximum ways of arranging atoms in a crystal system. They are:

P – Primitive lattice (which has atoms only at the corners of the cell)

C – Base centered lattice (has an extra atom at the center of the base)

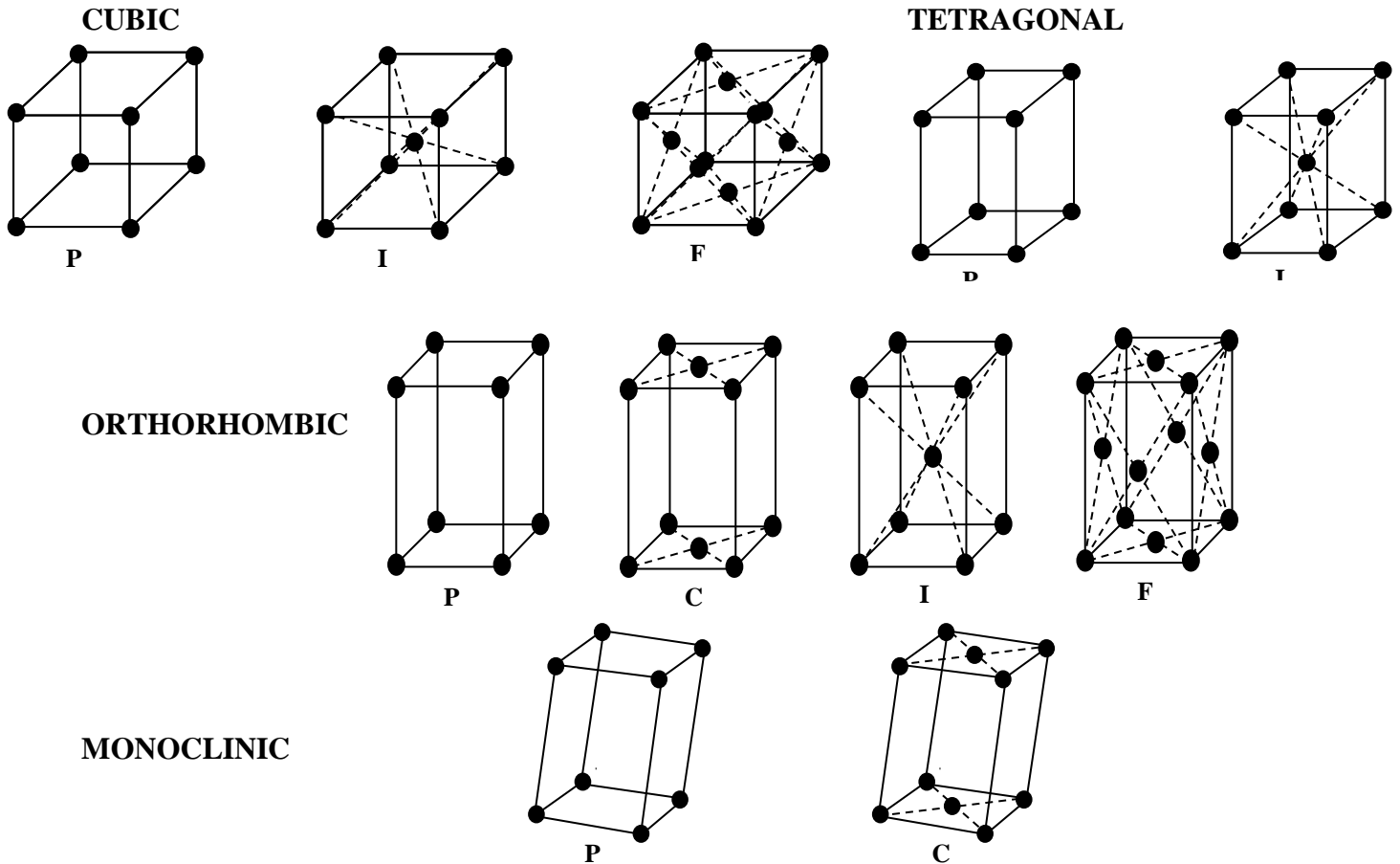
I – Body centered lattice (has an extra atom at the center of the base)

F – Face centered lattice (has an extra atom at the center of each face of the cell)

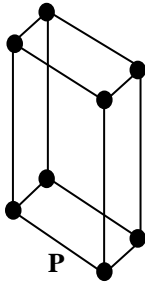
In three dimensions, we have altogether, 14 Bravais lattices for the seven crystal systems. Of these 7 are primitive and 7 are non-primitive.

The 14 Bravais lattices are shown in the figure below:

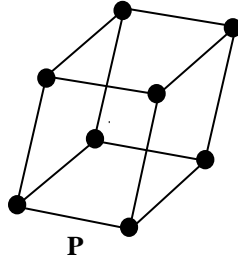
SYSTEM	BRAVAIS LATTICES	UNIT CELL	NO. OF LATTICES IN THE SYSTEM
Cubic	P, F, I	$\bar{a} = \bar{b} = \bar{c},$ $\alpha = \beta = \gamma = 90^\circ$	3
Tetragonal	P, I	$\bar{a} = \bar{b} \neq \bar{c},$ $\alpha = \beta = \gamma = 90^\circ$	2
Orthorhombic	P, C, I, F	$\bar{a} \neq \bar{b} \neq \bar{c},$ $\alpha = \beta = \gamma = 90^\circ$	4
Monoclinic	P, C	$\bar{a} \neq \bar{b} \neq \bar{c},$ $\alpha = \beta = 90^\circ \neq \gamma$	2
Triclinic	P	$\bar{a} \neq \bar{b} \neq \bar{c},$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$	1
Trigonal	P	$\bar{a} = \bar{b} = \bar{c},$ $\alpha = \beta = \gamma \neq 90^\circ < 120^\circ$	1
Hexagonal	P	$\bar{a} = \bar{b} \neq \bar{c},$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	1



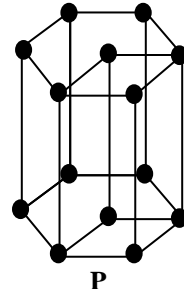
## TRICLINIC



## TRIGONAL



## HEXAGONAL



## IMPORTANT PARAMETERS

**Coordination Number:** The coordination number is defined as, the number of equidistant neighbours that an atom has in a given crystal structure. Greater coordination number indicates the close packing of the atoms in the crystal.

**Packing Factor:** { packing fraction or packing density} It is defined as, the ratio of the volume occupied by the atoms in the unit cell to the volume of the unit cell. The packing fraction varies from 0.34 to 0.74 for different crystal structures.

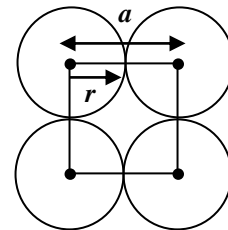
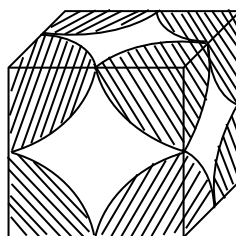
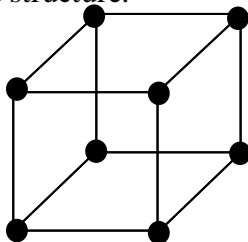
**Nearest Neighbor Distance:** The distance between the centers of two nearest neighboring atoms is called the nearest neighbor distance.

**Atomic Radius:** It is defined as half the distance between the nearest neighbors in a crystal of pure element.

## SIMPLE CUBIC STRUCTURE

In a simple cubic lattice, there is one lattice point at each of the eight corners of the unit cell. The lattice parameters of cubic structure is  $\bar{a} = \bar{b} = \bar{c}$ ,  $\alpha = \beta = \gamma = 90^\circ$

**Coordination number** If we take an atom at one corner as a center, it is observed that this atom is surrounded by six atoms at same distance. Hence, the coordination number is **6**. So, it is a loosely packed structure.



**Polonium** exhibits this structure.

**Nearest neighbor distance** Now, if we consider a unit cell of simple cubic structure, we see that the atoms touch each other along the edge of the cube. Hence, the nearest neighbor distance is  $2r$ . This is nothing but the edge of the cube i.e.  $2r = a$



**Atomic radius** it is half the nearest neighbor distance. Since 'a' is the nearest neighbor distance, the atomic radius is  $\frac{a}{2}$ .

### Effective number of atoms per unit cell

Each corner atom is shared equally by eight neighboring unit cells so that each unit cell shares only  $1/8^{\text{th}}$  part of the atom.

Hence, equivalent or effective number of atoms in a unit cell of a simple cube =  $8 \times \frac{1}{8} = 1$

Hence, this cell is a primitive cell.

### Atomic packing factor

If we assume that the shape of the atom is spherical, then its volume  $v$  is given by  $\frac{4}{3} \pi r^3$

But, the volume of the unit cell,  $V$  is  $a^3 = (2r)^3 = 8r^3$

Now, the packing factor =  $\frac{v}{V}$

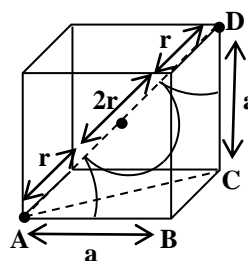
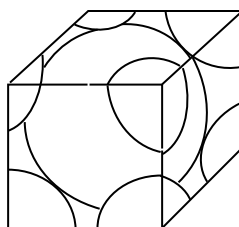
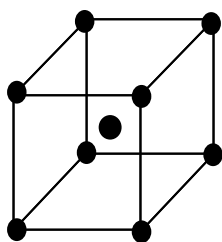
$$\therefore \text{Packing factor} = \frac{\frac{4}{3} \pi r^3}{8r^3} = \frac{\pi}{6} = 0.52 \text{ or } 52\%$$

This indicates that, in simple cubic structure, only 52% of the unit cell is occupied by the atoms and the remaining 48% is left empty.

## BODY CENTERED CUBIC STRUCTURE

In this structure, there are eight atoms at the eight corners and another at the center of the body.

**Coordination number** Here, if we consider the body-centered atom as the origin, we find eight equidistant neighbors to this atom. Thus, the coordination number is **8**.



Elements that exhibit this structure are **Li, Na, K, and Cr**.

The corner atoms do not touch each other but the corner atoms touch the body center atom along the body diagonal. The nearest neighbor distance is  $2r$ . Now let us calculate the nearest neighbor distance in a body centered cubic structure.

We see that the triangles ABC & ACD are right angled at B & C respectively. Now applying the Pythagoras theorem for the  $\Delta ABC$ , we get

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

$$\Rightarrow AC^2 = a^2 + a^2 = 2a^2$$

Similarly, in  $\Delta ACD$

$$AD^2 = AC^2 + CD^2$$

$$\Rightarrow AC^2 = 2a^2 + a^2 = 3a^2$$

But, from the figure we can say that  $AD = 4r$

$$\therefore (4r)^2 = 3a^2 \quad \Rightarrow a^2 = \frac{(4r)^2}{3}$$

$$\text{Hence, } a = \frac{4r}{\sqrt{3}}$$

**Effective number of atoms per unit cell** As the body-centered atom is situated inside the cell, the corner atoms, each, are shared by eight cells. Thus, the effective number of atoms in BCC is given by  $8 \times \frac{1}{8} + 1 = 2$

**Atomic packing fraction**

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

$$\text{Volume occupied by the atoms, } v = 2 \times \frac{4}{3} \pi r^3$$

Hence, the packing fraction is given by,  $\frac{v}{V} \therefore$

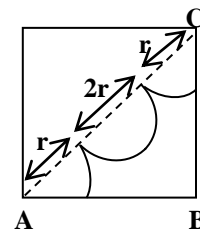
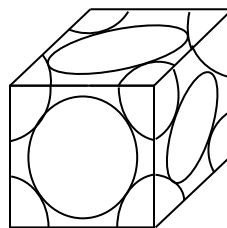
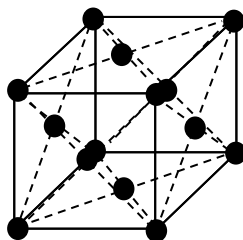
$$\text{P.F} = \frac{2 \times \frac{4}{3} \pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3} = \frac{\pi\sqrt{3}}{8} = 0.68 = 68 \%$$

i.e. 68% of the unit cell is occupied by the atoms and the remaining 32% is left empty. By comparing this fraction with that of the simple cubic structure, we can say that, BCC is relatively closely packed than the simple cubic structure.

### FACE CENTERED CUBIC STRUCTURE

In this structure, besides the eight atoms at the corners of the cube, we have six atoms at the center of each face of the cube.

**Coordination number** Considering the atom at a face center as the origin, it can be found that this face is common to two unit cells and there are twelve points surrounding it situated at a distance equal to half the face diagonal of a unit cell. Thus, the coordination number of FCC structure is **12**.



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

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

**Atomic radius** we know that the atomic radius is half the distance between the nearest neighbor atoms. Hence, radius of the atom is  $r = \frac{a}{2\sqrt{2}}$

**Effective number of atoms** In the FCC structure, there are eight atoms at the corners of the unit cell and six atoms at the centers of the each face of the unit cell. A face centered atom is shared by two unit cells. Thus, each atom gives only half of its volume to a particular cell.

Hence, the equivalent number of atoms in FCC structure is **Nearest neighbor distance** Here, the face centered atom touches the corner atoms along the face diagonal. The corner atoms do not touch each other. The nearest neighbor distance  $2r$  can be calculated in the following way

If we consider the triangle ABC we see that it is right angled at B. then applying the Pythagoras theorem we get

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

given by  $8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$

**Atomic packing fraction**

Volume of the unit cell  $V = a^3 = (2\sqrt{2})^3 r^3$

Volume occupied by the atoms  $v = 4 \times \frac{4}{3} \pi r^3$

Hence, Atomic packing fraction =  $\frac{v}{V} = \frac{4 \times \frac{4}{3} \pi r^3}{(2\sqrt{2})^3 r^3} = \frac{\pi}{3\sqrt{2}} = 0.74$  or 74 %

i.e. 74% of the unit cell is occupied by the atoms and the remaining 26% of the unit cell volume is left empty.

Thus, of the three Bravais lattices of the cubic crystal system we see that FCC structure is closely packed of all the structures.

**DIRECTIONS IN CRYSTALS**

Due to the anisotropy of crystals, several crystals exhibit different value for certain physical properties in different directions. Therefore, to relate the values of physical properties with corresponding directions, we need to identify or name the directions and planes in the crystals.

Let us consider the directions OA, OB, OC, and OD. A direction in a crystal is described by giving the first integer point (x, y) through which the line passes.

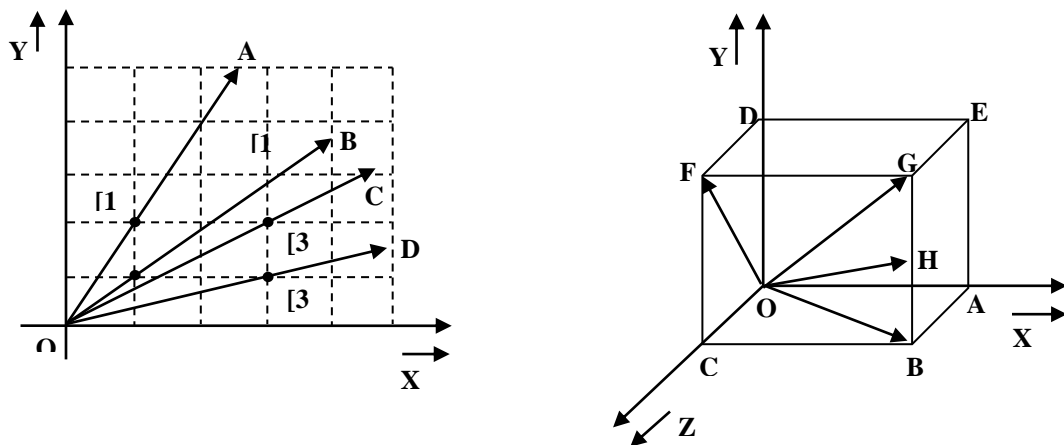
For example, the line OA is passing through the first point [x = 1 y = 2]. Similarly, the directions of OB, OC and OD are represented by [1 1], [3 2] and [3 1] respectively. **As a convention, square brackets are used to represent directions.**

In 3-D, it is represented by the first whole number point [x y z] through which the line passes. The directions of OA, OB, OF, OG and OH are represented by [1 0 0], [1 0 1], [0 1 1], [1 1 1], [1 2 1] respectively.

**CRYSTAL PLANES**

These are the two dimensional surfaces consisting of lattice points. The lattice points forming a space lattice may be thought of as occupying various set of parallel planes.

For a given lattice, a plane is not a single plane but it represents the planes, which are parallel to the earlier plane i.e. a set of parallel planes.



**A crystal is made up of a large number of parallel and equidistant planes passing through lattice points. These planes are called lattice planes.** These planes can be chosen in various number of ways. The perpendicular distance between the adjacent planes is called the **interplanar spacing**.

**MILLER INDICES**

A given space lattice may have an infinite set of lattice planes having its characteristic interplanar spacing. The set of planes are represented by certain numbers called **Miller indices**. Miller has given a method to designate a set of parallel planes in a crystal by three numbers (h k l) called, Miller indices. Now let us discuss the procedure of naming the planes in a crystal.

**Determination of Miller Indices**

The following are the steps to determine the Miller indices:

- Determine the coordinates of the intercepts made by the plane along the crystallographic axes
- Express the intercepts as the multiples of unit cell dimensions, or lattice parameters along the axes.
- Determine the reciprocals of these numbers
- Reduce the reciprocals to the smallest set of integral numbers and enclose them in brackets.

### Example

Consider a plane ABC, which intercepts X, Y, Z, axes at  $2a$ ,  $3b$ ,  $c$ . then the Miller indices of the plane are obtained as follows:

Step 1: obtain the intercepts made by the plane on the crystallographic axes.

$$\begin{array}{ccc} X & Y & Z \\ 2a & 3b & c \end{array}$$

Step 2: express the intercepts as multiples of unit cell dimensions

$$\begin{array}{ccc} \frac{2a}{a} & \frac{3b}{b} & \frac{c}{c} \\ 2, & 3, & 1 \end{array}$$

Step 3: determine the reciprocals of these numbers

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

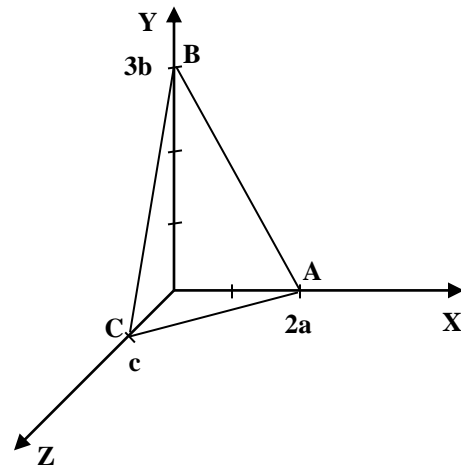
Step 4: convert these reciprocals into set of smallest integral number and enclose them in brackets.

$$6 \times \frac{1}{2}, 6 \times \frac{1}{3}, 6 \times 1 \text{ i.e. } (3 \ 2 \ 6)$$

In general, it is denoted by  $(h \ k \ l)$ . We also notice that,

$$\frac{1}{p} : \frac{1}{q} : \frac{1}{r} = h : k : l$$

$$\text{Here, } \frac{1}{2} : \frac{1}{3} : 1 = 3:2:6$$



Hence, **Miller indices can be defined as the reciprocals of the intercepts made by the crystallographic axes when reduced to smallest number.**

### Important Features of Miller Indices

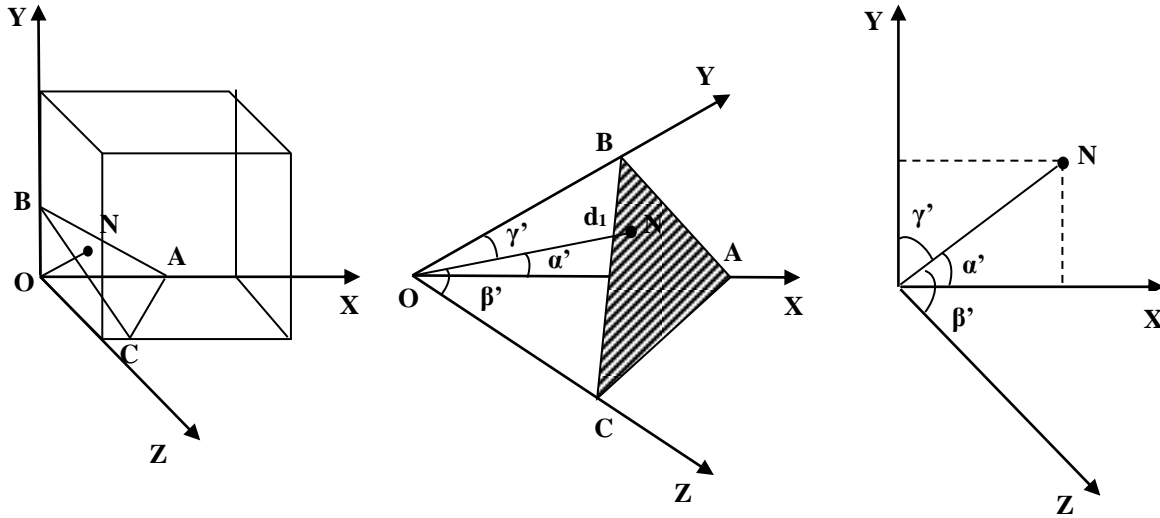
- All the parallel and equidistant planes have the same  $(h \ k \ l)$  values. Therefore, Miller indices define a set of parallel planes.
- If any plane is parallel to one of the axes, then its intercept is taken as infinity
- Any plane passing through the origin is defined in terms of parallel planes having non-zero intercepts.

- If  $(h k l)$  are the Miller indices of a plane, then the plane cuts the axes into  $h, k, l$  equal parts respectively.

### SEPARATION BETWEEN SUCCESSIVE $(h k l)$ PLANES

Let us derive an expression for the separation between two parallel planes in a crystal. Let us consider a cube with edge 'a'. Let  $(h k l)$  represent the Miller indices of the plane ABC. This plane belongs to a family of planes whose Miller indices are  $(h k l)$  because; these numbers represent a set of parallel planes.

Let  $ON = d$  be the perpendicular distance of the plane ABC from origin. Let  $\alpha', \beta', \gamma'$  be the angles made by  $ON$  with the coordinate axes respectively.



The intercepts made by the plane on the three axes are:

$$OA = \frac{a}{h}, OB = \frac{a}{k}, OC = \frac{a}{l} \quad \longrightarrow \quad (1)$$

From the figures we have,

$$\cos \alpha' = \frac{d_1}{OA}; \cos \beta' = \frac{d_1}{OB}; \cos \gamma' = \frac{d_1}{OC} \quad \longrightarrow \quad (2)$$

From figure (2), we have

$$\begin{aligned} ON^2 &= x^2 + y^2 + z^2 \\ \text{i.e. } d_1^2 &= [d_1^2 \cos^2 \alpha' + d_1^2 \cos^2 \beta' + d_1^2 \cos^2 \gamma'] \\ \Rightarrow [\cos^2 \alpha' + \cos^2 \beta' + \cos^2 \gamma'] &= 1 \quad \longrightarrow \quad (3) \end{aligned}$$

Substituting equation (3) in equation (2), we get

$$\begin{aligned} \left(\frac{d_1}{OA}\right)^2 + \left(\frac{d_1}{OB}\right)^2 + \left(\frac{d_1}{OC}\right)^2 &= 1 \\ \Rightarrow \left(\frac{d_1}{a/h}\right)^2 + \left(\frac{d_1}{a/k}\right)^2 + \left(\frac{d_1}{a/l}\right)^2 &= 1 \\ \frac{d_1^2}{a^2} (h^2 + k^2 + l^2) &= 1 \end{aligned}$$

$$\Rightarrow d_1^2 = \frac{a^2}{(h^2 + k^2 + l^2)}$$

$$\therefore d_1 = \frac{a}{\sqrt{(h^2 + k^2 + l^2)}} \longrightarrow (4)$$

Let  $OM = d_2$  be the perpendicular distance of the next plane parallel to the first plane ABC. The intercepts of this plane on the three crystallographic axes are,

$$OA' = \frac{2a}{h}, OB' = \frac{2a}{k}, OC' = \frac{2a}{l} \longrightarrow (5)$$

$$\text{and } \cos \alpha' = \frac{d_2}{OA'}; \cos \beta' = \frac{d_2}{OB'}; \cos \gamma' = \frac{d_2}{OC'} \longrightarrow (6)$$

$$OM^2 = [d_2^2 \cos^2 \alpha' + d_2^2 \cos^2 \beta' + d_2^2 \cos^2 \gamma']$$

$$\text{i.e. } d_2^2 = [d_2^2 \cos^2 \alpha' + d_2^2 \cos^2 \beta' + d_2^2 \cos^2 \gamma']$$

$$\Rightarrow [\cos^2 \alpha' + \cos^2 \beta' + \cos^2 \gamma'] = 1 \longrightarrow (7)$$

Now by substituting equations (5) & (6) in equation (7), we get

$$\Rightarrow \left(\frac{d_1}{2a/h}\right)^2 + \left(\frac{d_1}{2a/k}\right)^2 + \left(\frac{d_1}{2a/l}\right)^2 = 1$$

$$\Rightarrow \frac{d_1^2}{4a^2} (h^2 + k^2 + l^2) = 1$$

$$\Rightarrow d_1^2 = \frac{4a^2}{(h^2 + k^2 + l^2)}$$

$$\therefore d_1 = \frac{2a}{\sqrt{(h^2 + k^2 + l^2)}} \longrightarrow (8)$$

Thus, the interplanar spacing between two adjacent parallel planes with Miller indices  $(h k l)$  in a cubic lattice is given by,

$$d = d_2 - d_1$$

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

If the crystal is not cubic, then in general the distance between two  $(h k l)$  planes in a crystal is given by,

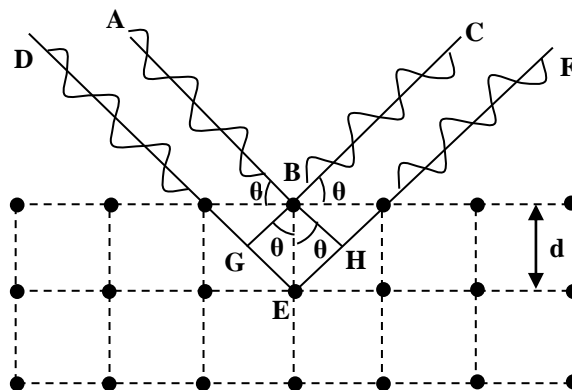
$$\therefore d = \frac{1}{\sqrt{\left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right)}}$$

### **BRAGG'S LAW**

Bragg's law predicts the conditions under which diffracted X-ray beams from a crystal are possible. In deriving it, we ignore the structure of the unit cell, which is related only to the intensities of these beams. W.L.Bragg has presented a simple explanation of observed angles of the diffracted beam from the crystal.

Consider a two-dimensional arrangement of atoms in a plane of a crystal as shown in the figure, which contains a set of parallel planes represented by straight lines. Suppose a parallel beam of X-rays is incident on the crystal, in a direction making a glancing angle  $\theta$  with surface of the planes.

As X-rays are much more penetrating than visible light, it is necessary to consider the rays reflected from several layers together. **There will be no diffracted beam unless the waves reflected from different planes are exactly in phase.** Now, they will reinforce themselves so that reflected waves are intensive in nature.



**The condition for the reflected waves to be in phase is that the path difference between the reflected waves from different planes must be integral multiples of the wavelength of the X-rays,  $\lambda$ .** When all the reflected waves are in phase, constructive interference takes place resulting in maximum intensity.

Consider two rays ABC & DEF which are reflected from different planes separated by a distance 'd', which is called interplanar separation. Let  $\theta$  be the angle made by the rays with different set of planes. The two rays are reflected from different points B & E from different planes. The path lengths of ABC & DEF are not same. Extend the ray AB to cut EF at H, and CB to cut DE at G. the path length of DEF is greater than that of the ray ABC by an amount (GE + EH)

Therefore, the path difference between two rays reflected form adjacent planes = (GE + EH)

From the geometry, it is understood that the angles GBE & EGH are each equal to  $\theta$ . The length of BE is equal to 'd'.

$$\therefore \frac{GE}{BE} = \frac{EH}{BH} = \sin \theta \Rightarrow GE = EH = (BE) \sin \theta$$

$$\Rightarrow GE + EH = d \sin \theta + d \sin \theta = 2d \sin \theta$$

The condition for diffraction maxima is that the path difference should be an integral multiple of wavelength, i.e.

$$\boxed{2d \sin \theta = n\lambda}$$

Where 'n' is the order of diffraction. **This is called Bragg's law.** This law gives the condition for the diffraction maxima for reflected X-rays from several planes. The angle of diffraction  $\theta$  is different for different diffraction orders.

If  $n = 0$ , it is called a zero order diffraction i.e. it has not experienced any diffraction.

$$\text{For first maxima, } n = 1, \theta_1 = \sin^{-1} \left( \frac{\lambda}{2d} \right) \quad \text{For second maxima, } n = 2, \theta_2 = \sin^{-1} \left( \frac{2\lambda}{2d} \right),$$

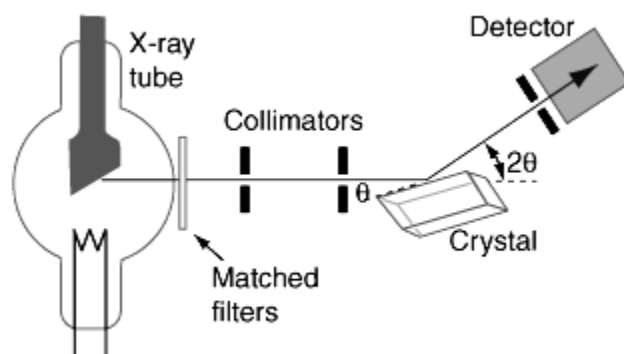
As the order of the maxima increases, their intensities decrease. The Bragg's law is a consequence of the periodicity of the space lattice. The intensity of different orders depends on the composition of atoms in the basis.



**Glancing angle:** the angle at which the reflection occurs is called the glancing angle. It is the angle between incident ray and the plane of reflection.

**Bragg's X-ray spectrometer:**

- The schematic diagram of Bragg's spectrometer is shown
- Collimated beams of X-ray are obtained by passing X-rays through the matched filters and collimators. This collimated beam of X-rays is allowed to fall on a crystal mounted on a circular table.
- The table can be rotated about vertical axis. Its position can be measured by verniers scale arrangement.
- A detector consists of an ionization chamber is fixed to the longer arm attached to the table.
- The position of which is measured by another verniers scale arrangement. An electrometer is connected to the ionization chamber to measure the ionization current produced by diffraction X-rays from the crystal.
- With help of electrometer we can measure the intensity of the diffracted beam. The slit made up of lead is provided just before the detector to limit the width of the diffracted beam.
- If X-rays incident at an angle  $\theta$  on the crystal, then reflected beam makes an angle  $2\theta$  with the incident beam.
- Hence the detector is precisely adjusted for  $2\theta$  to get the reflected beam till the rate of deflection is maximum. A plot of ionization current for different incident angles to study the X-ray diffraction spectrum is shown in fig.
- The rise in ionization current for different values of  $\theta$  shows that Bragg's law is satisfied for various values of n. i.e.  $2d\sin\theta = \lambda$  or  $2\lambda$  or  $3\lambda$  etc. peaks are observed at  $\theta_1, \theta_2, \theta_3$  etc. with intensities of  $I_1, I_2, I_3$  etc.
- i.e.  $2d\sin\theta_1 : 2d\sin\theta_2 : 2d\sin\theta_3 = \lambda : 2\lambda : 3\lambda$
- The crystal interplaner spacing  $d$  can be measured using  $2d\sin\theta = n\lambda$ .



## UNIT-III

### MAGNETIC PROPERTIES

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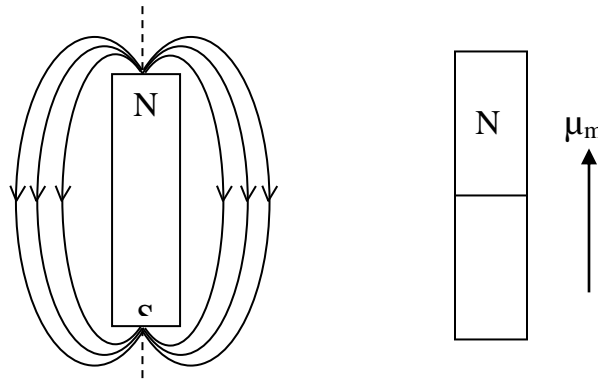
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#### INTRODUCTION

The iron ore magnetite is known to exhibit magnetic properties for more than two thousand years. The development of quantum physics helped to understand the phenomenon of magnetism to a great extent. It was established that the **magnetism of materials is mainly a consequence of the interactions of uncompensated magnetic moments of atoms or molecules.** Magnetic materials play a prominent role in modern technology. They are widely used in industrial electronics, computer industry etc.

#### MAGNETIC FIELD

The magnetic effects are greatly exhibited at the two ends of a bar magnet. These ends are called magnetic poles, the north and south poles. It is found that magnetic poles always occur in pairs and cannot be isolated. **The space around a magnet where its influence is experienced is known as the magnetic field.** The Danish physicist, Oersted discovered in 1819, that a current carrying conductor also produces a magnetic field.



#### FLUX

A magnetic field is schematically represented in diagrams by magnetic lines of force which are also called lines of magnetic induction. A line of induction is a curve whose tangent at each point indicates the direction of orientation of a small magnetic compass needle. These lines are collectively termed as flux.

#### MAGNETIC FLUX DENSITY (B)

The concentration of magnetic flux is called magnetic flux density. It is defined as the number of flux lines passing through unit area of cross-section. The unit of B in SI system is tesla (T) or  $\text{Wb/m}^2$ . The CGS unit for B is gauss (G).

$$1\text{G} = 10^{-4}\text{ T}$$

## MAGNETIC FIELD STRENGTH (H)

The magnetic field strength is defined as the force experienced by a unit north pole placed at a point in the field. The units of H are ampere-turns per meter, A/m in SI system and oersted, Oe in Gaussian system.

## MAGNETIC PERMEABILITY ( $\mu$ )

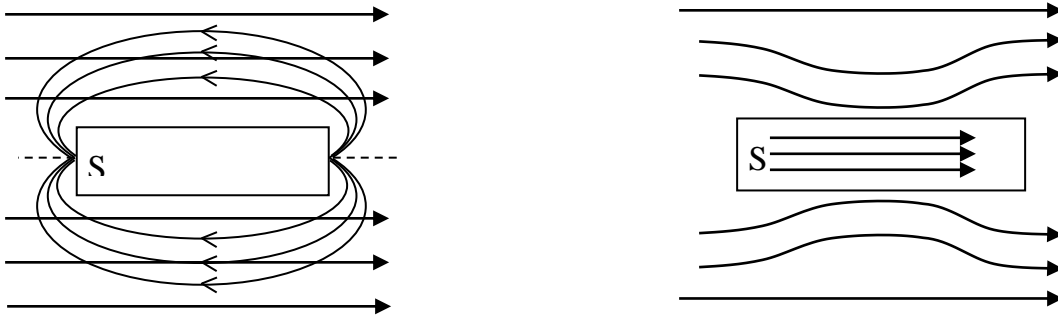
Consider an unmagnetised bar of magnetic material in a uniform magnetic field. The bar gets magnetized by induction and attains polarity. The magnetic lines in the bar emanate north pole pass through the outer region and reenter the bar from south pole, forming a closed loop.

The lines of the bar oppose the lines of original field outside the magnet and favor inside the magnet. Because of this, magnetic field strength H is increased inside the bar and decreased outside. Similarly, B becomes high inside the bar and low outside the bar.

Thus,  $\mathbf{B} \propto \mathbf{H}$

i.e.  $\mathbf{B} = \mu\mathbf{H}$

where  $\mu$  is a constant of proportionality, called absolute permeability of the medium.



If the flux density is established in the air or vacuum, or in a non-magnetic material, then

$$\mathbf{B}_0 = \mu_0\mathbf{H}$$

The ratio of  $\mu / \mu_0$  is called relative permeability, denoted by  $\mu_r$ . i.e.  $\mu_r = \mu / \mu_0 = B / B_0$ , where  $\mu_0 = 4\pi \times 10^{-7}$  henry/m

## MAGNETIZATION

The process of converting a non-magnetic specimen into a magnetic specimen is referred to as magnetization.

It may be regarded that each element in the volume of the solid behaves as a small magnet and the magnetic moment of the solid as a whole is a vector sum of the magnetic moments of all such elements.

Thus, **the magnetization M of the solid is defined as induced magnetic moment per unit volume.**

$$\text{i.e. } M = \frac{1}{V} \sum \mu_{mi}$$

Where  $\Delta v$  is the elementary volume and  $V$  is the total volume of the solid.

If a solid is placed in a magnetic field, the magnetic field lines are redistributed as compared with their distribution when the solid is not in the field. The solid somehow enhances the magnetic field induction. The resultant field may be viewed as the contribution from two sources; the primary field  $B_0$  and the field created by the solid.

$$\text{Thus, } B = B_0 + B_{\text{SOLID}}$$

$$\text{i.e. } B = \mu_0 H + \mu_0 M$$

$$B = \mu_0 (M + H)$$

## MAGNETIC SUSCEPTIBILITY

The magnetization of the material is proportional to the applied field  $H$ .

$$M = \chi H \Rightarrow \chi = \frac{M}{H}$$

where  $\chi$  is the proportionality constant, called magnetic susceptibility. **It is defined as the ratio of magnetization to the magnetic field strength.**

### RELATION BETWEEN $\chi$ & $\mu$

$$\begin{aligned} \text{We know that, } B &= \mu_0 (M + H) \\ &= \mu_0 (\chi H + H) \\ &= \mu_0 H (1 + \chi) \end{aligned}$$

$$\text{But, } B = \mu_r \mu_0 H$$

$$\mu_r = 1 + \chi$$

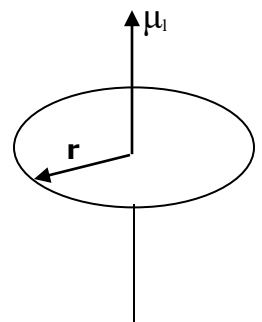
## ORIGIN OF MAGNETIC MOMENT

According to the Ampere's hypothesis, a plane current loop is equivalent to a magnetic dipole. i.e., a stationary loop carrying current in a plane produces a magnetic field, which at large distances may be described as resulting from a magnetic dipole whose moment is given by,

$$\mu = i \times A,$$

where 'i' is the current flowing through the loop and  $A$  is the area of the loop. The dipole direction is perpendicular to the plane of the loop. Electrons in an atom move in certain path about the nucleus of the atom. The electron motion can be described by assigning a certain angular momentum to each electron.

The magnetic properties of the substance are determined by the state of angular momentum which the electron may possess. **The state of the angular momentum depends not only on the orbital motion of electrons, but also on the spin of the electrons and the spin of the nucleus.**



## Magnetic Moment Due To Orbital Motion of Electron

Let's consider an electron moving with a constant speed  $v$  along a circular orbit of radius ' $r$ '. Let ' $T$ ' be the time taken to complete one revolution and ' $e$ ' be the charge on the electron. The charge that crosses any point in the orbit is,  $e/T$ . This is the current passing in the orbit.

$$\therefore I = \frac{e}{T} \longrightarrow (1)$$

The magnetic moment associated with the orbit according to Ampere's hypothesis is,

$$\mu_l = i \times A \longrightarrow (2)$$

where  $A$  is the area of the orbit. Since we have considered that the orbits are circular,  $A = \pi r^2$ .

$$\therefore \mu_l = \frac{e}{T} \times \pi r^2 \longrightarrow (3)$$

The angular velocity  $\omega = \frac{2\pi}{T} \Rightarrow T = \frac{2\pi}{\omega}$

$$\therefore \mu_l = \frac{e r^2 \omega}{2} \longrightarrow (4)$$

But, the angular momentum associated with the electron is,

$$P_l = mvr = m(r\omega) r = mr^2\omega$$

Hence, the equation (4) becomes,

$$\mu_l = \frac{e}{2m} P_l \longrightarrow (5)$$

The orbital angular momentum  $P_l$  in terms of orbital quantum number  $l$  can be written as follows

$$P_l = l \frac{h}{2\pi}$$

$$\therefore \mu_l = \frac{e}{2m} \cdot \frac{lh}{2\pi} = \frac{eh}{4\pi m} l \longrightarrow (6)$$

If  $l = 0$ ,  $\mu_l = 0$ . If  $l = 1$ ,  $\mu_l = \frac{eh}{4\pi m}$  and so on.

The quantity  $\frac{eh}{4\pi m}$  represents the smallest unit of magnetic moment and is called **Bohr**

**Magneton ( $\mu_B$ )**

$$\mu_l = \mu_B l$$

The value of Bohr Magneton  $\mu_B = 9.264 \times 10^{-24} \text{ A/m}^2$ . The ratio of orbital magnetic moment to the orbital angular momentum,  $\frac{\mu_l}{P_l}$  is called the **Gyro magnetic ratio, denoted by G**.

$$\therefore G = \frac{\mu_l}{p_l} = \frac{e}{2m}$$

It can also be written as,  $G = g \frac{e}{2m}$ , where 'g' is called Lande's splitting factor. Here, g = 1 for the orbital motion of the electron.

### Magnetic Moment Due To Electron Spin

The spinning electron behaves like a tiny magnet. Due to the spin motion, it possesses a spin magnetic moment. It is given by,

$$\mu_s = 2 \frac{e}{2m} p_s$$

where  $p_s$  is the spin angular momentum given by,

$$p_s = s \cdot \frac{h}{2\pi}$$

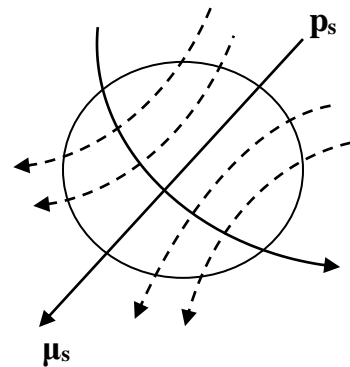
$$\text{Thus, } \mu_s = 2 \cdot \frac{e}{2m} \frac{sh}{2\pi} = 2s \frac{eh}{4\pi m}$$

But, the spin quantum number has only one value  $\frac{1}{2}$ .

$$\text{Thus, } s = \frac{1}{2}$$

$$\therefore \mu_s = \frac{eh}{4\pi m} = \mu_B$$

$$\therefore \mu_s = \mu_B$$



### Magnetic Moment Due To Nuclear Spin

Another contribution to the total magnetic moment of the atom may arise from nuclear magnetic moment. It was found that nucleus also possesses spin motion. Due to this spin motion of the positively charged nucleus, a magnetic moment is produced according to Ampere's theorem.

By analogy with the Bohr Magneton, the Nuclear Magnetron arises due to the spin of the nucleus, and is given by,

$$\mu_n = \frac{eh}{4\pi m_p}$$

where  $m_p$  is the mass of the proton. The value of  $\mu_N$  is  $5.05 \times 10^{-27} \text{ Am}^2$

### Spatial Quantization

Bohr's theory suggests that the magnitude and directions of the orbital angular momentum vector 'l' are quantized. This concept is referred to as spatial quantization. This introduces another

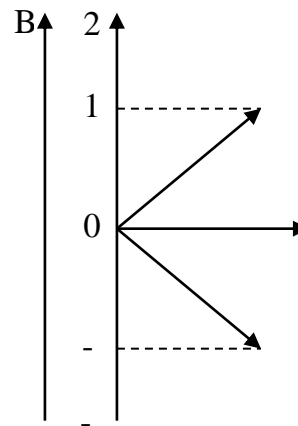
set of quantum numbers known as magnetic quantum number, denoted by  $m_l$ . this quantum number can assume the values from '1' to '-1'.

$$\text{i.e. } m_l = l, l-1, l-2, \dots, 0, \dots, -(l-2), -(l-1), -l$$

i.e.,  $(2l + 1)$  values.

**The equation  $\mu_l = \mu_B \cdot l$  implies that the electron in an atom can take only certain specified values of magnetic moment depending upon  $l$ .**

- In any magnetic field, the orientation of the atomic magnets tends to change.
- The orbital magnetic moment vector,  $\mu_l$  can take only those orientations for which the projections of the angular momentum vector along the field direction are integers specified by the magnetic quantum number.
- Let us consider a d-electron whose  $l = 2$ . The angular momentum vectors OA, OB, OC, and OE along the direction of the magnetic field, B are 2, 1, 0, -1, -2.
- $\mu_l = \mu_B \cdot m_l$ . The total magnetic moment contributed by the orbital motion of electrons in an atom can be vectorially added.
- Completely filled shell contributes nothing to the total magnetic moment of the atom.
- Even if there are unfilled shells, the contribution of their  $\mu_l$  to the total magnetic moment  $\mu$  is negligible, since it was found that the orbital magnetic moments of these elements and their compounds are **FROZEN**.
- i.e., they behave like immobile magnetic dipoles, which cannot be aligned by the external magnetic fields.



### TOTAL MAGNETIC MOMENT OF AN ATOM

The total magnetic moment of an atom is the vector sum of the orbital magnetic moment  $\mu_l$ , spin magnetic moment  $\mu_s$  and the nuclear magnetic moment  $\mu_N$ . Now let us discuss to what extent these three factors contribute to the total magnetic moment of the atom.

- The spatial quantization of the orbital angular momentum vector  $\mu_l$  does not allow it to align in the direction of the applied field. Hence, the contribution of  $\mu_l$  to the total magnetic moment,  $\mu$  of an atom is negligible.
- Since the mass of the proton is much larger than that of an electron the value of nuclear Magneton,  $\mu_N$  is so small. Hence, it provides no substantial contribution to the total magnetic moment of the atom.
- Since the magnitude of the spin magnetic moment is always the same, the external field can only influence its direction.
- If the electrons are not paired, then they are free to orient themselves in the direction of the external field.

- If the electrons in an atom are all paired up, then the spin magnetic moment of each electron is cancelled by that of the other such that the total spin magnetic moment,  $\mu_s$  is zero.
- Thus, if there exist any unpaired electrons in an atom, the resulting spin magnetic moment,  $\mu_s$  will be the vector sum of all those.
- Hence, **the total magnetic moment depends on  $\mu_s$  largely compared to  $\mu_l$  and  $\mu_N$ .**

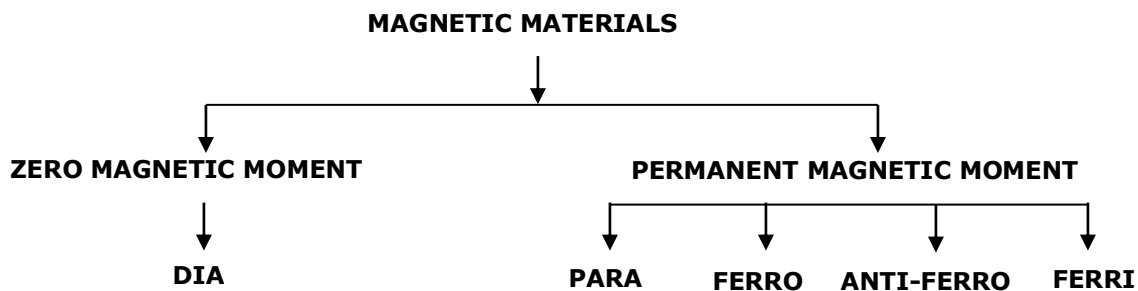
### CLASSIFICATION OF MAGNETIC MATERIALS

Any substance when placed in a magnetic field, behaves in a particular way, which is not the same for all the substances. This behavior depends on the magnetic dipoles associated with an atom in that particular substance.

Based on the permanent magnetic dipole moments, magnetic materials are classified into two broad groups.

- Materials composed of atoms having zero magnetic moment, called **diamagnetic**, and
- Materials composed of atoms having permanent magnetic moment. This class of materials is further classified into four types based on the interaction between the adjacent atoms. They are **paramagnetic, ferromagnetic, anti-ferromagnetic and ferromagnetic.**

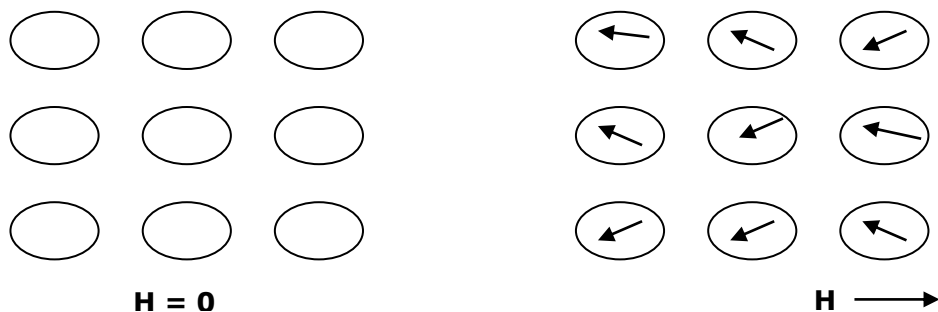
This classification can be schematically represented as follows.



### DIAMAGNETIC MATERIALS

**If in a material, the arrangement of the orbits and orientation is such that the vector sum of magnetic moment is zero, then the material is said to be a diamagnetic.**

The atoms in these materials do not possess permanent magnetic moment. When the material is placed in a magnetic field, the orbits of the electrons undergo a precessional motion. This is called Larmor's precession. This precessional motion of charge produces a current, which induces a magnetic field inside the atom. **This intrinsic magnetic field is opposite in direction to the external field. Thus, a diamagnetic material repels the external field.**





## PROPERTIES

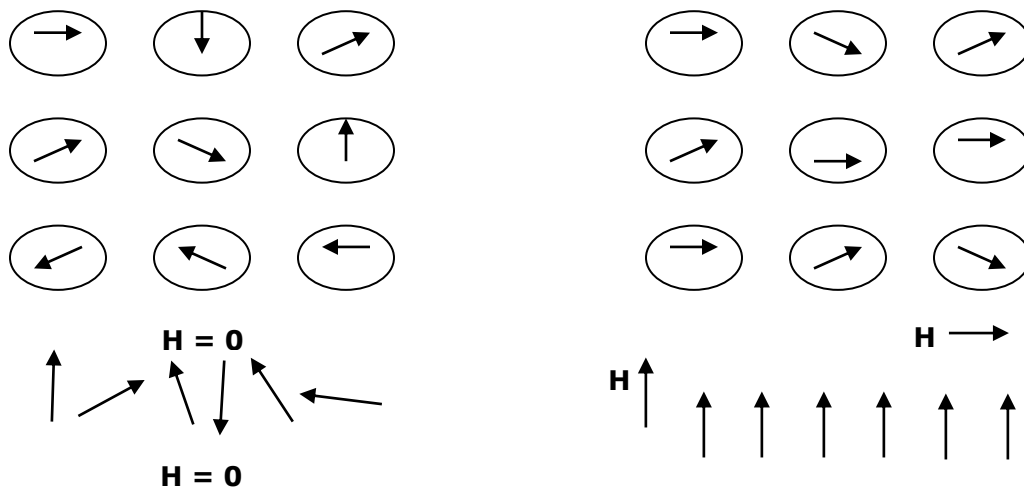
- The magnetic susceptibility  $\chi$  is negative and small. Temperature has no effect on the susceptibility of diamagnetic materials.
- The relative permeability  $\mu_r$  is less than 1, but positive. This means lines of magnetic field become less dense in the material than in the air.
- In general, the substances whose atoms possess paired electrons exhibit diamagnetism. There are some exceptions like Cu to this behavior.
- Examples of a diamagnetic substance are, bismuth (Bi), zinc (Zn), copper (Cu), silver (Ag), gold (Au), diamond, NaCl, water, nitrogen, hydrogen.

## PARAMAGNETIC MATERIALS

If in a material, the arrangement of orbits and the orientation is such that the vector sum of magnetic moments is non-zero, but small, then such substance is called a paramagnetic substance.

Paramagnetic materials are substances whose molecules possess a net permanent magnetic moment even in the absence of the field. These magnetic moments are randomly oriented in the absence of the external field. Hence, the net magnetization of the material is zero.

When the material is subjected to the influence of the magnetic field, the magnetic dipoles tend to align in the direction of the field, and the material becomes feebly magnetized.



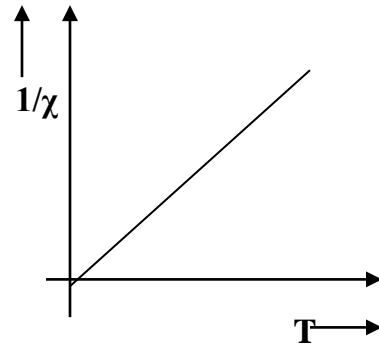
## PROPERTIES

- The magnetic susceptibility is small and positive ( $10^{-3}$  to  $10^{-5}$ )
- The relative permeability  $\mu_r$  is greater than 1 but small. This indicates that when a paramagnetic substance is placed in a uniform magnetic field, the field in the material will be more than the applied field.

- These substances have unpaired electrons in their valence orbit.
- **Temperature Dependence**

The thermal agitation tends to counteract the orientation of the dipoles. With an increase in the temperature, the increase in the thermal agitation tends to randomize the dipole directions thus decreasing the magnetization. Thus, the magnetic susceptibility decreases with magnetization.

$$\chi \propto \frac{1}{T} \Rightarrow \chi = \frac{C}{T}$$



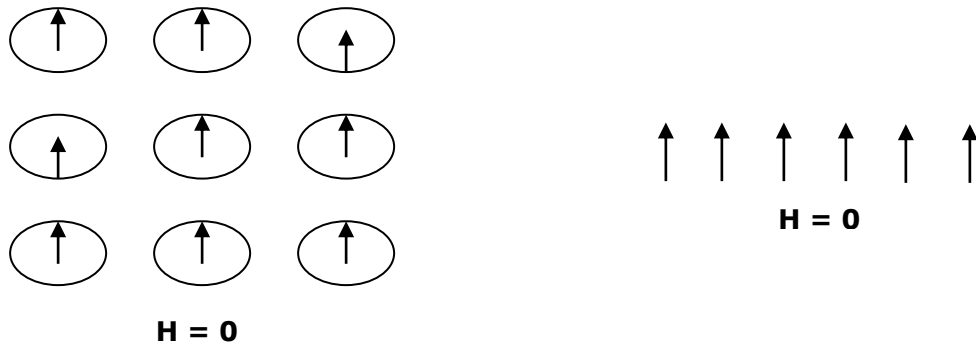
This law is called **Curie's law**, and C is called the Curie's constant.

### FERROMAGNETIC MATERIALS

**If in a material the orbits are so oriented that the atom as a whole possesses a large magnetic moment, then the material is called a ferromagnetic material.**

The spin magnetic moments are greatly responsible for ferromagnetism. In definite conditions, the spin moments of electrons become aligned parallel to one another even in the absence of external magnetic field. Thus, ferromagnetic materials are those which possess a magnetization even in the absence of magnetic field. This is called the **spontaneous magnetization**.

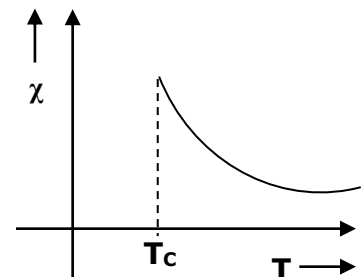
When placed in an external field, these substances get easily magnetized to a large value.



### PROPERTIES

- The susceptibility is very high and positive. (  $10^2$  to  $10^6$  )
- The relative permeability is also very high. Lines of force are very dense in ferromagnetic substances
- **Ferromagnetic substances exhibit hysteresis.**
- **Temperature Dependence**

The susceptibility is fairly high and constant up to certain temperature according to the equation,



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

This law is called **Curie-Weiss law**. 'T' is called the Curie temperature. When the temperature of the ferromagnetic substance is increased above a temperature called Curie temperature, thermal agitations dominate the existing interaction between the electron spins leading to randomization of the dipoles. Thus, **the spontaneous magnetization is lost above T' and the substance behaves as a paramagnetic material.**

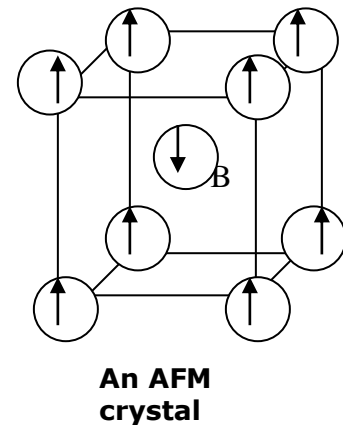
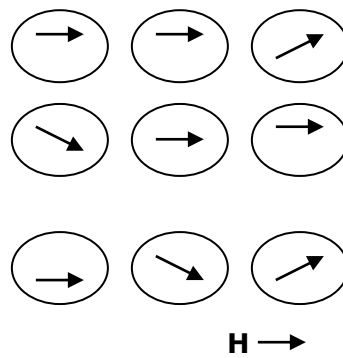
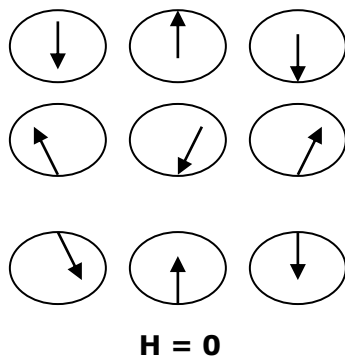
Examples ferromagnetic materials are, iron (Fe), nickel (Ni), cobalt (Co), Gadolinium (Gd).

### ANTIFERROMAGNETIC MATERIALS

This is the property of the substances whose spin moments of neighboring atoms are oriented in an anti-parallel order. i.e., **the alternate atoms have spin moments parallel to each other but, the adjacent atoms have not.**

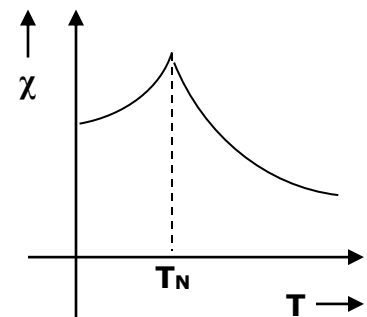
These crystals are composed of two interpenetrating sub-lattices A & B, one lattice consisting of atoms with moments in one direction and the other lattice consisting of atoms with moments in opposite direction.

If no external field is applied, the net magnetization of an anti ferro magnetic substance will be zero because; the moments exactly cancel when summed up over the entire crystal. If the field is applied, a small magnetization, in the direction of the field results.



### PROPERTIES

- The susceptibility of an anti ferro magnetic substance is small and positive, since the magnetization is small.
- **Temperature Dependence**  
The magnetization increases as the temperature increases.



Above a particular temperature called Neel's temperature, thermal agitations dominate the orientation of the dipoles in the field direction. The temperature dependence of the susceptibility for an antiferro magnetic material is given by the relation,

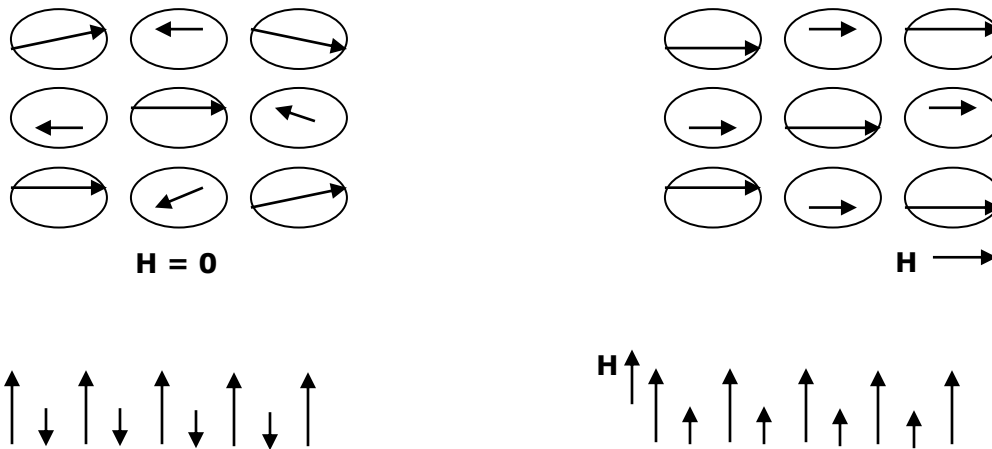
$$\chi = \frac{C}{T + T_N}$$

This is called Curie-Weiss law for anti ferro magnetic materials where  $T_N$  is the Neel's temperature. Hence, above Neel's temperature, the magnetization decreases with increase in temperature and the specimen turns out to be a paramagnetic material.

- Few examples of anti ferro magnetic materials are salts of transition elements, MnO, MnS, MnTe, MnF<sub>2</sub>, FeCl<sub>2</sub> etc.

### FERRIMAGNETIC MATERIALS

This kind of materials is much similar to ferromagnetic materials in their macroscopic magnetic characteristics. The magnetic moments of the sub-lattices in this material are unequal spins and opposite in direction.



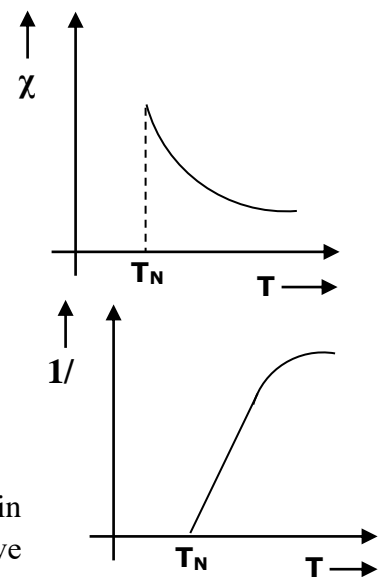
The adjacent atoms in ferri magnetic materials differ in the magnitude of the magnetic moments and their directions also. Thus, the net magnetization of a ferri magnetic material has a non-zero value. i.e., they possess a small value of magnetization.

Thus, **ferri magnetism can also be referred to as uncompensated anti ferromagnetism**. When placed in external magnetic field, they orient in the direction of the field. Due to the prevalence of spontaneous magnetization, they get easily magnetized.

#### **PROPERTIES**

- The value of susceptibility,  $\chi$  is large and positive.
- **Temperature Dependence**

The spontaneous magnetization decreases with the increase in temperature above a temperature called Neel's temperature. i.e., above



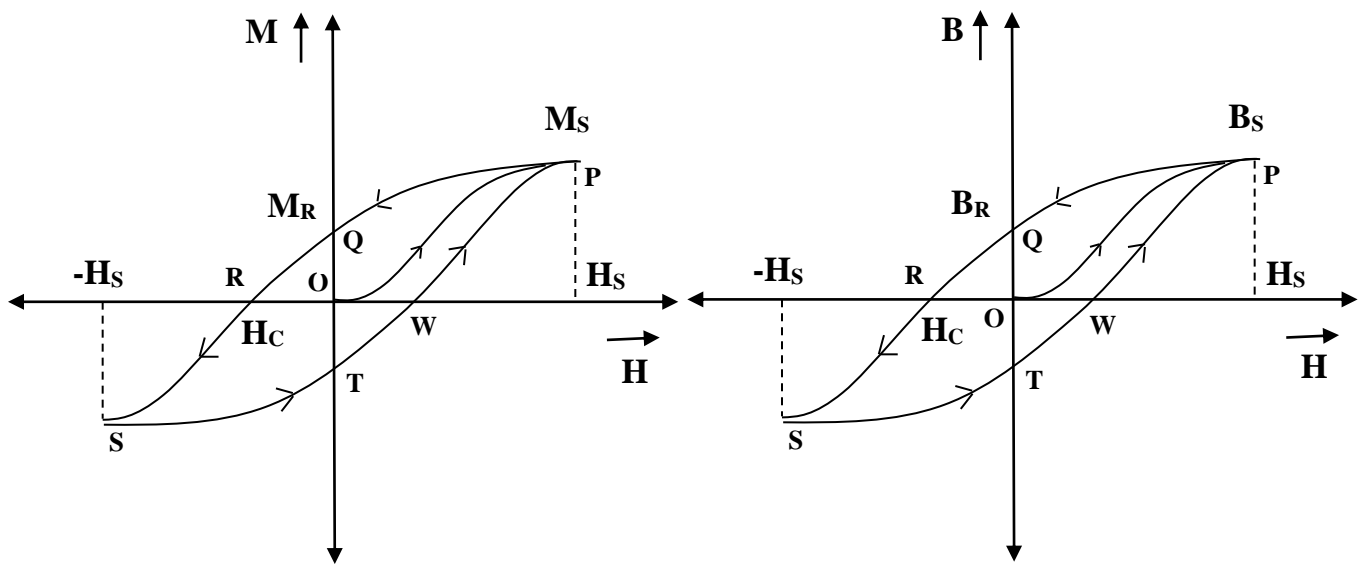
$T_N$  it converts itself into a paramagnetic material. But in paramagnetic state, the linear relation between  $\chi$  &  $T$  is not maintained. The curvature in the plot of  $1/\chi$  vs.  $T$  is a characteristic feature of a ferri magnetic substance.

- Ferrites like  $\text{CuFe}_2\text{O}_4$ ,  $\text{MnFe}_2\text{O}_4$ ,  $\text{ZnFe}_2\text{O}_4$ ,  $\text{FeFe}_2\text{O}_4$ , are examples of this kind.

### **HYSTERESIS CURVE**

**Hysteresis means retardation or lagging of an effect behind the cause of the effect.** When a ferromagnetic substance is placed in an external magnetic field, it is magnetized. However, the magnetization of the specimen does not vary linearly with the applied field. **The magnetization  $M$  lags behind the field  $H$ . This lagging of magnetization behind magnetic field is known as hysteresis.**

Hysteresis loop of a specimen is thus, a curve showing the change in magnetic induction in it, when the applied field is varied from  $H_S$  to  $-H_S$  and back again.



The above process is explained in the following steps

- Initially the magnetization  $M$  is zero when there is no field.
- When the external field  $H$  is gradually increased,  $M$  also increases gradually.
- The  $M$  value reaches a maximum called **saturation magnetization  $M_S$**  shown by point  $P$  in the figure.
- **Saturation magnetization is defined as the maximum extent up to which a ferromagnetic substance can be magnetized.**
- When  $H$  is decreased back gradually,  $M$  does not retrace original path  $OP$ . Rather, it follows a new curve  $PQ$ . This indicates hysteresis is an irreversible process.
- When the field is reduced completely to zero, ( $OQ$ ) some magnetization is still retained.
- This value of  $M$  is called **residual magnetization or retentivity, or remanance.**

- In order to demagnetize the specimen completely, we need to apply a magnetic force in the reverse direction.
- When a reverse field is applied, the magnetization  $M$  gradually reduces and become zero at a value  $H = -OR$ . **The reverse field where the magnetization reduces to zero is called the coercive force or coercivity.**
- Further increase of the reverse field results in process similar to that in the positive field and reaches saturation  $-M$  at the point  $S$ .
- If the field is decreased,  $M$  begins to decrease from  $-M$  but, this doesn't retrace old path  $RS$ , rather it proceeds along  $STW$ .
- Hereafter,  $M$  increases with further increase in  $H$  in the positive direction and will reach  $M_s$  finally.
- The closed loop  $PQRSTWP$  is known as hysteresis loop.

### **IMPORTANCE OF HYSTERISIS LOOP**

Study of hysteresis loop in ferromagnetic materials is important because, it allows estimation of many magnetic properties and based on that we can judge whether a material is useful or not for a specified application.

The significance of hysteresis loop is discussed below:

- Area of the loop gives the energy loss per cycle per  $m^3$
- Steepness of the curve indicates whether the magnetization is quick or not
- **Energy Product:** the product of retentivity and coercivity is called the energy product of the specimen. Materials that are used as permanent magnets should have high energy product value.

### INTRODUCTION

From the electrical conductivity point of view, materials are classified into three categories; conductors, semiconductors and insulators. All the metals contain free electrons which give rise to electrical conductivity.

Dielectric materials do not have such free electrons in them and their conductivity is negligible. These dielectrics possess both positive and negative charges which are bound together at an equilibrium state. However in the presence of an external electric field, the equilibrium gets disturbed and these charges get displaced giving rise to polarization.

Thus, dielectrics are electrically insulating materials. They can be defined as, **the substances which have the ability of getting polarized and in which an electric field can exist for a long period.**

Dielectrics possess high resistivity value in the range  $10^6$  to  $10^{16}$   $\Omega$ -m. Under high voltage bias, they allow a very little current in the range  $10^{-6}$  to  $10^{-14}$  A. The electric properties of a dielectric are associated with its inherent property of possessing electric dipole.

In this chapter, we learn about the dielectric properties of the materials in the presence of electric field which are useful in the fabrication of various devices.

### IMPORTANT DEFINITIONS

#### Electric dipole

A system consisting of two equal and opposite charges separated by a distance is called an electric dipole.

#### Dipole moment

The dipole moment is defined as the product of the magnitude of the charge and the separation between them. It is denoted by  $\mu$ .

$$\bar{\mu} = q\bar{r}$$

Where  $q$  is magnitude of the charge and  $r$  is the distance between the charges. This dipole moment is a vector quantity and its direction is always from negative to positive charge. Its unit is **debye**.

$$1 \text{ debye} = 3.33 \times 10^{-30} \text{ coulomb-meter}$$

If each particle (atom or molecule) of a substance possesses a dipole moment, the net dipole moment of the sample is given by,

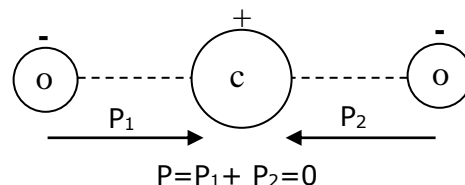
$$\bar{\mu}_i = \sum q_i \bar{r}_i$$

## TYPES OF DIELECTRICS

Dielectric materials are broadly classified into two types; they are polar dielectrics and non-polar dielectrics.

### Non-polar dielectrics

In these molecules, which are usually diatomic, composed of two atoms of the same type, each atom possesses a positive nucleus of charge 'q' surrounded by a symmetrically distributed electron cloud of charge '-q'. In the absence of external field the centre of gravity of the positive charge coincides with the center of gravity of the negative charge. Hence, the net dipole moment is zero.



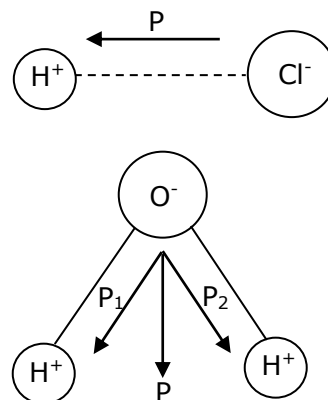
When they are placed in external field then both the positive and negative charges tend to move according to the direction of the field. Such materials are called non-polar dielectrics.

Eg: H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, CO<sub>2</sub>, C<sub>6</sub>H<sub>6</sub> etc

### Polar dielectrics

Generally, polyatomic substances contain molecules in which the center of gravity of the positive charge does not coincide with that of the negative charge and hence every molecule possesses a dipole moment even in the absence of the electric field.

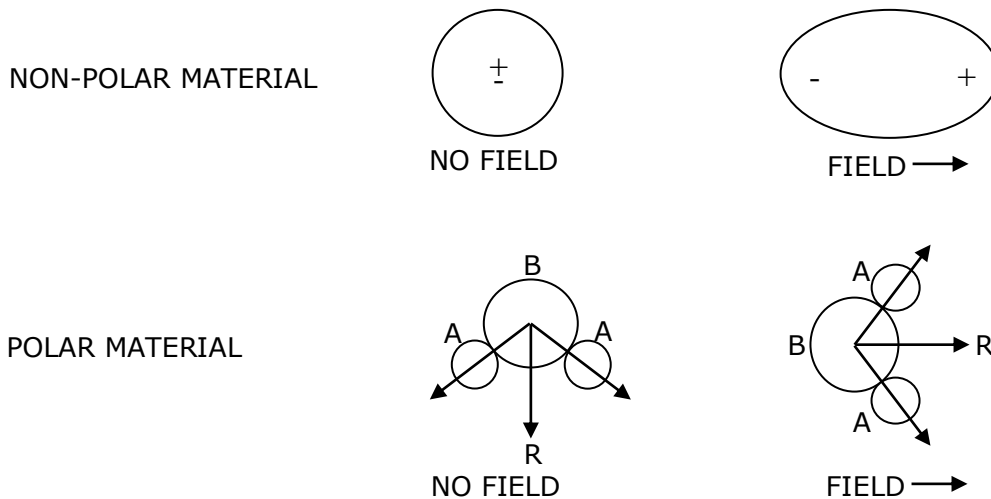
But, these molecules are oriented randomly and hence, the net dipole moment is zero in the absence of the field. When placed in external field they orient in the direction of the field. Such materials are called polar dielectrics.



Eg: H<sub>2</sub>O, CO<sub>2</sub>, N<sub>2</sub>O, NH<sub>3</sub> etc

## POLARIZATION

The process of inducing dipole moment in a dielectric by an applied electric field is known as polarization. Polarization can take place in both polar and non-polar dielectrics as shown in the figure below.





When a non-polar molecule or an atom is subjected to an external electric field E, then the centers of negative charge and positive charge distributions get separated. Then the atoms or molecules acquire a net dipole moment.

When a polar substance is exposed to an external field, each of the molecular dipole experiences a unique torque. As a consequence, they tend to orient themselves in the direction of the field. Hence, a net dipole moment is induced in the substance.

### **POLARIZATION VECTOR ( $\bar{P}$ )**

It is defined as the dipole moment per unit volume of a dielectric. If there are 'N' number of atoms per unit volume and  $\bar{\mu}$  is the average dipole moment, then

$$\bar{P} = N \times \bar{\mu}$$

Units of polarization are coulomb/m<sup>2</sup>.

### **PERMITTIVITY, ( $\epsilon$ )**

Permittivity is a quantity which represents the dielectric property of a medium. The ability of a material to get polarized easily is determined by the permittivity of the material.

The permittivity of the free space  $\epsilon_0 = 8.85 \times 10^{-12}$  F/m.

### **DIELECTRIC CONSTANT (or relative permittivity), $\epsilon_r$**

The dielectric constant or relative permittivity of a medium can be defined as the ratio between the permittivity of a medium to the permittivity of the free space.

$$\epsilon_r = \frac{\epsilon}{\epsilon_0} = \frac{C_d}{C_0} = \frac{E_0}{E_d} = \frac{V_0}{V_d}$$

### **ELECTRIC FIELD INTENSITY (E)**

Electric field intensity E at any point in the field is mathematically equal to the force experienced by a unit positive charge placed at that point.

### **DISPLACEMENT VECTOR (or DIELECTRIC DISPLACEMENT)(D)**

The number of lines of force received by unit area is called flux density or electric displacement vector. Mathematically, it can be stated as

$$D = \frac{q}{4\pi r^2}$$

The electric field at a point in a medium is given by,

$$E = \frac{q}{4\pi \epsilon r^2}$$

Hence, the relation between D & E can be given as, **D =  $\epsilon$ E**.

## ELECTRIC SUSCEPTIBILITY( $\chi$ )

When a dielectric is placed in an electric field of strength  $E$ , polarization takes place. The polarization vector is proportional to electric field strength.

$$\therefore \bar{P} \propto \bar{E} \Rightarrow \bar{P} = \chi \bar{E}$$

Where the constant ' $\chi$ ' is known as electric susceptibility.

$$\therefore \chi = \frac{\bar{P}}{\bar{E}}$$

## RELATION BETWEEN FLUX DENSITY AND POLARIZATION ( $D = \epsilon_0 E + P$ )

To derive the above relation first let us discuss Gauss law of electrostatics, which states that, the outward normal flux from a closed surface is equal to  $1/\epsilon_0$  times the total charge present in the surface.

$$\text{i.e. } \int E \cdot dA = \frac{1}{\epsilon_0} q$$

Now, let us apply Gauss' theorem to a parallel plate capacitor. Let us consider a capacitor without dielectric and dielectric. In the first case, when no dielectric is present, the  $E_0$  at any point on the Gaussian surface is given by,

$$\int E_0 \cdot dA = \frac{1}{\epsilon_0} q$$

$$\Rightarrow E_0 \cdot A = \frac{q}{\epsilon_0}$$

$$\therefore E_0 = \frac{q}{A\epsilon_0} \longrightarrow (1)$$

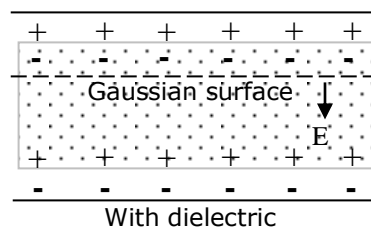
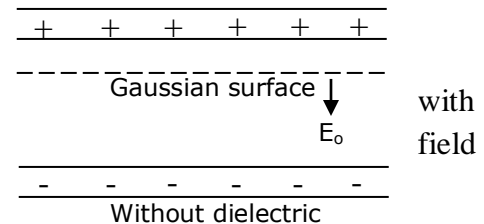
In the second case, when dielectric is present the net charge within the Gaussian surface is  $q - q'$  where  $q'$  is the induced charge and the field is given by,

$$\int E \cdot dA = \frac{q - q'}{\epsilon_0}$$

$$\Rightarrow E = \frac{q - q'}{A\epsilon_0} \longrightarrow (2)$$

The expression for capacitance of a capacitor with and without the dielectric respectively can be given as,

$$C' = \frac{A\epsilon_0\epsilon_r}{d} = \frac{q'}{V_d}$$



$$C_0 = \frac{A\epsilon_0}{d} = \frac{q}{V_0}$$

$$\therefore \frac{C'}{C_0} = \epsilon_r = \frac{V_0}{V_d} = \frac{E_0}{E}, \text{ since } \epsilon_r = \frac{V_0}{V_d} = \frac{E_0}{E}$$

$$\therefore E = \frac{E_0}{\epsilon_r} = \frac{q}{A\epsilon_0\epsilon_r} \longrightarrow (3)$$

Now, using relation (2), equation (3) can be written as,

$$\Rightarrow \frac{q}{A\epsilon_0\epsilon_r} = \frac{q}{A\epsilon_0} - \frac{q'}{A\epsilon_0}$$

$$\Rightarrow \frac{q}{A} = \epsilon_0 \left( \frac{q}{A\epsilon_0\epsilon_r} \right) + \frac{q'}{A}$$

The last term of the above expression is the induced charge per unit area, called the electric polarization  $\bar{P}$ . Substituting  $E = \frac{q}{A\epsilon_0\epsilon_r}$  and  $q/A = D$  in the above relation we get,

$$\bar{D} = \epsilon_0 \bar{E} + \bar{P} \longrightarrow (4)$$

This is the relation between the flux density and polarization. In the space, if there is no dielectric then  $\bar{P} = 0$ . Hence, we can write

$$\bar{D} = \epsilon_0 \bar{E} \longrightarrow (5)$$

Now considering the relations (4) and (5), we can write

$$\epsilon \bar{E} = \epsilon_0 \bar{E} + \bar{P}$$

$$\Rightarrow \epsilon_0 \epsilon_r \bar{E} = \epsilon_0 \bar{E} + \bar{P}$$

$$\epsilon_r = 1 + \frac{\bar{P}}{\epsilon_0 \bar{E}}$$

$$\boxed{\therefore \epsilon_r - 1 = \frac{\bar{P}}{\epsilon_0 \bar{E}} = \chi}$$

## **THE MICROSCOPIC CONCEPT OF POLARIZATION**

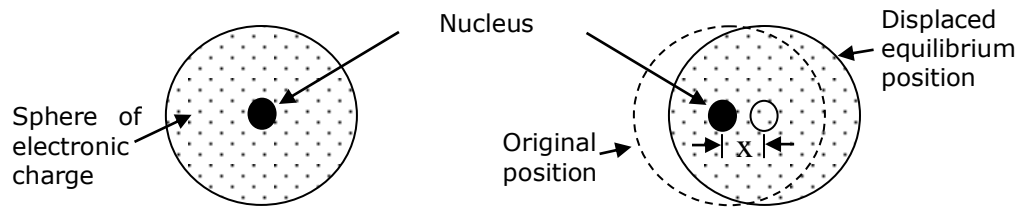
Dielectric polarization is nothing but the displacement of charged particles under the action of an electric field to which they are subjected. The displacement of electric charges results in the formation of electric dipole moment in atoms or ions or molecules of the material. The three important types of polarization that exist in dielectric substances are;

- Electronic polarization

- Ionic polarization
- Orientation polarization

### Electronic polarization

Electronic polarizability arises from the displacement of electrons in an atom relative to the nucleus in the presence of an electric field. We can explain this process by a classical model. In classical approach we assume that electrons form a uniformly charged spherical cloud surrounding the nucleus of an atom, i.e. an electric cloud of charge  $-Ze$  is distributed in the sphere of radius  $R$ .



When an electric field is applied, the center of the electron cloud and that of the nucleus gets displaced. A separation is created between these two. Hence, the opposite charges are displaced from each other with a distance between them. Hence the atom acts as a dipole and acquires dipole moment.

Let us consider a nucleus of charge  $Ze$  surrounded by a negative charge  $-Ze$  distributed in the sphere of radius  $R$ . The charge density  $\rho$  is given by,

$$\rho = \frac{-Ze}{\frac{4}{3}\pi R^3} = \frac{-3}{4} \left( \frac{Ze}{\pi R^3} \right) \longrightarrow (1)$$

When this system is subjected to an external field of intensity  $E$ , the nucleus and the electron experiences Lorentz forces of magnitude  $ZeE$  in opposite directions. Therefore, the nucleus and the electron cloud are pulled apart. As they are pulled apart, a Coulomb force develops between them, which tends to counter the displacement. Hence, the actual magnitude of the displacement is small and is of the order of  $10^{-17}m$  for a field of  $30kV/m$ .

Let the small displacement be  $x$ . To calculate the induced dipole moment, it is firstly assumed that only the electron cloud is displaced by the field.

Now the Lorentz force which acts on the electron cloud is  $-ZeE \longrightarrow (2)$

and the Coulombian force =  $\frac{Ze \times \text{charge enclosed in the sphere}}{4\pi\epsilon_0 x^2}$

Now, we have to calculate the charge enclosed in the sphere of radius  $x$ .

Hence, the enclosed charge = density x volume of the sphere

$$= \frac{4}{3}\pi x^3 \rho$$

$$= \frac{4}{3} \pi x^3 \times \left( \frac{-3 Ze}{4 R^3} \right)$$

$$= \frac{-Zex^3}{R^3}$$

$$\text{The Coulombian force} = \frac{Ze}{4\pi\epsilon_0 x^2} \times \left( \frac{-Zex^3}{R^3} \right) = \frac{-Z^2 e^2 x}{4\pi\epsilon_0 R^3}$$

At equilibrium, Lorentz force = Coulombian force

$$\therefore -ZeE = -\frac{Z^2 e^2 x}{4\pi\epsilon_0 R^3}$$

$$\Rightarrow E = \frac{Zex}{4\pi\epsilon_0 R^3}$$

$$\boxed{\therefore x = \frac{4\pi\epsilon_0 R^3 E}{Ze}}$$

The above equation indicates that the displacement of the electron cloud is proportional to the applied field.

Now, the induced dipole moment is given by,

$$\mu_e = Zex$$

$$= Ze \left( \frac{4\pi\epsilon_0 R^3 E}{Ze} \right)$$

$$= 4\pi\epsilon_0 R^3 E$$

$$\boxed{\Rightarrow \mu_e = \alpha_e E}$$

$$\boxed{\therefore \mu_e = \alpha_e E}$$

Where  $\alpha_e = 4\pi\epsilon_0 R^3$  is the electronic polarizability.

Now, electronic polarization is given by,

$$P_e = N \mu_e = N \alpha_e E$$

Where N is number of atoms per  $m^3$ .

But,  $P = E\epsilon_0(\epsilon_r - 1)$

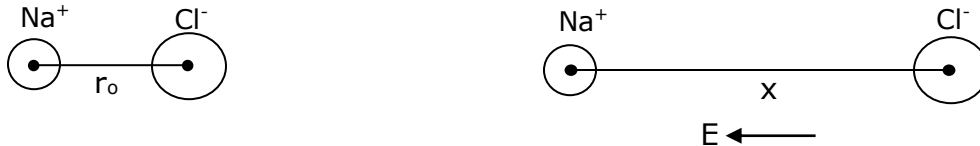
$$\Rightarrow N \alpha_e E = E \epsilon_0 (\epsilon_r - 1)$$

$$\boxed{\Rightarrow \epsilon_r - 1 = \frac{N \alpha_e}{\epsilon_0}}$$

## Ionic Polarization

Generally, this polarization will happen in ionic substances like NaCl, H<sub>2</sub>O etc. ionic polarization arises because of relative displacement of positive and negative ions of a molecule in the presence of an external electric field.

For example, let us consider the NaCl molecule. When this NaCl is subjected to electric field, then Na<sup>+</sup> and Cl<sup>-</sup> ions are displaced in an opposite because of Lorentz force. This results in the formation of a dipole.



### Derivation of $\alpha_i$

Let us consider a molecule having two equal and opposite charges. Let  $m_1$  and  $m_2$  be the masses of +ve and -ve charges respectively. When an electric field  $E$  is applied to this molecule, these ions displace in opposite directions. let  $x_1$  and  $x_2$  be the displacements of +ve and -ve ions respectively.

$$\text{Hence, net distance between the two ions is, } x = x_1 + x_2 \longrightarrow (1)$$

$$\left. \begin{array}{l} \text{The Lorentz force acting on +ve ion} = eE \\ \text{The Lorentz force acting on -ve ion} = -eE \end{array} \right\} \longrightarrow (2)$$

When ions are displaced from their original positions in opposite directions then restoring force appears on the ions, which tends to move the ions back to the mean positions.

$$\left. \begin{array}{l} \text{The restoring force acting on +ve ion} = -k_1x_1 \\ \text{The restoring force acting on -ve ion} = k_2x_2 \end{array} \right\} \longrightarrow (3)$$

where  $k_1$  and  $k_2$  are restoring force constants.

At equilibrium, Lorentz force and restoring forces are equal and opposite. Hence,

$$\begin{aligned} eE &= k_1x_1 \quad \text{and} \quad eE = k_2x_2 \\ \therefore x_1 &= \frac{eE}{k_1} \quad \text{and} \quad \therefore x_2 = \frac{eE}{k_2} \end{aligned}$$

where  $k_1 = m_1\omega_0^2$  and  $k_2 = m_2\omega_0^2$

$$\therefore x_1 = \frac{eE}{m_1\omega_0^2} \quad \text{and} \quad \therefore x_2 = \frac{eE}{m_2\omega_0^2}$$

$$\begin{aligned}\therefore x_1 + x_2 &= \frac{e}{\omega_0^2} \left( \frac{1}{m_1} + \frac{1}{m_2} \right) E \\ \mu_i &= (x_1 + x_2)e = \frac{e^2}{\omega_0^2} \left( \frac{1}{m_1} + \frac{1}{m_2} \right) E \\ \therefore \mu_i &\propto E \\ \Rightarrow \mu_i &= \alpha_i E\end{aligned}$$

$$\boxed{\therefore \alpha_i = \frac{e^2}{\omega_0^2} \left( \frac{1}{m_1} + \frac{1}{m_2} \right)}$$

### Orientation Polarization

Certain substances, called polar substances, consist of molecules that have permanent dipoles even in the absence of external field. But, all the dipoles are oriented randomly in the absence of external field, such that the net dipole moment is zero.

However, when they are placed in external field, molecular dipoles align in the field direction, resulting in a net dipole moment. This kind of polarization is called orientation polarization or dipolar polarization.

The dipole moment induced will depend upon the external field intensity.

$$\begin{aligned}\mu_o &\propto E \\ \text{i.e. } \mu_o &= \alpha_o E\end{aligned}$$

where  $\alpha_o$  is known as orientation polarizability. The value of  $\alpha_o$  is  $\frac{\mu^2}{3k_b T}$ . Here,  $\mu$  is the dipole moment of individual molecule.

### LOCAL OR INTERNAL FIELD

**The total electric field which a dipole experiences in a medium is called the local field or internal field or Lorentz field denoted by  $E_L$ .** This is different from externally applied field.

Suppose a dielectric substance consists of large number of molecules. When this is subjected to an electric field, then each molecule is associated with a dipole moment and it is equal to the product of polarizability and electric field intensity.

If we consider a dipole, in addition to the external field, the remaining dipoles impose an internal electric field on the molecule under consideration. Therefore, an effective field exists on every molecule, which is equal to the sum of the external field and the field due to all the other dipoles around it.

This total field is known as internal field or local field or Lorentz field,  $E_L$ .

### Expression for local field of a cubic system

This was evaluated by Lorentz. For this, let us consider a dielectric which is placed between two electrodes as shown in the figure.

Imagine a dipole which is surrounded by a spherical cavity of radius 'r' at the center A. the sphere contains many molecules but small compared with the dimensions of the whole dielectric. The total electric field acting on the molecular dipole which is at the center of the cavity is given by,

$$E_L = E_1 + E_2 + E_3 + E_4$$

where,

$E_1$  is the field intensity due to charge density on the plates of capacitor (i.e. field without dielectric)

$E_2$  is the field intensity due to the polarized charges on the plane surface of the dielectric i.e. depolarization field

$E_3$  is the field due to all the dipoles inside the spherical cavity. This field depends on symmetry of the crystal

$E_4$  is the field due to the polarized charges on the spherical cavity.

Now, we have to calculate the values of  $E_1, E_2, E_3, E_4$ .

If we observe  $E_1$  and  $E_2$ , we know that the sum of  $E_1$  and  $E_2$  is equal to the net macroscopic field inside the dielectric material.

$$\text{Hence, } E_1 + E_2 = E$$

$$\therefore E_L = E + E_3 + E_4$$

In the present case,  $E_3 = 0$ . This is because the spherical cavity is highly symmetric and all the dipoles inside it are randomly distributed, such that the net field caused by them is zero.

$$\therefore E_L = E + E_4$$

Now let us calculate  $E_4$ . Here it should be remembered that, induced charge is distributed uniformly on the surface of the spherical cavity and there is no charge inside the cavity. Suppose the surface charge density is  $\sigma$ .

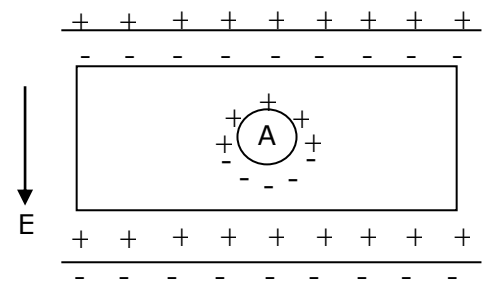
Now to calculate  $E_4$ , let us divide the spherical cavity into number of rings. Consider one such ring PQRS lying between  $\theta$  and  $d\theta + \theta$  as shown in figure, where  $\theta$  is the direction with respect to the field.

$$\text{The area of the ring} = dA = 2\pi r l$$

$$dA = 2\pi (BR) \times (RP)$$

$$\text{From the figure } RP = r d\theta, BR = r \sin \theta$$

$$\therefore dA = 2\pi r^2 \sin \theta d\theta$$





Charge  $dq$  on the ring  $dA$  is equal to the parallel component of the polarization multiplied by the surface area.

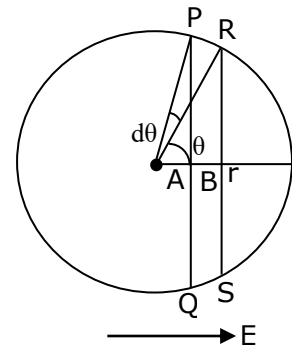
$$\therefore dq = P \cos \theta dA = P \times 2\pi r^2 \sin \theta \cos \theta d\theta$$

The field due to the charge at A is denoted by  $dE_4$  and is given by,

$$dE_4 = \frac{dq}{4\pi\epsilon_0 r^2} = \frac{P \cos \theta dA}{4\pi\epsilon_0 r^2}$$

$$dE_4 = \frac{P \cos \theta \times 2\pi r^2 \sin \theta \cos \theta d\theta}{4\pi\epsilon_0 r^2}$$

$$dE_4 = \frac{P \cos^2 \theta \sin \theta d\theta}{2\epsilon_0}$$



Now, the total field  $E_4$  due to the charges on the surface of the entire cavity is obtained by integrating above equation.

$$E_4 = \int dE_4 = \frac{P}{2\epsilon_0} \int_0^\pi \cos^2 \theta \sin \theta d\theta$$

put  $\cos \theta = x \Rightarrow -\sin \theta = dx$

$$\therefore E_4 = \frac{-P}{2\epsilon_0} \int_1^{-1} x^2 dx$$

$$= \frac{P}{2\epsilon_0} \int_1^{-1} x^2 dx = \frac{P}{3\epsilon_0}$$

$$\therefore E_4 = \frac{P}{3\epsilon_0}$$

Hence, local field  $E_L = E + \frac{P}{3\epsilon_0}$

The above equation is known as Lorentz field or local field. Here, it should be observed that the local field is greater than the electric field applied.

### **CLAUSIUS-MOSOTTI RELATION**

This equation relates the macroscopic quantity dielectric constant and the microscopic quantity polarizability.

Consider a single atom or molecule. When it is placed in an electric field, then dipole moment induced will be proportional to the local field i.e.  $\mu = \alpha E_L$ , where  $\alpha$  total polarizability.

If there are  $N$  atoms per unit volume, then dipole moment per unit volume i.e. polarization vector is given by,

$$P = N \alpha E_L \longrightarrow (1)$$

But, we know that  $P = \epsilon_0 E (\epsilon_r - 1)$

$$\begin{aligned} \epsilon_0 E (\epsilon_r - 1) &= N \alpha E_L \\ \therefore \epsilon_r &= 1 + \frac{N \alpha E_L}{\epsilon_0 E} \longrightarrow (2) \end{aligned}$$

We know that,  $E_L = E + \frac{P}{3\epsilon_0} = E + \frac{N \alpha E_L}{3\epsilon_0}$  [from (1)]

$$\Rightarrow E = E_L \left( 1 - \frac{N \alpha}{3\epsilon_0} \right)$$

$$\therefore \frac{E_L}{E} = \frac{1}{1 - \frac{N \alpha}{3\epsilon_0}} \longrightarrow (3)$$

Substituting equation (3) in (2), we get

$$\begin{aligned} \therefore \epsilon_r &= 1 + \frac{N \alpha}{\epsilon_0} \left[ \frac{1}{1 - \frac{N \alpha}{3\epsilon_0}} \right] \\ &= \frac{\epsilon_0 \left( 1 - \frac{N \alpha}{3\epsilon_0} \right) + N \alpha}{\epsilon_0 \left( 1 - \frac{N \alpha}{3\epsilon_0} \right)} \\ &= \frac{1 + \frac{2}{3} \left( \frac{N \alpha}{\epsilon_0} \right)}{1 - \frac{1}{3} \frac{N \alpha}{\epsilon_0}} \\ \text{Now, } \frac{\epsilon_r - 1}{\epsilon_r + 2} &= \frac{\frac{1 + \frac{2}{3} \left( \frac{N \alpha}{\epsilon_0} \right)}{1 - \frac{1}{3} \left( \frac{N \alpha}{\epsilon_0} \right)} - 1}{\frac{1 + \frac{2}{3} \left( \frac{N \alpha}{\epsilon_0} \right)}{1 - \frac{1}{3} \left( \frac{N \alpha}{\epsilon_0} \right)} + 2} = \frac{N \alpha / \epsilon_0}{3} \end{aligned}$$

$$\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{N\alpha}{3\epsilon_0}$$

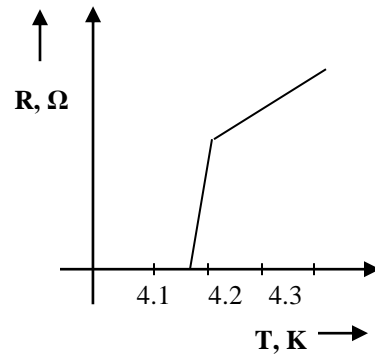
This relation is called Clausius-Mosotti equation. Multiplying both sides of the above equation by the molar volume, we get

$$\frac{\epsilon_r - 1}{\epsilon_r + 2} \frac{M_A}{\rho} = \frac{N\alpha}{3\epsilon_0} \frac{M_A}{\rho} = \frac{N_A\alpha}{3\epsilon_0} = P_M$$

where  $M_A$  is molecular weight and  $P_M$  is called molar polarization.

**THE DISCOVERY**

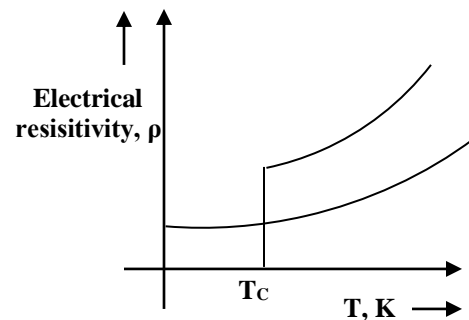
In 1908, a Dutch physicist, Kammerlingh Onnes studied the variation of electrical resistance of metals at low temperatures. He discovered that, the electrical resistance of highly purified mercury dropped abruptly to zero at 4.15K. He called this new phenomenon, superconductivity. Subsequently, this was discovered in Lead (Pb), Tin (Sn), Zinc (Zn), Aluminum (Al), other metals and alloys.



**SUPERCONDUCTIVITY**

**The sudden disappearance of electrical resistance in materials when cooled below a certain temperature is called superconductivity and the temperature at which a normal material turns into a superconductor is called the critical temperature  $T_c$ .**

The superconducting transition is sharp for a chemically pure and structurally perfect specimen, while the transition range is broad in impure or structurally imperfect specimen.



**GENERAL FEATURES**

- The transition temperature is different for different substances
- Superconductivity is found to occur in metallic elements with valence electrons between 2 and 8
- Transition metals having odd number of valence electrons are favorable to exhibit superconductivity, while metals with even number of valence electrons are unfavorable
- Materials having high normal resistivity exhibit superconductivity
- There is no change in the crystal structure at superconducting state as revealed by x-ray diffraction.
- The superconducting property of a superconductor is not lost by adding impurities to it, but the critical temperature is lowered.
- Ferromagnetic and antiferromagnetic materials are not superconductors
- The magnetic flux lines are rejected out of the superconductor
- There is a discontinuous change in specific heat
- There occur small changes in thermal conductivity and volume of the material

## EFFECT OF MAGNETIC FIELD

Superconducting state of a metal mainly depends on temperature and the strength of the magnetic field in which the metal is placed. Superconductivity disappears if the temperature of the specimen is raised above the transition temperature or a strong magnetic field is applied.

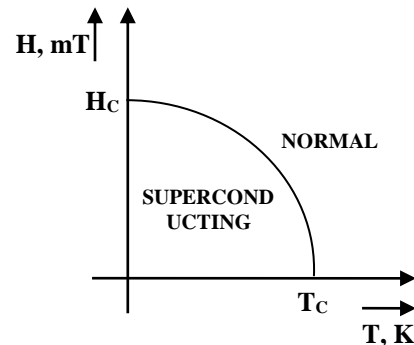
Superconductivity can be destroyed or its normal resistivity may be restored if the material is exposed to a magnetic field of sufficient field strength. The minimum amount of field required to destroy the superconductivity of a material and bring it to normal state is called the critical field, denoted by  $H_C$ . The critical field  $H_C$  varies with temperature according to the equation

$$H_C = H_0 \left[ 1 - \left( \frac{T}{T_C} \right)^2 \right]$$

Where  $H_0$  is constant

At  $T = T_C$ ,  $H_C = 0$ . At temperatures below  $T_C$ ,  $H_C$  increases.

Where,  $H_C(0)$  is the critical field at  $0^0\text{K}$ .  $H_C(0)$  and  $T_C$  are constants and characteristic of the material.



## MEISSNER EFFECT

In 1933, Meissner and Oschenfeld measured the flux distribution inside Tin and Lead specimens, which were cooled below their transition temperatures while in a magnetic field. They found that, at the transition temperatures, the specimens spontaneously became perfectly diamagnetic, canceling all the flux.

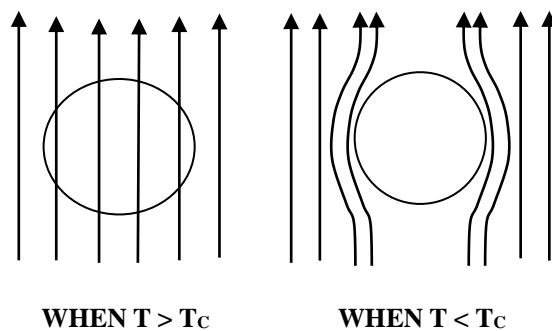
This demonstrated that, superconductors are something more than the materials which are perfectly conducting; they have an additional property that a merely resistance less metal would not possess i.e. **The expulsion of magnetic lines of force from the body of the superconductor when it is cooled below its transition temperature is known as Meissner Effect.**

This effect is reversible. That means, when the temperature is raised, from below  $T_C$ , at  $T = T_C$ , the flux lines suddenly start penetrating and the specimen returns back to the normal state.

We know that, the magnetic induction inside the specimen is given by,

$$\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M}) \quad \longrightarrow \quad (1)$$

Where  $H$  is the external field,  $M$  is the magnetization produced inside the specimen.



When the specimen is superconducting, according to Meissner effect, inside the bulk superconductor,  $\mathbf{B} = \mathbf{0}$ .

$$\text{i.e. } \mu_0(\mathbf{H} + \mathbf{M}) = \mathbf{0} \Rightarrow \mathbf{M} = -\mathbf{H} \longrightarrow (2)$$

The magnetic susceptibility  $\chi = \frac{\mathbf{M}}{\mathbf{H}} = -1 \longrightarrow (3)$  which is the maximum value for a diamagnet. Thus, the material is perfectly diamagnetic.

Let us consider a superconducting material under normal state, whose resistivity is ' $\rho$ '. Let ' $J$ ' be the current passing through the material. From Ohm's law,  $E = J \rho$ . On cooling the material to its transition temperature  $\rho$  tends to zero.

If  $J$  is held finite,  $E$  must be zero.

$$\text{From Maxwell's equation} \quad \nabla \times \mathbf{E} = - \frac{d\mathbf{B}}{dt} \longrightarrow (4)$$

Under superconducting state, since  $E$  is zero,  $\frac{d\mathbf{B}}{dt} = 0$  i.e.  $\mathbf{B}$  is constant.

**This means that the magnetic flux passing through the specimen should not change on cooling to the transition temperature.**

But, the Meissner effect contradicts this result. **According to this, perfect diamagnetism is an essential property of defining the superconducting state.**

**Thus, from zero resistivity,  $E = 0$**

**From Meissner effect,  $\mathbf{B} = \mathbf{0}$ .**

## CRITICAL CURRENT

The magnetic field, which causes a transition from superconducting state to normal state, need not be necessarily an external applied field. It may arise because of electric current flow in the superconductor. If a superconducting wire of radius ' $r$ ' carries a current ' $I$ ', it produces a magnetic field. The magnetic field when exceeds the critical field destroys the superconductivity. That means the superconductor can hold current up to one particular value, beyond which it becomes normal.

**The maximum current that can be passed in a superconducting sample without destroying its superconductivity is called the critical current,  $I_C$ .**

It is given as,  $I_C = 2\pi r H_C$ . **This is also called Silsbee rule.**

## ISOTOPE EFFECT

Maxwell and Reynold first observed this effect in 1950, in case of Mercury. According to this effect, the transition temperature is different for different isotopes of an element. It decreases with increasing atomic mass. The mass and the critical temperature of an isotope are related in the following way

$$T_C \propto M^{-\alpha} \quad \text{i.e. } T_C M^\alpha = \text{constant}$$

Usually,  $\alpha = 1/2$ . Thus, the superconducting substances with heavy ions possess less critical temperature compared to that of one with lighter ions.

## PENETRATION DEPTH

The Meissner effect explains that in the presence of a magnetic field, a superconductor behaves as a diamagnetic material. i.e. it expels all the lines of magnetic force.

In 1935, F.London & H.London stated that **the applied field does not suddenly drop to zero at the surface of the superconductor but decays exponentially according to the equation,**

$$H = H_0 \exp(-x/\lambda)$$

Where  $H_0$  is the magnetic field at the surface and  $\lambda$  is the characteristic length called **penetration depth**.

Thus, **penetration depth may be defined as; the depth from the surface at which the magnetic flux density falls to 1/e of its initial value at the surface.** The penetration depth does not have a fixed value but varies with temperature according to the equation,

$$\lambda = \frac{\lambda_0}{1 - \left(\frac{T}{T_C}\right)^4}$$

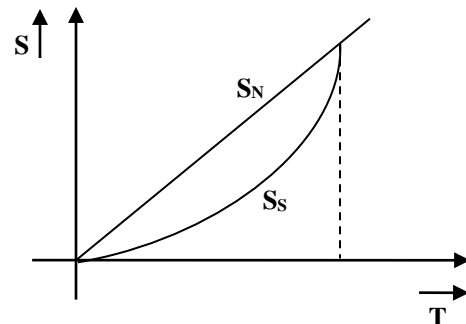
**This concept of penetration depth tells us that when a superconducting specimen is placed in a weak magnetic field, the specimen does not completely expel the flux. It retains some flux at the surface.**

## THERMAL PROPERTIES

### Entropy

In all superconductors, the entropy decreases markedly on cooling below the critical temperature.

Entropy is a measure of disorder of the system. Hence, the decrease in entropy between the normal state and the superconducting state tells us that the superconducting stage is more ordered than the normal state.



## Specific Heat

The specific heat of a metal is of the form  $C = aT + bT^3$

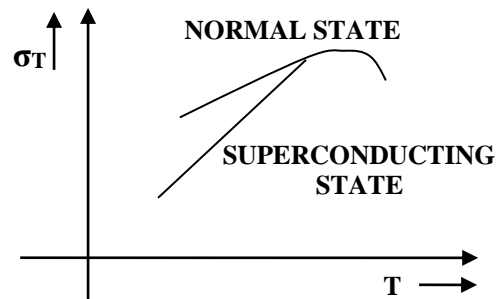
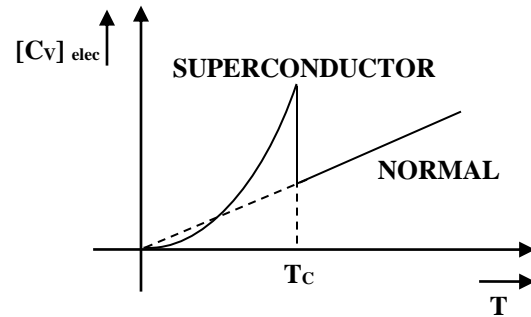
The first term is the specific heat of electrons in the metal and the second term is the contribution of the lattice vibrations at low temperatures. The specific heat of the superconductors shows a jump at  $T_C$ . Because the lattice vibration part remains unaffected, the second term has the same value in normal and superconducting states. By neglecting this term, we find that electronic specific heat is not linear with the temperature as in the case of the normal metals. It rather fits an exponential form

$$[C_V]_{\text{elec}} = A \exp(-\Delta/K_B T)$$

Where  $\Delta$  is the energy gap. This exponential form is an indication of the existence of a finite gap in the energy spectrum of the electrons in a superconductor.

## Thermal Conductivity

This thermal conductivity of the superconductor undergoes a continuous change between two phases and is usually lower in superconducting phase, indicating that the electronic contribution drops playing no part in heat transfer.



## TYPE-I & TYPE-II SUPERCONDUCTORS

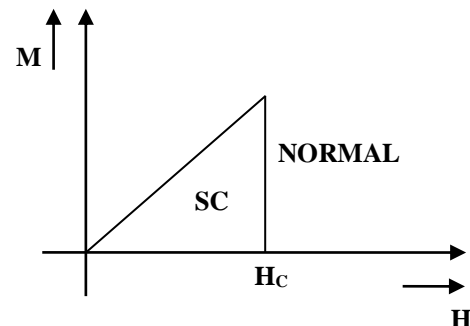
Superconductors are divided into two types depending upon the way in which the transition from superconducting state to normal state takes place, when the magnetic field exceeds the critical value  $H_C$  i.e. based on the diamagnetic response of the substance in an external magnetic field.

They are **Type-I or soft superconductors**

**Type-II or hard superconductors**

### Type – I Superconductors

Superconductors exhibiting a complete Meissner effect (perfect diamagnetism) are called type-I superconductors. When the magnetic field strength is gradually increased from its initial value  $H < H_C$ , at  $H_C$ , the diamagnetism abruptly disappears and the transition from superconducting to the normal state is sharp. These are also referred to as soft





superconductors.

E.g. Al, Zn, Hg and Sn (pure specimens)

### Type – II Superconductors

In type-II, up to a field  $H_{c1}$ , called the **lower critical field**, the specimen is in the superconducting state. The magnetic flux lines are rejected. When the field is increased beyond  $H_{c1}$ , flux lines start penetrating. Between  $H_{c1}$  &  $H_{c2}$  the specimen is in a mixed state (neither superconducting state nor normal state). This  $H_{c2}$  is called the **upper critical field**.

Above  $H_{c2}$ , the specimen is in a normal state. This means that, the Meissner effect is incomplete in the region between  $H_{c1}$  &  $H_{c2}$ . This region is called **vortex region**. These are also called hard superconductors. These are of great practical interest because of the high current densities that can carry.

E.g.: Ta, V, and Nb.

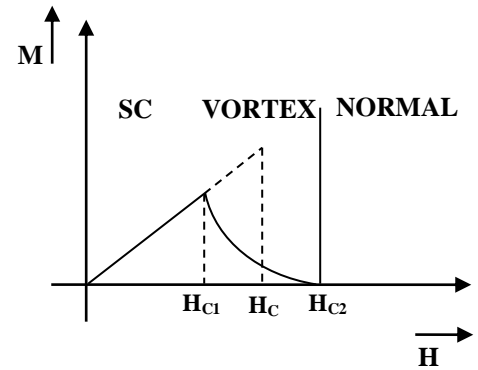
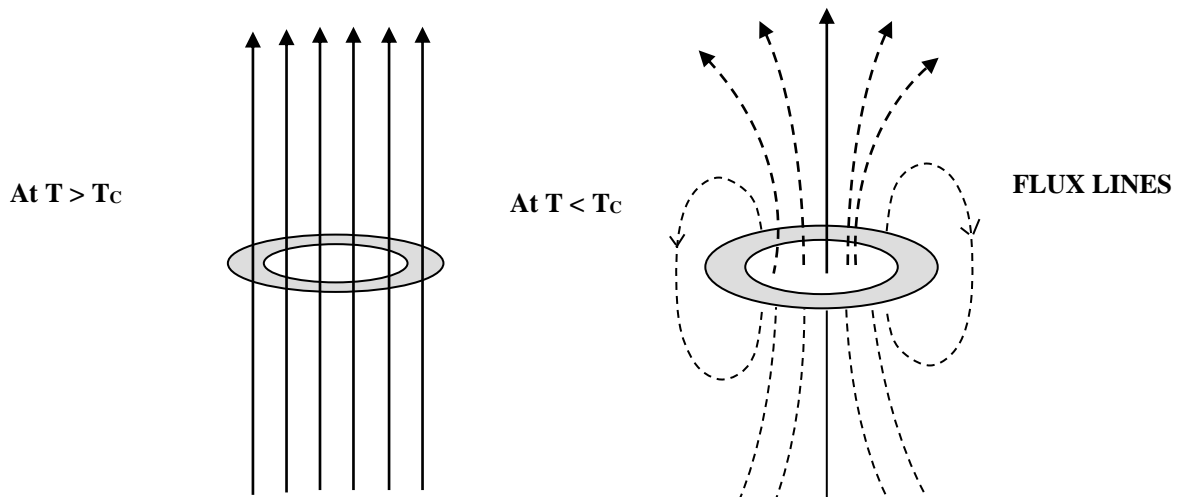
### FLUX QUANTIZATION

Consider a metal in the form of a ring. Let us apply magnetic field while the ring is in normal state. Then, the magnetic flux penetrates through the ring. Due to this current is induced. When the ring is cooled to the transition temperature while the field is on; the flux is excluded from the body of the ring.

Now remove the field, even in the absence of field, the current, which is induced, persists over a long period without attenuation, such currents are known as persistent currents. Due to these currents magnetic flux  $\phi$  generates, which the superconducting ring traps. The flux  $\phi$ , which is trapped inside the ring, is quantized (i.e.) **the magnetic flux trapped is the integral multiples of  $h/q$  where  $q = 2e$ , charge of the electron pair.**

$$\therefore \phi_0 = n \frac{h}{2e}$$

The value of  $h/q$  was found to be  $2.07 \times 10^{-15}$  Wb. This confirmed the existence of electron pair in a superconductor.



## **BCS THEORY**

The microscopic theory put forward by Bardeen, Cooper, Schrieffer provides the better explanation of superconductivity and accounts very well for the most of the properties exhibited by superconductors.

The bases of formulation of BCS theory are two experimental facts:

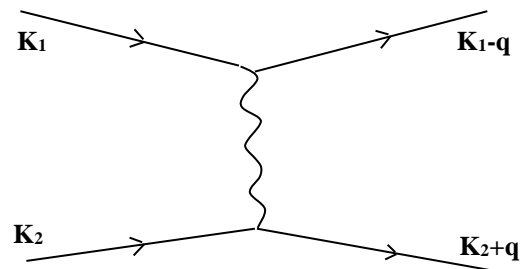
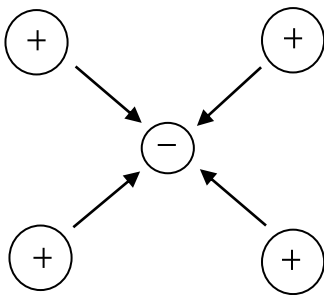
- Isotope effect,  $T_C M^{1/2} = \text{constant}$ .
- Variation of specific heat

From the above, we can infer that the transition resulting in superconducting state must involve the dynamics of ion motions. In addition,  $T_C$  attains a zero value when  $M$  approaches infinity. This suggests that non-zero transition temperature is a consequence of the ions, which can contribute phonons by their vibrations.

Froehlich and Bardeen pointed out that an electron moving through a crystal lattice has a self-energy accompanied by virtual phonons. The superconductivity is explained by BCS theory in the following way.

### **Electron – Lattice – Electron interaction**

- Let us assume that an electron approaches a positive ion core, it suffers attractive Coulomb interaction. Due to this attraction, ion core is set in motion leading to the distortion of the lattice. Smaller the mass of the positive ion core, greater will be the distortion.
- Another electron comes in that way sees this distorted lattice, then the interaction between the two, the electron and distorted lattice occurs.
- The two electrons interact via the lattice deformation resulting in the lowering of energy of the second electron. The lowering of electron energy implies that the force between the two electrons is attractive.
- This type of interaction is called **electron-lattice-electron interaction**. This interaction is strongest when the two electrons have equal and opposite momenta and spins.

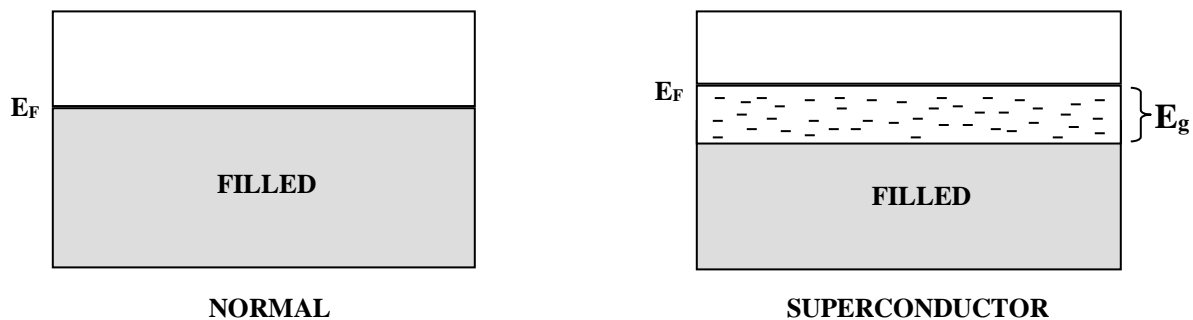


- The distortion of the lattice is quantized and **the quantum of lattice vibration is called a phonon**. Hence, the two electrons interact with each other by exchange of phonons.
- Let an electron of wave vector  $K_1$  emits a virtual phonon of vector  $q$ , an electron with wave vector  $K_2$  absorbs this phonon.  $K_1$  is thus scattered as  $K_1 - q$  and  $K_2$  as  $K_2 + q$ .
- Thus, superconductivity occurs when an attractive interaction between two electrons, by means of phonon exchange, dominates the usual repulsive interaction.
- After the exchange of phonon, the electrons get paired together due to the attractive force between them. This pair of electrons is termed as **Cooper pair**.
- The energy of the pair of electrons in the bound state is less than the energy of the pair in the free state. The difference of energy between the two states is the binding energy of the cooper pair and this energy should be supplied, if the pair is to be broken.
- At temperatures less than critical temperature, electron-lattice-electron interaction is stronger than electron- electron Coulomb repulsion. Hence, the electrons tend to pair up. This pairing is complete at  $0^\circ\text{K}$  and is completely broken at critical temperature.

### Energy Gap of a Semiconductor

The energy difference between the free state of electrons and paired state appears as the energy gap at the Fermi surface. The normal electron states are above the energy gap and the superconducting states are below the energy gap. Since the pairing is complete at  $0^\circ\text{K}$ , the difference in free and paired electron states is at maximum and this occurs as energy gap at absolute zero.

At  $T = T_C$ , the pairing is dissolved and energy gap reduces to zero. There are many excited states for Cooper pairs across the energy gap. At critical temperature, this coherence disappears and pairs are broken resulting in the transition of superconducting state to normal state.



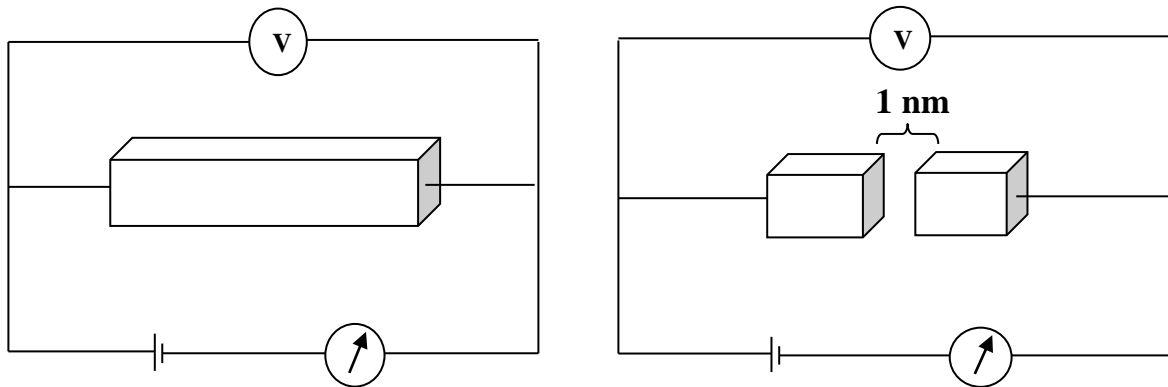
BCS theory explains several experimentally observed features of superconductivity such as general properties, existence of critical fields, penetration depth, coherence length, flux quantization, isotope effect, and Meissner effect. However, this theory failed in explaining which materials are superconductors and which are not. It could not also explain why excellent conductors at room temperature are not superconductors even at temperatures close at  $0^\circ\text{K}$ .

## JOSEPHSON EFFECT

In 1962, B.D. Josephson predicted that a super current could be made to flow across an insulating gap between two superconductors, provided the gap is small enough.

A current is made to flow in a bar of superconductor as in figure. The voltmeter indicates a drop in voltage to zero across the conductor. Suppose the bar is cut into two pieces. These are separated by 1 cm. No current will flow and voltmeter indicates a voltage equal to the open circuit voltage.

If the distance between the pieces is reduced to 1 nm, the voltmeter suddenly shows zero voltage showing that a current flows across the gap. This is known as **DC Josephson Effect**.



If the voltmeter indicates some value, i.e. if some voltage is applied across the gap, then electromagnetic waves of high frequency emanate from the gap, indicating the presence of high frequency alternating current in the gap. This phenomenon is called **AC Josephson effect**.

The frequency of this current is given as,

$$v = 2eV/h$$

## APPLICATIONS OF SUPERCONDUCTORS

### **Electric generators**

Superconducting generators are very smaller in size and weight when compared with conventional generators. The low loss superconducting coil is rotated in an extremely strong magnetic field. Motors with very high powers, as large as 2500 kW, could be constructed at a very low voltage as low as 450V.

### **Low loss transmission lines**

Since the resistance is almost zero at superconducting phase, the power loss during transmission is negligible. Hence, electric cables are designed with superconducting wires.

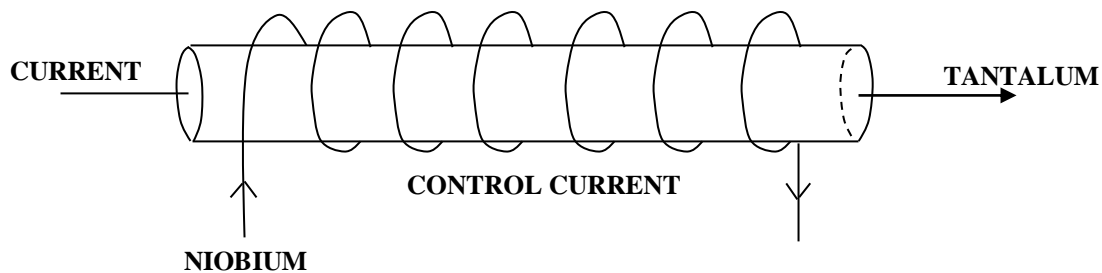
## Magnetic levitation

Diamagnetic property of a superconductor is the basis of magnetic levitation. A superconducting material can be suspended in air against the repulsive force from a permanent magnet. This effect can be used for high speed transportation.

## Fast electrical switching

A superconductor possesses two states, the superconducting and normal. The application of a magnetic field greater than the critical field can initiate a change from superconducting to normal and removal of the field reverses the process. This principle is applied in development of switching element called **CRYOTRON**.

This cryotron consists of a tantalum core around which a niobium wire is wound. Tantalum is the gate and niobium is the control. Allowing a control current to pass through niobium winding, a magnetic field sufficient to change tantalum from its superconducting state to normal state is produced. This closes the gate for the flow of current through tantalum. Removal of control current reopens the gate. Using this kind of elements, one can develop extremely fast large scale computers.



## **SQUIDS (Superconducting Quantum Interference Devices)**

SQUID is a double junction quantum interferometer. Two Josephson junctions mounted on a superconducting ring forms an interferometer. These are based on the flux quantization a superconducting ring. The total magnetic flux passing through the ring is quantized.

These SQUID sensors detect very minute magnetic signals. These are used to study tiny magnetic signals from the brain and heart. SQUID magnetometers are used to detect the paramagnetic response in the liver. This gives information about the amount of iron held in the liver accurately.

**ABSORPTION:** Different surfaces absorb sound energy differently. An open window passes all the sound waves falling on it, and hence an open window is taken as a perfect absorber. The extent of absorption by a surface is expressed in terms of the quantity absorption coefficient.

**ABSORPTION COEFFICIENT:** The Absorption coefficient( $\alpha$ ) is defined as the ratio of sound energy absorbed by the surface to the sound energy absorbed by an equal area of a perfect absorber given as

$$\alpha = \frac{\text{sound energy absorbed by the surface}}{\text{sound energy absorbed by an equal area of a perfect absorber}}$$

**REVERBERATION:** The sound produced by a source in a hall suffers successive reflections from the wall, floor, Ceiling and other reflecting materials in the hall. The listeners hear a series of sound waves. This gives the listener a persistence of sound even after the original sound has cutoff. This is called reverberation.

**REVERBERATION TIME:** The time interval required for the intensity to drop to one millionth of its original value is called reverberation time. It can be expressed in dB. If the incident intensity is  $I_i$ , then the final intensity  $I_f$  is one millionth of  $I_i$ ,

That is  $I_f = 10^{-6} I_i$

$$\frac{I_i}{I_f} = 10^6$$

In terms of dB's

$$dB_i = 10 \log \frac{I_i}{I}$$

$$dB_f = 10 \log \frac{I_f}{I}$$

$$\begin{aligned} dB_i - dB_f &= 10 \log \frac{I_i}{I_f} \\ &= 10 \log 10^6 \\ &= 10 \times 6 \\ &= 60 \end{aligned}$$

In other words, reverberation time for a hall is the time required for the intensity to drop by 60 dB.

**SABINE'S FORMULA:** The relation between reverberation time, the volume of the hall( $V$ ), the area ( $S$ ) and the absorption coefficient ( $\alpha$ ) is known as the sabine's formula. Let  $\alpha_1, \alpha_2, \alpha_3, \dots$  be

the absorption coefficients of the materials in the hall whose surface areas exposed to sound be  $s_1, s_2, s_3, \dots$ . Respectively. Then the average value of the absorption coefficient is given as

$$\alpha = \frac{\alpha_1 s_1 + \alpha_2 s_2 + \alpha_3 s_3 + \dots}{s_1 + s_2 + s_3 + \dots} = \frac{\sum \alpha_i s_i}{s}$$

$$\sum_i \alpha_i s_i = \alpha s$$

Where  $s$  is the total surface area of all surfaces exposed to sound.

By statistical method sound travels an average distance of  $4V/S$ ,

Where  $V$  is the volume of the hall between two successive reflections. This distance is known as **mean free path**.

$$\text{Time taken between two successive reflections} = \frac{4V}{sv}$$

Where  $v$  is the velocity of sound

$$\text{The avg. no. of reflections per sec is } n = \frac{sv}{4V}$$

Let  $I_t$  be the avg. intensity per unit volume of the hall at any given instant and  $dI$  the drop in intensity in a small interval of time  $dt$ . Then

The no. of reflections in time  $dt = ndt$

Drop in intensity per reflection =  $\alpha I$

Drop in intensity for  $ndt$  reflections =  $-\alpha I ndt$

The -ve sign is to indicate the drop in intensity. Substituting the value of  $n$ , we get

$$dI = \frac{-\alpha I s v dt}{4V}$$

$$\frac{dI}{I} = \frac{-\alpha s v dt}{4V}$$

On integration,

$$\ln I_t = -\frac{\alpha s v t}{4V} + \text{const}$$

Denoting the initial intensity by  $I_0$ , we obtain

$$\ln \frac{I_t}{I_0} = -\frac{\alpha s v t}{4V}$$

$$\frac{I_t}{I_0} = e^{-\frac{\alpha s v t}{4V}}$$

Using eq.  $\frac{I_t}{I_0} = 10^{-6}$ , we obtain  $e^{-\frac{\alpha s v T}{4V}} = 10^{-6}$  where  $T$  is the reverberation time.

$$\frac{\alpha s v T}{4V} = 6 \ln 10$$

$$= 6 \times 2.3026$$

Taking velocity of sound as 330m/s then, reverberation time

$$T = \frac{6 \times 2.3026 \times 4V}{330 \times \alpha s}$$

#### EYRING'S FORMULA:

Without approximating  $\log_e(1 - \bar{\alpha}) = -\bar{\alpha}$ , we get

This is known as Eyring's formula for relatively high absorption coefficients.

### Basic Requirements for the Acoustically Good Halls:

According to Prof. W.C.Sabine, the following are the basic requirements for the acoustically good halls.

1. The sound should be sufficiently loud at all parts of the hall.
2. There should be no echoes
3. The speech must be clear and distinct.
4. Noise and effect of resonance should be avoided.
5. There should be sufficient number of windows and ventilators in the hall.
6. Sound should be uniform throughout the hall.
7. The reverberation time should neither be too large nor too small.

### Problems:

- 1. An auditorium has a volume of 8400 m<sup>3</sup> required to have reverberation time 1.2 seconds. What is the total absorption in the hall?**

Solution: Given

The volume of an auditorium,  $V = 8400 \text{ m}^3$

The reverberation time,  $T = 1.2$  seconds

The reverberation time is given by

$$T = \frac{0.167V}{A}$$

$$\Rightarrow A = \sum aS = \frac{0.167V}{T}$$

Substituting the values then,  $A = 0.167 \times \frac{8400}{1.2}$

$$\therefore A = 1155 \text{ m}^2 \text{ O.W.U.}$$

- 2. The volume of a hall is 475 m<sup>3</sup>. The area of wall is 200 m<sup>2</sup>, area of the floor and ceiling each is 100m<sup>2</sup>. If the absorption coefficient of the wall, ceiling and floor are 0.025, 0.02 and 0.55 respectively, calculate the reverberation time for the hall.**

Solution:

Given volume of the hall,  $V = 475 \text{ m}^3$

$$\text{Reverberation time, } T = \frac{0.167V}{\sum aS}$$

$$\sum aS = (200 \times 0.025 + 100 \times 0.02 + 100 \times 0.55)$$

$$= 5 + 2 + 55 = 62$$

$$\therefore T = \frac{0.167 \times 475}{62} = 1.264 \text{ seconds.}$$

- 3. A hall has dimensions 20×15×5 m<sup>3</sup>. The reverberation time is 3.5 sec. calculate the total absorption coefficient.**

Solution: Given volume of the hall,  $V = 20 \times 15 \times 5 \text{ m}^3$

Reverberation time,  $T = 3.5$  sec.

$$\text{Total absorption, } A = \sum aS = \frac{0.167V}{T}$$



$$= \frac{0.167 \times 20 \times 15 \times 5}{3.5}$$

$$\therefore A = 70.714 \text{ O.W.U.}$$

$$\text{Average absorption coefficient} = \frac{\text{Total absorption}}{\text{surface area}} = \frac{70.714}{950} = 0.074 \text{ sabine/m}^2.$$

**4. The reverberation time of an auditorium is 1.5 s. The volume of the auditorium is  $6 \times 10^4 \text{ m}^3$  and the effective reflecting area with in the auditorium is  $4 \times 10^4 \text{ m}^2$ . Find the coefficient of absorption of the auditorium.**

Solution: Given Reverberation time,  $T = 1.5$  seconds

$$\text{Volume of the auditorium, } V = 6 \times 10^4 \text{ m}^3$$

$$\text{Total surface area, } S = 4 \times 10^4 \text{ m}^2$$

$$\text{Sabine's formula for reverberation time is } T = \frac{0.167V}{\sum aS}$$

$$\text{Coefficient of absorption, } a = \frac{0.167V}{TS} = \frac{0.167 \times 6 \times 10^4}{1.5 \times 4 \times 10^4}$$

$$\therefore a = 0.165$$

**DEL OPERATOR ( $\nabla$ ):** An operator which is capable of differentiating both vector and scalar called Del or nabla. It is defined as

$$\nabla = \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z}$$

Where i,j and k are the unit vectors.

The Del operator has three possible types of vector multiplications.They are gradient,diverence and curl.

**GRADIENT OF A SCALAR:** Thevector differential operator  $\nabla$  is operated on a scalar function  $\phi$  then It is called gradient of a scalar and is a vector . It is defined as

$$Grad \phi = \nabla \phi = \hat{i} \frac{\partial \phi}{\partial x} + \hat{j} \frac{\partial \phi}{\partial y} + \hat{k} \frac{\partial \phi}{\partial z}$$

For example the electric field vector is  $\nabla E = -Grad V = -\nabla V$

**DIVERGENCE OF A VECTOR:** The multiplication of a del operator with a vector called dot or scalar product.The divergence of a vector A can be written as

$$\begin{aligned} Div A = \nabla \cdot A &= \left( \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \right) \cdot (\hat{i} A_x + \hat{j} A_y + \hat{k} A_z) \\ &= \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} \end{aligned}$$

Where  $A_x, A_y$  and  $A_z$  are components of vector A in the direction of x,y and z respectively.

**CURL OF A VECTOR:**

$$\begin{aligned} Curl A = \nabla \times A &= \hat{i} \left( \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right) + \hat{j} \left( \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \right) + \hat{k} \left( \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \\ \nabla \times A &= \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix} \end{aligned}$$

**GAUSS THEOREM:** If 's' is a closed surface surrounding the volume V, the divergence for any vector A is expressed as

$$\int_s A \cdot ds = \int_v (\nabla \cdot A) dV$$

Where  $ds = \hat{n} ds$ , ds an element of area on s and  $\hat{n}$  the unit normal on ds.

**STOKES THEOREM:** If C is the closed contour around the edge of the open surface S, then stokes theorem states that

$$\int_l A \cdot dl = \int_s (\nabla \times A) \cdot ds$$

## EQUATION OF CONTINUITY:

$$\int_s J \cdot ds = -\frac{d}{dt} \int_v \rho dv$$
$$\int_s J \cdot ds = -\int_v \frac{\partial \rho}{\partial t} dv$$
$$\int_v \nabla \cdot J dv = -\int_v \frac{\partial \rho}{\partial t} dv$$
$$\nabla \cdot J = -\frac{\partial \rho}{\partial t}$$

## MAXWELL'S EQUATIONS:

**Maxwell's electric flux equation:** According to Gauss's law, the total electric displacement through the surface enclosing a volume is equal to the total charge within the volume.

$$\int_s D \cdot ds = q \quad \longrightarrow \quad (1)$$

Where D is the electric displacement density and q, the electric charge. In terms of charge density  $\rho$

$$q = \int_v \rho dv \quad \longrightarrow \quad (2)$$

from eqns 1 and 2

$$\int_s D \cdot ds = \int_v \rho dv$$

Using Gauss theorem we get,

$$\int_v \nabla \cdot D dv = \int_v \rho dv$$

$$\nabla \cdot D = \rho \quad \longrightarrow \quad (3)$$

Equation (3) is called **Maxwell's electric flux equation.**

**Maxwell's magnetic flux equation:** According to Gauss theorem in magnetostatics, the net magnetic flux emerging through any closed surface is zero.

$$\int_s B \cdot ds = 0 \quad \longrightarrow \quad (4)$$

Where B is the magnetic flux density which is magnetic flux per unit area. Converting the surface integral of eqn to volume integral, we get,

$$\int_v \nabla \cdot B dv = 0$$
$$\nabla \cdot B = 0 \quad \longrightarrow \quad (5)$$

Equation (5) is called **Maxwell's magnetic flux equation.**

**Maxwell's equation for induced electric field:** According to Faraday's law of electromagnetic induction, the negative time rate of change of magnetic flux linked with a circuit is equal to the emf induced in the circuit.

$$\int_l E \cdot dl = -\frac{\partial}{\partial t} \int_s B \cdot ds \quad \longrightarrow \quad (6)$$

Where E is the electric field strength and B is the magnetic flux density. Converting the line integral to surface integral using Stokes theorem,

$$\int_s (\nabla \times E) \cdot ds = \int_s -\frac{\partial B}{\partial t} \cdot ds \rightarrow (7)$$

$$\nabla \times E = -\frac{\partial B}{\partial t} \rightarrow (8)$$

Equation (8) is called **Maxwell's equation for induced electric field.**

**Maxwell's equation for induced magnetic field:**

“The magnetomotive force around a closed path is equal to  $\mu_0$  times the current enclosed by the path”.

i.e., the line integral of magnetic flux about any closed path is equal to  $\mu_0$  times the current enclosed by the closed loop.

$$\int_l H \cdot dl = i$$

$$i = \int_s J \cdot ds$$

$$\int_l H \cdot dl = \int_s J \cdot ds$$

Applying Stoke's theorem, we have

$$\int_s (\nabla \times H) \cdot ds = \int_s J \cdot ds$$

$$\nabla \times H = J$$

$$\nabla \cdot (\nabla \times H) = \nabla \cdot J = 0$$

$$\nabla \cdot J = 0$$

$$\nabla \cdot J = -\frac{\partial(\nabla \cdot D)}{\partial t}$$

$$\nabla \cdot \left(\frac{\partial D}{\partial t} + J\right) = 0$$

$$\int_s \left(\frac{\partial D}{\partial t} + J\right) \cdot ds = 0$$

$$\nabla \times H = \frac{\partial D}{\partial t} + J$$

**Maxwell's Electromagnetic equations:**

The set of four equations i.e. Gauss's laws of electrostatics and magnetostatics, Faraday's law of electromagnetism and Ampere's law are known as Maxwell's equations.

***Maxwell's equations in Integral form:***

$$(i) \iint_s \vec{D} \cdot d\vec{S} = \iiint_v \rho \, dV \quad \text{or} \quad \iint_s \vec{E} \cdot d\vec{S} = \frac{q}{\epsilon_0}$$

$$(ii) \iint_s \vec{B} \cdot d\vec{S} = 0$$

$$(iii) \oint \vec{E} \cdot d\vec{l} = -\frac{\partial}{\partial t} \iint_s \vec{B} \cdot d\vec{S}$$

$$(iv) \oint \vec{H} \cdot d\vec{l} = \iint_s \left( \vec{J} + \frac{\partial \vec{D}}{\partial t} \right) \cdot d\vec{S}$$

**Maxwell's equations in Differential form:**

$$(v) \vec{\nabla} \cdot \vec{D} = \rho \quad \text{or} \quad \text{Div } \vec{D} = \rho$$

$$(vi) \vec{\nabla} \cdot \vec{B} = 0 \quad \text{or} \quad \text{Div } \vec{B} = 0$$

$$(vii) \vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad \text{or} \quad \text{Curl } \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$(viii) \vec{\nabla} \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t} \quad \text{or} \quad \text{Curl } \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t}$$

## UNIT-V

### QUANTUM MECHANICS

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#### INTRODUCTION

The phenomenon such as interference, diffraction and polarization established the wave nature of light. A bold attempt was made by Max Planck, who proposed quantum theory and said that light behaves like a particle and is emitted in the form of discrete packets of energy. Experiments like photo-electric effect and Compton effect firmly established the particle nature of light. Hence, the dual nature of light was established by 1920.

In 1924, a French scientist, Louis de Broglie put forth a new concept. Just as particles associated with radiation are called photons, the waves associated with the moving particles are called matter waves.

Classical mechanics failed to explain atomic phenomenon involving electrons; protons etc, whose size and interacting distances are extremely small. This has led to the development of the quantum theory.

## WAVE-PARTICLE DUALITY

The universe we see today is the manifestation of matter and energy. Both of them exist in different forms. Einstein showed that mass and energy are mutually convertible, through his relation of mass-energy equivalence

$$E = mc^2$$

To understand the wave-particle duality, it is necessary to know what is a wave and what is a particle.

The concept of the **particle** is easy to understand. It is a representative unit of matter. It is a **discrete entity with particular mass, and occupies a definite position in space at any instant of time**. Thus, a particle is defined by,

- Mass, m
- Velocity, v
- Momentum, p
- Energy, E

The concept of a **wave** is a bit tedious one. A wave can be defined as, **the propagation of a disturbance in a medium without causing any change in the medium**. It is characterized by the following properties

- Frequency,  $\nu$
- Wavelength,  $\lambda$
- Amplitude, A
- Intensity, I
- Phase,  $\phi$

Prior to the intervention of the quantum mechanics, it was believed that the energy propagates in the form of continuous wave trains. Considering the above facts, it appears difficult to accept the idea that the radiation has dual nature. But, it is necessary to accept this because radiation sometimes behaved like a wave and sometimes like a particle. This behavior of the radiation is termed as the **wave-particle duality**.

It is important to note that, radiation can't exhibit both the particle and wave nature simultaneously in a single event. This is called **the principle of complementarity**.

## DE-BROGLIE'S HYPOTHESIS

It was established that light has dual nature. The manifestation of the properties depends upon the conditions under which the particular phenomenon occurs. **Louis de Broglie**, in 1924, extended the wave-particle parallelism of optics to all the fundamental entities of matter such as electrons, protons, neutrons, atoms and molecules.

He boldly suggested that, **nature loves symmetry**. That means the correspondence between wave and particle should not be confined only to electromagnetic radiation, but should also be valid for material particles i.e. **like radiation, matter also has dual nature. He proposed that, a moving particle has always got a wave associated with it. He called these waves matter waves or pilot waves or de-Broglie waves.**

The wavelength of such a wave is given as,

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

Where 'm' is the mass of the particle, 'p' its momentum.

### Expressions For de-Broglie Wavelength

According to Planck's quantum theory, energy of a photon is given by,

$$E = h\nu = h \frac{c}{\lambda} \longrightarrow (1)$$

According to Einstein's mass-energy equivalence,  $E = mc^2 \longrightarrow (2)$

Hence from (1) and (2),  $mc^2 = \frac{hc}{\lambda}$

$$\therefore \lambda = \frac{h}{mc}$$

If we consider the case of a material particle of mass 'm' moving with velocity 'v', then

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

If E is the kinetic energy of the particle, then

$$E = \frac{1}{2}mv^2 = \frac{1}{2} \frac{m^2v^2}{m} = \frac{p^2}{2m}$$

$$\Rightarrow p = \sqrt{2mE}$$

Hence, the de-Broglie wavelength is

$$\lambda = \frac{h}{\sqrt{2mE}}$$

When a charged particle carrying a charge 'q' is accelerated by a potential difference V, then its K.E is,  $E = qV$ .

Then the de-Broglie wavelength is given by,

$$\lambda = \frac{h}{\sqrt{2mqv}}$$

When a material particle is in thermal equilibrium at temperature T, then  $E = \frac{3}{2} K_B T$ , where  $K_B$  is the Boltzmann constant.

Then the de-Broglie wavelength is given as,

$$\lambda = \frac{h}{\sqrt{3mKT}}$$

### de-Broglie Wavelength Associated With The Electron

Let us consider an electron of rest mass  $m_0$  and charge 'e', which accelerated by potential V volts, from rest to velocity v, then  $\frac{1}{2} m_0 v^2 = eV$ , then  $v = \sqrt{\frac{2eV}{m_0}}$

$$\therefore \lambda = \frac{h}{m_0 v} = \frac{h \sqrt{m_0}}{m_0 \sqrt{2eV}} = \frac{h}{\sqrt{2eV m_0}}$$

$$\Rightarrow \lambda = \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 1.6 \times 10^{-19} \times V \times 9.1 \times 10^{-31}}}$$

$$\therefore \lambda = \frac{12.26}{\sqrt{V}} \text{ \AA}$$

### PROPERTIES OF MATTER WAVES

- Lighter is the particle, greater is the wave length associated with it, and vice-versa.
- When  $v = 0$ , then  $\lambda = \infty$ , i.e. wave becomes indeterminate and when  $v = \infty$ , then  $\lambda = 0$ . This shows that matter waves are generated by the motion of the particles.
- The de-Broglie wavelength is independent of charge.
- The velocity of matter waves depends on the velocity of the particle, i.e. it is not constant, whereas the velocity of electromagnetic wave is constant.
- A particle in motion, associated with a matter wave, has different velocities ; one due to the mechanical motion of particle v, and the second due to the propagation of the wave represented by  $\omega$

We know that  $E = h\nu$  and  $E = mc^2$ . Hence,  $\nu = \frac{mc^2}{h}$

The wave velocity,  $\omega = \nu \times \lambda = \frac{mc^2}{h} \times \frac{h}{mv}$



$$\therefore \omega = \frac{c^2}{v}$$

As the particle velocity  $v$  cannot exceed  $c$ ,  $\omega > c$ .

- The wave nature of the matter introduces an uncertainty in the location of the position of the particle because, a wave cannot be said to be existing exactly at one point.

Where the wave is strong, there is a good chance of finding the particle while, where the wave is small (weak), there is a small chance of finding the particle.

## SCHRÖDINGER'S TIME-INDEPENDENT WAVE EQUATION

Classical mechanics failed to provide a correct explanation for the properties of the physical systems with sub-atomic dimensions. According to the de-Broglie theory, a material particle is associated with a wave. A wave motion can be described effectively if we have a parameter related to that wave which varies in space and time. Hence, we need a parameter, which varies in space and time, to explain the nature of the matter waves.

**This mathematical reformation to the wave nature, called wave mechanics was developed by Schrödinger in 1926. He described the amplitude of matter waves by a complex quantity  $\psi(x,y,z,t)$  known as wave function or the state of the system.** It describes the particular dynamical system under observation.

According to de-Broglie theory, a particle of mass 'm' is always associated with a wave whose wavelength is given by  $\lambda = \frac{h}{mv}$ . If the particle has wave properties, it is expected that there should be some sort of wave equation which describes the behavior of the particle.

Consider a system of stationary waves associated with the particle. Let  $x,y,z$  be the coordinates,  $\psi$  be the displacement of the matter wave at any time  $t$ . this wave function is assumed to be finite, single-valued and periodic function.

The differential equation of a wave motion is given by,

$$\frac{\partial^2 \psi}{\partial t^2} = v^2 \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) = v^2 \nabla^2 \psi \longrightarrow (1)$$

Where  $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ , is a Laplacian operator, 'v' is the wave velocity.

The solution of the equation (1) is given by

$$\psi = \psi_o \sin \omega t = \psi_o \sin 2\pi \nu t \longrightarrow (2)$$

Where  $\nu$  is the frequency of the stationary wave associated with the particle.

Differentiating equation (2) twice with respect to  $t$ , we get

$$\frac{\partial \psi}{\partial t} = \psi_o (2\pi \nu) \cos 2\pi \nu t$$

$$\text{and } \frac{\partial^2 \psi}{\partial t^2} = -\psi_0 (2\pi\nu)^2 \sin 2\pi\nu t$$

$$\therefore \frac{\partial^2 \psi}{\partial t^2} = -4\pi^2 \nu^2 \psi = -\frac{4\pi^2 \nu^2}{\lambda^2} \psi \longrightarrow (3) \quad (\because \nu = \frac{v}{\lambda})$$

Substituting the value of  $\left(\frac{\partial^2 \psi}{\partial t^2}\right)$  from eqn. (3) in eqn.(1), we get

$$\begin{aligned} v^2 \nabla^2 \psi &= -\frac{4\pi^2 \nu^2}{\lambda^2} \psi \\ \Rightarrow \nabla^2 \psi + \frac{4\pi^2}{\lambda^2} \psi &= 0 \longrightarrow (4) \end{aligned}$$

Now from the de-Broglie relation,  $\lambda = \frac{h}{mv}$

$$\text{Hence, eqn. (4) becomes } \nabla^2 \psi + \frac{4\pi^2}{h^2} m^2 v^2 \psi = 0 \longrightarrow (5)$$

If E and V are the total and potential energies of the particle respectively, then its kinetic energy is given by,

$$\begin{aligned} \frac{1}{2} m v^2 &= E - V \\ \text{or } m^2 v^2 &= 2m(E - V) \longrightarrow (6) \end{aligned}$$

From eqn. (5) and (6) we have

$$\begin{aligned} \nabla^2 \psi + \frac{4\pi^2}{h^2} 2m(E - V)\psi &= 0 \\ \nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E - V)\psi &= 0 \longrightarrow (7) \end{aligned}$$

Substituting  $\hbar = \frac{h}{2\pi}$  in eqn. (7), we get

$$\boxed{\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V)\psi = 0} \longrightarrow (8)$$

This equation is known as **Schrödinger time independent wave equation**. For a free particle, V=0, hence the Schrödinger wave equation can be written as

$$\boxed{\nabla^2 \psi + \frac{2mE}{\hbar^2} \psi = 0}$$

### PHYSICAL SIGNIFICANCE OF THE WAVE FUNCTION

The wave function  $\psi$  was introduced by Erwin Schrödinger to explain the properties of the matter waves. Let us now see the physical concept behind the introduction of this quantity.

The wave function can be defined in such a way that any meaningful question about the result of an experiment performed upon the system can be answered if the wave function is known. At first, it was considered that the wave function  $\psi$  is merely an auxiliary mathematical quantity employed to make the calculations related to the experimental results.

The first interpretation of  $\psi$  was given by Schrödinger. We know that in any electromagnetic wave system, if  $A$  is the amplitude of the wave, then the energy density (energy per unit volume) is equal to  $A^2$ . Thus, the number of photons per unit volume is equal to  $\frac{A^2}{h\nu}$  i.e. the photon density is proportional to  $A^2$  as  $h\nu$  is a constant.

If  $\psi$  is the amplitude of the matter waves at any point in space, then the particle density at that point may be taken as proportional to  $\psi^2$ . Thus,  $\psi^2$  is a measure of particle density. When this is multiplied by the charge of the particle, charge density is obtained. In this way,  $\psi^2$  is a measure of charge density.

But,  $\psi$  is largely different from zero within some finite region known as wave packet. Now, the question that arises immediately is, “where is the particle situated in the wave packet?”

To explain this, Max Born suggested a new idea about the physical significance of  $\psi$  which is generally accepted. **According to Max Born,  $\psi \psi^* = |\psi|^2$  gives the probability of finding the particle in the state  $\psi$  i.e.  $\psi^2$  is a measure of probability density.**

The probability of finding a particle in volume  $d\tau = dxdydz$  is given by  $|\psi|^2 dxdydz$ . The total probability of finding the particle somewhere is unity i.e. particle is certainly to be found somewhere in the space.

$$\iiint |\psi|^2 dxdydz = 1$$

$\psi$  satisfying above requirement is said to be normalized. Besides being normalized, the wave function  $\psi$  must fulfill the following requirements.

- **It must be finite everywhere.** If  $\psi$  is infinite at a particular point, then it would mean an infinitely large probability of finding the particle at that point. That is not possible. Hence  $\psi$  must be finite or zero value at any point.
- **It must be single valued.** Let us consider that  $\psi$  has more than one value at any point. It means that there is more than one value of probability of finding the particle at that point. This is obviously ridiculous.

- **It must be continuous.** For Schrödinger equation to be valid,  $\left(\frac{\partial^2 \psi}{\partial x^2}\right)$  must be finite everywhere. This is possible only when  $\left(\frac{\partial \psi}{\partial x}\right)$  has no discontinuity at any boundary

where potential changes. This implies that  $\psi$  too must be continuous across a boundary.

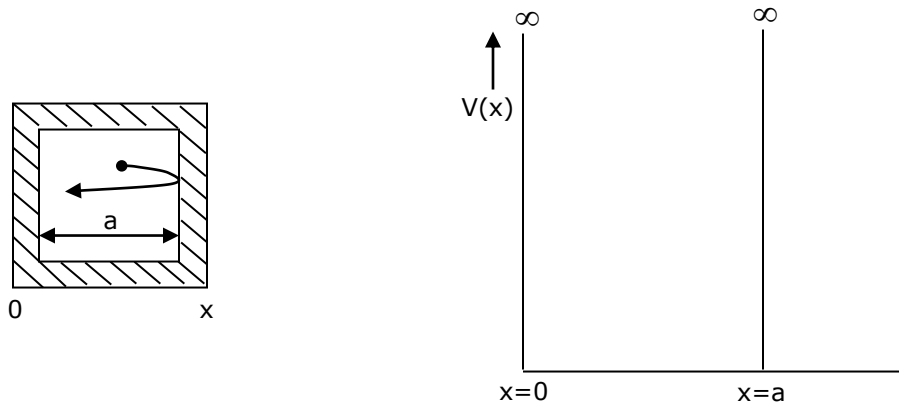
## PARTICLE IN ONE-DIMENSIONAL POTENTIAL BOX

### Bound State Problem

When the motion of the particle is confined to a limited region such that the particle moves back and forth in the region, the particle is said to be in bound state.

If one-dimensional motion of a particle is assumed to take place with zero potential energy over a fixed distance and if the potential energy is assumed to become infinite at the boundaries, then it is described as particle in one-dimensional box, which is the simplest among all the bound state problems.

Schrödinger wave equation can be used to derive the energy associated with particle moving in one-dimensional box.



Let us consider the case of a particle of mass 'm' moving along X-axis between the two rigid walls A and B at  $x=0$  and  $x=a$ . The particle is free to move between the walls. The potential energy of the particle between the two walls is constant because no force is acting on the particle. this constant value of the potential is taken as zero for simplicity.

When the particle strikes any one of the walls, it is reflected back immediately as the walls are perfectly rigid. Now the force acting on the particle abruptly changes from zero to a finite value  $F$  within a distance of zero at the wall.

We know that  $|F| = \frac{\partial V}{\partial x}$ , we should have  $\Delta V \rightarrow \infty$  as  $\Delta x \rightarrow 0$  such that  $\frac{\partial V}{\partial x}$  has a finite value. So the potential energy of the particle becomes infinite at the walls. Thus, the potential function is defined in the following way:

$$\left. \begin{array}{l} V(x) = \infty \text{ for } x < 0 \text{ and } x > a \\ \text{and } V(x) = 0 \text{ for } 0 \leq x \leq a \end{array} \right\} \longrightarrow (1)$$

The Schrödinger wave function for the particle is given by,

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

As  $V=0$  between the walls, the above equation takes the following form

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2} E\psi = 0 \longrightarrow (2)$$

Let  $\frac{8\pi^2 m}{h^2} E = k^2$ . Then the eqn. (2) takes the form

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \longrightarrow (3)$$

The general solution of the eqn. (3) is of the form,

$$\psi(x) = A \sin kx + B \cos kx \longrightarrow (4)$$

Where A & B are constants. The values of these constants can be obtained by applying the boundary conditions of the problem. They are

- $\psi = 0$  at  $x=0$  and
- $\psi = 0$  at  $x=a$

Applying the first condition, we have

$$0 = A \sin 0 + B \cos 0 \text{ i.e. } B=0$$

$$\therefore \psi(x) = A \sin kx$$

By applying the second boundary condition, we have  $0 = A \sin ka \therefore \psi(x) = 0$  when  $x=a$ .

$$\Rightarrow A \sin ka = 0$$

Here either  $A=0$  or  $\sin ka = 0$  but  $A \neq 0$  because, if  $A=0$ , the entire function will be zero as  $B=0$ .

$$\therefore \sin ka = 0 \text{ or } ka = n\pi \text{ (} n=1,2,\dots\text{)}$$

$$\therefore k = \frac{n\pi}{a} \longrightarrow (5)$$

Here we cannot take  $n=0$ , because for  $n=0$ ,  $k=0$ ,  $E=0$  and hence, every where in the box i.e. a particle in the box cannot have zero energy.

$$\psi(x) = 0$$

Now, the wave function becomes

$$\psi(x) = A \sin \frac{n\pi x}{a} \longrightarrow (6)$$

From eqn. (5)  $k^2 = \frac{n^2 \pi^2}{a^2}$  and we have used the relation  $\frac{8\pi^2 m}{h^2} E = k^2$ .

$$\therefore \frac{8\pi^2 m E_n}{h^2} = \frac{n^2 \pi^2}{a^2}$$

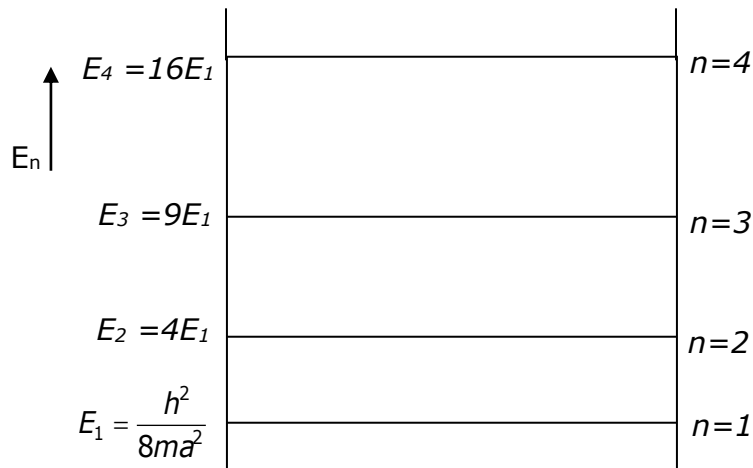
$$\boxed{\therefore E_n = \frac{n^2 h^2}{8ma^2}} \longrightarrow (7)$$

Where  $n=1,2,3,\dots$ , it is clear from the equation (7) that **inside an infinitely deep potential well, the particle can have only discrete set of values of energy i.e. the energy of the particle is quantized.**

The discrete energy values are given by:

$$E_1 = \frac{h^2}{8ma^2} \text{ for } n=1, E_2 = \frac{4h^2}{8ma^2} \text{ for } n=2, E_3 = \frac{9h^2}{8ma^2} \text{ for } n=3, \dots \text{ and so on.}$$

The energy levels are shown in the figure.



Equation (7) reveals that,

- the lowest energy of the particle is obtained by putting  $n=1$ , and is given by  $E_1 = \frac{h^2}{8ma^2}$  and  $E_n = n^2 E_1$ . This lowest possible energy is called **zero point energy**.
- The spacing between the  $n^{\text{th}}$  level and the next higher energy level increases as  $(n+1)^2 E_1 - n^2 E_1 = (2n+1)E_1$

Corresponding to each value of  $E_n$ , there will be one wave function which is given by,

$$\psi(x) = A \sin \frac{n\pi x}{a}$$

The constant A can be obtained by applying the normalization condition

$$\int_{-\infty}^{\infty} \psi_n(x) \psi_n^*(x) dx = 1$$

$$\therefore \int_0^a |\psi(x)|^2 dx = 1 \quad \because (0 < x < a)$$

$$\int_0^a A^2 \sin^2 \frac{n\pi x}{a} dx = 1$$

$$\Rightarrow A^2 \int_0^a \frac{1}{2} \left[ 1 - \cos \frac{2n\pi x}{a} \right] dx = 1$$

$$\Rightarrow \frac{A^2}{2} \left[ x - \frac{a}{2\pi n} \sin \frac{2n\pi x}{a} \right]_0^a = 1$$

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

$$\therefore A = \sqrt{\frac{2}{a}}$$

$$\therefore \psi(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

The above equation gives the wave functions of the particle enclosed in infinitely deep potential well.

The wave functions for the first three values of  $n$  are shown in the figure.

It is evident from the figure that,  $\psi_1$  has two nodes at  $x=0$  and  $x=a$ . similarly,  $\psi_2$  has three nodes at  $x=0$ ,  $x=a/2$  and  $x=a$ .

In general,  $\psi_n(x)$  has  $(n+1)$  nodes.

### Probability of the location of the particle

We know that the probability of finding a particle over a small distance  $dx$  at  $x$  is given by,

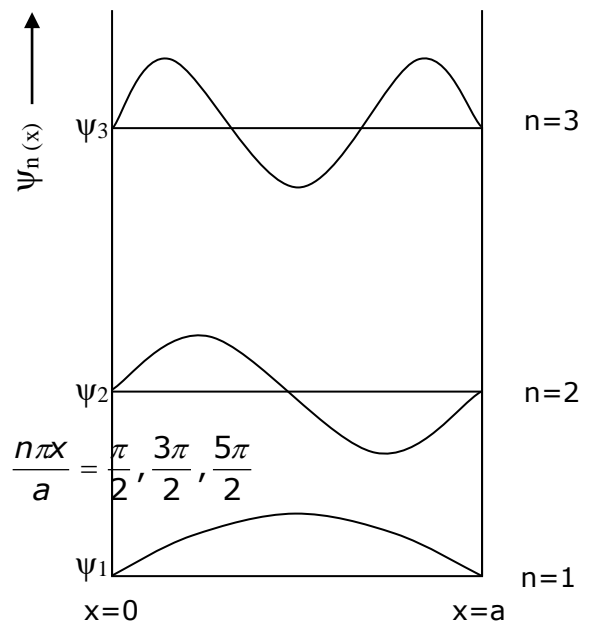
$$p(x)dx = |\psi_n|^2 dx$$

$$\therefore p(x)dx = \frac{2}{a} \sin^2 \frac{n\pi x}{a} dx$$

The probability density is maximum when

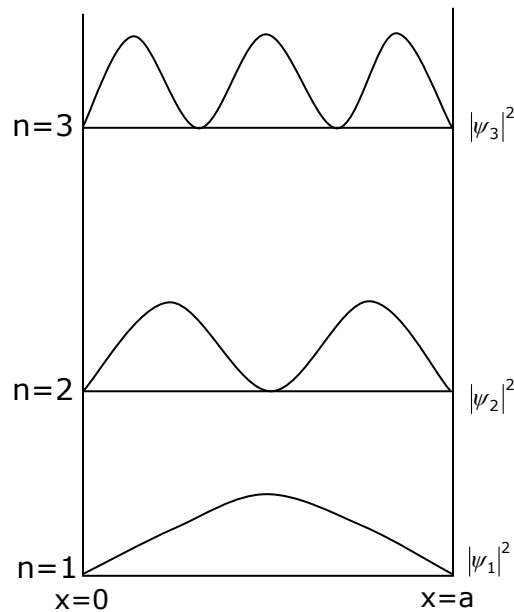
i.e. when  $x = \frac{a}{2n}, \frac{3a}{2n}, \frac{5a}{2n}$

Thus, for the  $n=1$  state, the most probable position of the particle is at  $x = \frac{a}{2}$



For  $n=2$ , the most probable positions are at  $x= \frac{a}{2} \frac{3a}{4}$

The probable positions in a particular state are shown in figure.



## FREE ELECTRON THEORY OF METALS

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### INTRODUCTION

The electrons in the outermost orbital of atom, which constitute the solid, determine its electrical properties. The electron theory of the solids aims to explain the structures and properties of solids through their electronic structure. This theory explains the electrical, thermal, magnetic and optical properties of conductors, semiconductors and insulators. The theory has been developed in three main stages:

- **The Classical free Electron Theory**

Drude & Lorentz developed this theory in 1900. According to this theory, the metals containing free electrons obey the laws of classical mechanics.

- **The Quantum Free Electron Theory**

Sommerfeld developed this theory during 1928. According to this theory, free electrons obey quantum mechanical laws.



- **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. This theory is also called **Band Theory of Solids**.

## PROPERTIES OF METALS

Let us have a brief view on the properties of metals and laws obeyed by them.

- The electrical conductivity ‘ $\sigma$ ’ of metals is very high ( $10^6$  to  $10^8$  mho/m). Therefore, the resistivity is very low ( $10^{-8}$  to  $10^{-6}$ ).
- Metals obey Ohm’s law, which states that the current flowing along a metallic wire is proportional to the potential difference  $V$  between the ends of the wire.

$$I \propto V \quad \Rightarrow I = \frac{V}{R}$$

Where ‘ $R$ ’ is the resistance of the wire.

- If ‘ $l$ ’ and ‘ $A$ ’ are length and area of cross-section of the wire, then  $R = \rho \frac{l}{A}$  where  $\rho$  is resistivity of material. If current density  $\mathbf{J} = \frac{I}{A}$ , electric field strength  $\mathbf{E} = \frac{V}{l}$ , then Ohm’s law can be written as,  $\mathbf{J} = \sigma \mathbf{E}$
- The resistance of a metal increases with the temperature  $T$  according to the rule,  $R(T) = R_0 + \alpha T$  where  $R_0$  is resistance at  $0^\circ\text{C}$ ,  $\alpha$  is temperature coefficient of resistance and  $T$  is temperature in  $^\circ\text{C}$ .
- At low temperature, the resistivity of a metal is proportional to the fifth power of absolute temperature, i.e.  $\rho \propto T^5$ . Above a particular temperature called Debye temperature,  $\rho \propto T$ .
- The resistivity of an impure metal is,  $\rho = \rho_0 + \rho(T)$ , where  $\rho_0$  is a constant for impure specimen,  $\rho(T)$  is temperature dependent resistivity of pure specimen. This is called Matheissen’s rule.
- The ratio between thermal to electrical conductivity of a metal is proportional to absolute temperature, which is known as Wiedemann-Franz law, (i.e)  $\frac{K}{\sigma} \propto T$ , where  $K$  is the thermal conductivity and  $\sigma$  is electrical conductivity of the metal.
- Near absolute zero, the resistivity of certain metals tends to zero i.e. exhibit the phenomenon of superconductivity.
- The conductivity of a metal varies in a magnetic field. This effect is known as magnetoresistance.
- For most metals, resistivity is inversely proportional to the pressure i.e.  $\rho \propto \frac{1}{P}$ .

## CLASSICAL FREE ELECTRON THEORY

This theory was proposed by Drude in 1900 and later developed by Lorentz. Many properties of the metals can be explained based on this theory.

We know that metal consist of valence electrons. These are loosely bound to the nucleus in an isolated atom. However, within the body of the metal, valence electrons are separated from the atoms. Therefore, they are free to move within the interatomic region. Such electrons are called free electrons. These are also referred to as conduction electrons since they are responsible for electrical conduction.

Following are the postulates of the Classical Free Electron Theory:

- Metals consist of large number of free electrons, which move about the whole volume of the metals like the molecules of a perfect gas in a container.
- These free electrons move in random directions and collide with either positive ion cores fixed to the lattice or other free electrons. All the collisions are elastic i.e. there is no loss of energy. Because of this random motion, the net current in the metal is zero.
- The movement of free electrons obeys the laws of classical kinetic theory of gases.
- The electron velocities in the metal obey the classical Maxwell-Boltzmann distribution of velocities.
- The free electrons move in a uniform potential field due to the ions fixed in the lattice, and the repulsion between the electrons is negligible.
- In between two collisions, the electrons may have uniform velocity but at every collision, both the magnitude and direction of the velocity will change.
- When an electric field is applied to the metal, the free electrons are accelerated in the direction opposite to the direction of the applied field and are responsible for conduction.

### **AVERAGE SPEED OF AN ELECTRON**

According to this theory, the free electrons are assumed to have average speed (or root mean square velocity), mean free path and mean lifetime. The value of  $v_{rms}$  can be calculated as follows.

According to the equipartition theorem, the expression for the pressure on the electron gas is given as,

$$P = \frac{1}{3} \rho v_{rms}^2$$
$$\text{i.e. } P = \frac{1}{3} mnv_{rms}^2$$

Where ' $P$ ' is the pressure on the electrons, ' $m$ ' is the mass of the electrons, ' $n$ ' is the number of electrons per unit volume,  $v_{rms}$  is the root mean square velocity of the electrons and  $\rho$  is the density of the electrons.

For the molar volume of the metal,  $P = \frac{1}{3} m \frac{N_A}{V_M} v_{rms}^2$ , where  $V_M$  is the molar volume and  $N_A$  is the Avogadro number.

$$\begin{aligned} \text{Now, } PV_M &= \frac{1}{3} m N_A v_{rms}^2 = R_u T \\ \Rightarrow m v_{rms}^2 &= 3 \frac{R_u}{N_A} T = 3 k_b T \end{aligned}$$

$$\therefore v_{rms}^2 = \frac{3 K_B T}{m} \quad \text{i.e. } v_{rms} = \sqrt{3 \frac{K_B T}{m}},$$

where  $R_u$  the universal gas constant and  $k_b$  is the Boltzmann constant.

The above equation indicates that, the average speed of an electron is directly proportional to the square root of absolute temperature.

### **MEAN FREE PATH**

The average distance traveled by the electrons between two successive collisions is called mean free path. It is given as,

$$\lambda = v_{rms} \tau$$

### **MEAN COLLISION TIME**

The average duration of time that elapses between two successive collisions is called mean collision time.

$$\tau = \frac{\lambda}{v_{rms}}$$

### **EXPRESSION FOR ELECTRICAL CONDUCTIVITY**

Owing to the random motion of electrons in a free field, the resultant motion is zero; hence, no current flows. When an electric field  $\mathbf{E}$  is applied to a conductor, an electric current begins to flow and the current density by Ohm's law is,

$$\mathbf{J} = \sigma \mathbf{E}$$

The constant  $\sigma$  is electrical conductivity of the specimen and its reciprocal is electrical resistivity  $\rho$ . Under the influence of external electric field, the electrons move in a direction opposite to that of the electric field. This directional motion of electrons is called **drift**. The average velocity gained during this motion is called **drift velocity**. The expression for drift velocity can be derived as follows.

The force acting on the electron moving under an electric field is given as,

$$F_E = - eE$$

During this accelerated motion, the electron collides with the lattice. This consequent scattering results in the loss of velocity it gained from the field. The effect of the lattice may be reduced considerably due to a retarding force. This force is proportional to the mass and velocity of the electron.

$$F_R = -\alpha m v$$

Hence, the equation of the motion of the electron is,

$$m \frac{dv}{dt} = F_E + F_R = -eE - \alpha m v \quad \longrightarrow \quad (1)$$

By the application of electric field, the velocity rises until the retarding force equals the force due to applied field. When these forces become equal, the acceleration ceases. After that, the electron moves with the drift velocity  $v_d$ .

$$\text{i.e. } -eE - \alpha m v_d = 0$$

$$\therefore v_d = \frac{-eE}{\alpha m} \quad \longrightarrow \quad (2)$$

The drift velocity per unit electric field is called the carrier mobility  $\mu$  i.e.  $\mu = \frac{-e}{\alpha m}$

Let us suppose that as soon as the velocity of the directional motion of the electrons attains a steady value, the field is cut-off (for e.g., at  $t = 0$  secs)

Because of the collision of the electrons with the lattice defects, the velocity starts decreasing. After sometime, the electron gas resumes its equilibrium condition. Such a process, which leads to the establishment of equilibrium in a system for which it was previously disturbed, is called the relaxation process.

When the applied field is cut-off, the equation of motion of the electrons becomes,

$$m \frac{dv}{dt} = -\alpha m$$

$$\Rightarrow \frac{dv}{v} = -\alpha dt$$

On integration,  $\log v = -\alpha t + C$

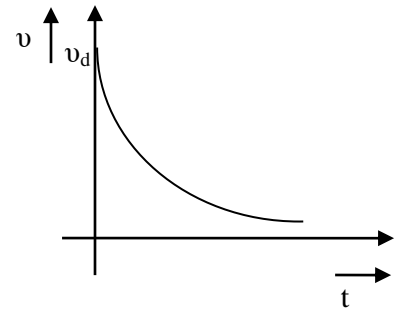
When  $t = 0$ ,  $v = v_d$ . i.e.  $\log v = -\alpha t + \log v_d$

$$\therefore v = v_d \exp(-\alpha t)$$

If at  $t = \tau$ ,  $v = v_d/e$ , then  $\frac{v_d}{e} = v_d \exp(-\alpha \tau)$

$$\Rightarrow \alpha = \frac{1}{\tau}$$

Thus, the time taken by the electron to attain a directional velocity, which is  $1/e$  of the drift velocity, is called the relaxation time,  $\tau$



Substituting this value of  $\alpha$  in equation (2), we get

$$v_d = -\frac{eE}{m} \tau \longrightarrow (3)$$

Let us assume that the distance between the layers, A & B is  $nv_d$ , with 'n' as number of free electrons in unit volume. Thus, the charge flowing through unit area for unit time at the layer B is  $nev_d$ . This is called the current density  $J$ .

$$J = -nev_d \quad \text{but,} \quad v_d = -\frac{eE}{m} \tau$$

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

We know that,  $J = \sigma E$ . Hence, by comparing the above equation with Ohm's law we can write that,

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

### Temperature Dependence of Resistivity

The relaxation time is given by,  $\tau = \frac{\lambda}{v_{rms}}$ . Now substituting this value in the equation of resistivity gives us,

$$\rho = \frac{m}{ne^2\lambda} v_{rms} = \frac{m}{ne^2\lambda} \sqrt{3 \frac{K_B T}{m}} = \frac{\sqrt{3K_B T m}}{ne^2\lambda}$$

$$\therefore \rho \propto \sqrt{T}$$

Since it was assumed in classical theory that  $\lambda$  is independent of temperature and is in the order of interatomic distance. But, it was found experimentally that,  $\rho \propto T$ . This discrepancy could not be explained by the classical theory. In addition, it is incorrect to treat  $\lambda$  to be independent of temperature.

### QUANTUM FREE ELECTRON THEORY

Classical theory based on its assumptions could explain Ohm's law, electrical conductivity and resistivity. It succeeded in explaining the Wiedemann-Franz law semi-quantitatively. Despite its merits, the theory equally left behind some concepts, about which it could not satisfy the experimental results.

Few most notable failures are;

- It could not predict the electronic contribution to the specific heat.

- It failed in predicting the exact value of Lorentz number in Wiedemann-Franz law.
- According to the assumptions of the theory, each electron has a magnetic moment associated with the spin and should give rise to paramagnetic susceptibility inversely proportional to temperature.

But, in reality, paramagnetism was found to be almost independent of temperature. **These drawbacks resulted because of the classical assumption that, all the free electrons in the metal absorb energy and participate in conduction, when energy is supplied to a metal externally. It was also assumed that all the electrons absorb equal amounts of energy.**

**Sommerfeld resolved these discrepancies in 1928, who replaced the Classical Maxwell-Boltzmann statistics by quantum Fermi-Dirac statistics. According to these statistics, the particles are indistinguishable and obey Pauli's exclusion principle.** He explained that only some of the (about 1%) free electrons could absorb energy and participate in conduction.

**He approximated the electron in a metal to be analogous to the particle in a one-dimensional potential box obeying the principles of quantum mechanics and Schrödinger equation. The electron was assumed to move inside the metal under a constant potential.**

**The electron encounters a huge difference in the potential at the surface of the metal, treated as walls of the potential well. Incapable of crossing the walls, the electron is treated to be trapped inside the metal, under normal conditions.** But, the concept of the free electron inside the metal was retained.

By considering these assumptions, he started attacking the problem by first discovering the possible energy states for an electron in the potential energy box and then considered the distribution of a large number of electrons in thermal equilibrium among these states with the help of Pauli's exclusion principle.

### **Electronic Distribution**

According to quantum mechanics, the energy of an electron in a 1-D potential is not continuous, but it is in discrete levels. The expression for the energy of the electron is given by,

$$E_n = \frac{n^2 h^2}{8ma^2} \text{ Where, } n = 1,2,3,\dots$$

and the wave function associated with the electron is,

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, \text{ where } n = 1,2,3,\dots$$

Now, if we assume that the metal is in the form of a cube of side 'a', the energy and the wave function transform as,

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

$$\psi_n(x, y, z) = \sqrt{\frac{8}{a^3}} \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{a} \sin \frac{n_z \pi z}{a} \text{ respectively.}$$

The wave function reduces to zero outside the box.

Now, let us see how Sommerfeld explained the distribution of the electrons in the metal.

- The electrons fill in the energy states with the help of Pauli's exclusion principle, which states that no two electrons will have same set of quantum numbers i.e. **not more than two electrons in any orbital state.**
- We now consider the building up of a free electron gas by dropping the electrons into a box one by one. The first electron, when dropped will occupy the minimum energy level, say  $E_0$ .
- The next electron will also be able to take the same state, provided it orients its spin antiparallel to the spin of the first electron.
- As already the minimum energy level was filled, the third electron when added to the box enters the next slightly higher energy level, say  $E_0 + \delta$  according to the Pauli's principle.
- This process will continue until all the available electrons (say  $N$ ,  $N$  being even) have been used.
- The first  $N/2$  energy levels will be filled with the electrons and all the higher energy levels are completely empty. This means that, the system is in its ground state ( $T = 0$ ).
- This  $N/2$ <sup>th</sup> level is called the Fermi level. **It is defined as, "the highest energy level that can be occupied at 0°K and energy corresponding to that level is called the Fermi energy,  $E_F$ ".**
- Thus, at  $T = 0$ , all the levels below the Fermi level are completely filled and all those above the Fermi level are completely vacant.

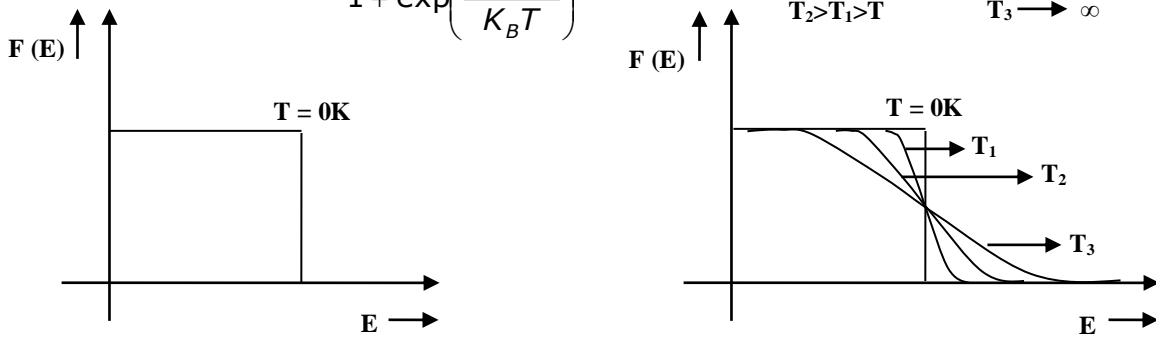
It was found that at non-zero temperatures, the distribution of the filled states would not end abruptly. Some of the states below the Fermi level are empty and some levels above the Fermi level are filled. Sommerfeld qualitatively explained the number of electrons available for conduction by introducing a function called Fermi distribution function.

## FERMI DISTRIBUTION FUNCTION

Sommerfeld introduced a parameter called Fermi distribution function, which qualitatively explains the electron conduction when energy is supplied to a metal externally. **This function gives the probability of occupation of an energy state by a single electron.**

The probability  $F(E)$  for the occupation of a particular energy level  $E$  by an electron is given by,

$$F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{K_B T}\right)}, \text{ Where } E_F \text{ is Fermi energy.}$$



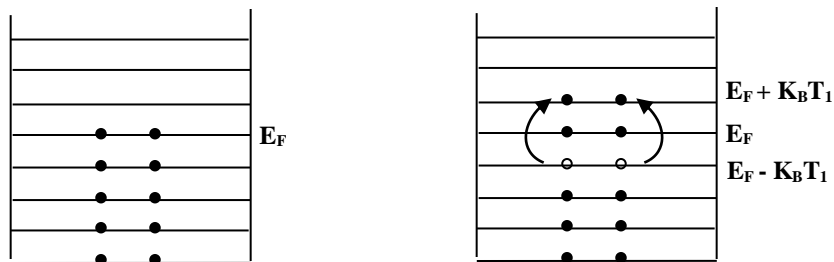
### FERMI DISTRIBUTION FUNCTION AT DIFFERENT TEMPERATURES

- At  $T = 0K$ , for  $E < E_F$ ,  $F(E) = 1$
- At  $T = 0K$ , for  $E > E_F$ ,  $F(E) = 0$
- At  $T$ , for  $E = E_F$ ,  $F(E) = 1/2$

This means that, at absolute zero, all quantum states below  $E_F$  are occupied while all those levels with energy greater than  $E_F$  are completely unoccupied. So,  $E_F$  is the maximum energy of the filled state. Fermi level is that level at which the probability of occupation is  $1/2$ .

We can see from the plot that with the increase in the temperature, the curve is slightly different. In addition, this difference is only near the Fermi level.

**Physically speaking, this explains that, when the temperature of the metal is increased, those free electrons, which are present in the  $K_B T$  range at Fermi level participate in conduction, but not all the free electrons.** i.e. when the temperature is  $T_1$ , only those electrons present in  $E_F - K_B T_1$  range move to  $E_F + K_B T_1$  range.



It is important to know, at this moment, about two more parameters related to the Fermi level.

- The velocity possessed by the electrons at the Fermi level called Fermi velocity,  $v_F$



- A parameter called Fermi temperature, which is defined as,  $T_F = \frac{E_F}{K_B}$

### HEAT CAPACITY OF ELECTRON GAS

Classical theory predicts that all the particles in an assembly would be able to absorb energy and hence contribute to the heat capacity. Thus, the electronic contribution to the heat capacity of a monovalent metal will be  $\frac{3}{2} N_A K_B = \frac{3R}{2}$ .

But, when the specimen is heated from absolute zero, only those electrons within an energy range  $K_B T$  of the Fermi level alone are excited thermally, and go to higher occupied states.

Thus, the minimum energy required for exciting all the free electrons will be  $E_F$ . Hence, the fraction of electrons absorbing energy are  $\frac{K_B T}{E_F}$ .

Hence, the energy associated with a kmol of metal will be,

$$U = N_A \frac{K_B T}{E_F} \frac{3}{2} K_B T = \frac{N_A K_B^2}{E_F} \frac{3T^2}{2}$$

$$\therefore C_{\text{Elec}} = \frac{dU}{dT} = 3 N_A K_B \frac{K_B T}{E_F}$$

For  $K_B T = 0.025\text{eV}$  (at  $T = 300\text{ K}$ ) and  $E_F = 5\text{eV}$  (on an average for all the metals).

$$C_{\text{Elec}} = 3R (0.005) = 0.015 R.$$

Where as, the lattice contribution is  $3R$ . This value of  $C_{\text{elec}}$  agrees with experimental value.

### WIEDEMANN-FRANZ LAW

According to the classical free electron theory, we have the expression for the thermal conductivity as,

$$K = \frac{3}{2} \frac{n K_B^2 T}{m} \tau, \sigma = \frac{ne^2 \tau}{m}$$

Now,  $\frac{K}{\sigma} = L T$  where,  $L = \frac{3}{2} \left( \frac{K_B}{e} \right)^2$

By applying quantum theory, a new expression was obtained for thermal conductivity, the value is,

$$K = \frac{\pi^2}{3} \frac{K_B^2 T n \tau_F}{m}, \sigma = \frac{ne^2 \tau_F}{m}$$

$$\therefore L = \frac{\pi^2}{3} \left( \frac{K_B}{e} \right)^2 = 2.45 \times 10^{-8} \text{ watt-ohm/ K}^2$$

Experimentally, it was verified that all the metals have the Lorentz number ‘L’ equal to the above value. Hence, the discrepancy in the value of Lorentz number was resolved by the quantum theory.

## SOURCES OF ELECTRICAL RESISTANCE IN METALS

The electrical resistance can be literally defined as the opposition to the flow of current in the metal, i.e. to the flow of free electrons. Regardless of the source of the disturbance to the path of electrons, their scattering results in an increase in the resistivity of the metal.

The prime sources, which contribute to the electron scattering, are;

**Thermal vibration of lattice**

**Presence of impurities**

**Other point defects**

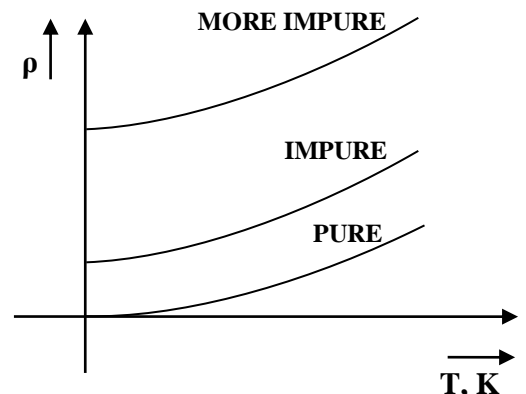
### Thermal Vibrations

When a metal is subjected to heat externally, it allows the atoms to vibrate with respect to their fixed positions. This prevents the atoms from being at their correct sites at same time. This results in frequent collisions of the electrons with the displaced atoms (exactly to speak, positive ion cores). The increased amount of electron scattering affects the mean free path of the electrons. Moreover, when the mobility of electron is limited in this way, the resistivity increases.

At very low temperatures, the impact of these lattice vibrations is not much substantial, and the conductivity increases.

### Impurities

Presence of any foreign substances in a metal act as scattering centers for mobile electrons, even in the absence of lattice vibrations. However, no real crystal is completely pure. Thus, the resistivity does not fall to zero at 0K. And, the resistivity curve is displaced upward by an amount, which reflects the extent to which these impurities are present and are effective as scatterers. The figure shows the variation in the resistivity value at different temperature for metals of varying purity.



For metals containing small amounts of impurities, the electrical resistivity,  $\rho$  is given as,

$$\rho = \rho_0 + \rho(T)$$

where  $\rho_0$  is a constant that depends directly on the impurity concentration and independent of temperatures, and  $\rho(T)$  is the temperature dependent part corresponding to the pure part of the metal.

This is called The Matheissen’s Rule. At high temperatures, the effect of lattice vibrations dominates this impurity factor.

## **Point Defects**

The existence of any vacancies or interstitialcies disturbs the lattice periodicity. This creates more number of collisions of free electrons with these defects, which act as effective centers of scattering.

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## **BAND THEORY OF SOLIDS**

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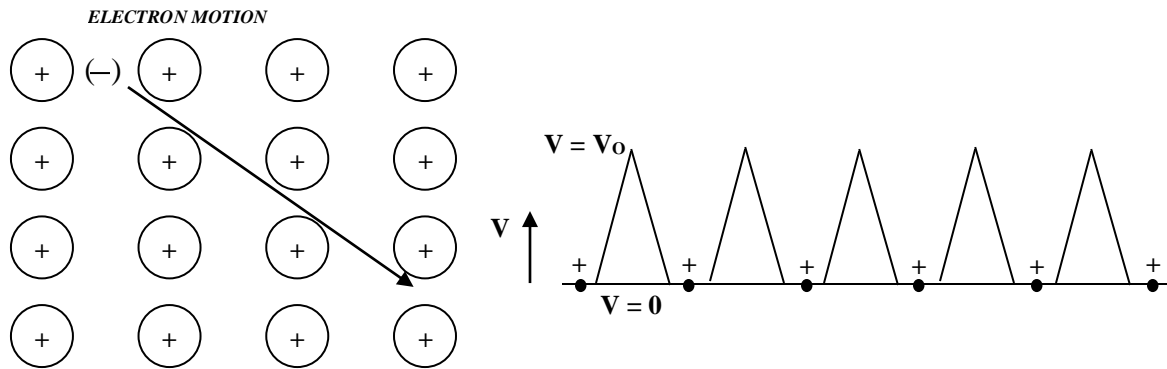
The quantum free electron theory successfully explains the phenomenon of specific heat, electrical conductivity, thermal conductivity and paramagnetism. Besides, it failed to explain the dependence of conductivity on temperature & pressure. The major pitfall of the theory is, it failed to explain why some solids are good conductors of electricity, some are semi conductors and some are insulators.

This problem was resolved by the introduction of the Zone theory or the band theory of solids by Bloch in 1928. Let us discuss the assumptions of the theory in brief.

### **Assumptions**

Contrary to the Sommerfeld's theory, it was assumed to disregard the surface and treat the crystal as an infinite array of lattice points. The attraction between the electrons and positive ion

cores is considered here. Hence, when an electron is moving inside the metal, the potential is minimum at the lattice points, where there is an attraction between electron and positive ion core; and maximum in the space between the lattice points.



Hence, one has to visualize that the electron is moving in a potential, which varies with the periodicity of the lattice. The concept of this periodic potential was found to illustrate many of the characteristic features regarding the behavior of the electrons.

### BLOCH'S THEOREM

Our objective is to study the motion of the electron in such a periodic lattice and the energy states it can occupy. According to Bloch, if the Schrödinger equation for the electron motion is of the form

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi = 0$$

i.e.  $\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} [E - V(x)] \psi = 0 \quad \longrightarrow (1)$

where the potential function  $V(x)$  has the periodicity of the lattice, i.e.  $V(x) = V(x + a)$ . Here, 'a' is the periodicity of the lattice, then the solution for such equation is of the form

$$\psi_{k(x)} = U_k e^{ikx} \quad \longrightarrow (2)$$

where  $U_k(x)$  has the periodicity of the lattice,

$$\text{i.e. } U_k(x) = U_k(x + a) \quad \longrightarrow (3)$$

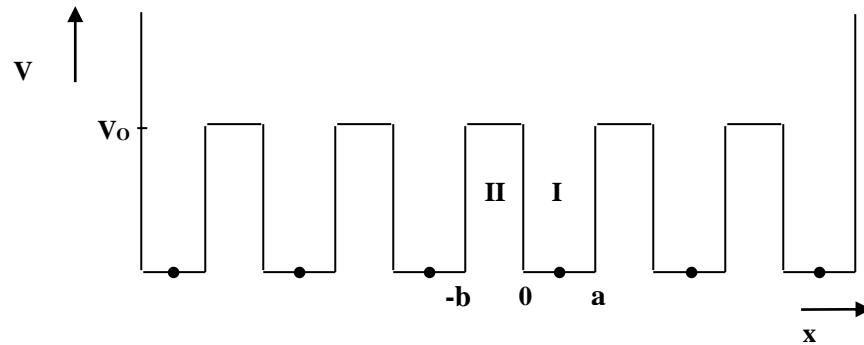
'k' represents the state of electron motion and  $k^{\text{th}}$  state corresponds to an electron having momentum  $\hbar k$ , and a de-Broglie wavelength,  $\lambda = \frac{2\pi}{k}$

In a one-dimensional model, we consider 'k' to be directed along X-axis. Generally, in 3-dimensional case, 'k' has to be treated as a vector and so called propagation vector.

The solution (2) consists of a plane wave  $e^{ikx}$  modulated by the periodic function  $U_k(x)$ .

### THE KRONIG – PENNEY MODEL

Kronig & Penney introduced a simpler shape of potential variation to make the application of Schrödinger equation easy. This shape of the potential is shown below;



The Kronig-Penney approximation is thus a periodic arrangement of potential wells and barriers. The time-independent Schrödinger equation takes the following forms for the two regions I & II.

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} E\psi = 0, \text{ for } 0 < x < a \quad \longrightarrow (4)$$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} [E - V_0]\psi = 0, \text{ for } -b < x < 0 \quad \longrightarrow (5)$$

Using Bloch's theorem, the solution of both the equations (4) and (5) is,

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

Assuming that the total energy  $E$  of the electron is less than the potential energy  $V_0$ , we define two real quantities  $\alpha$  &  $\beta$ , such that

$$\alpha^2 = \frac{8\pi^2mE}{h^2} \quad \longrightarrow (6)$$

$$\beta^2 = \frac{8\pi^2m}{h^2} (V_0 - E) \quad \longrightarrow (7)$$

Thus, equations (4) & (5) can be written as,

$$\frac{d^2\psi}{dx^2} + \alpha^2 \psi = 0, \text{ for } 0 < x < a \quad \longrightarrow (8)$$

$$\frac{d^2\psi}{dx^2} - \beta^2 \psi = 0, \text{ for } -b < x < 0 \quad \longrightarrow (9)$$

Differentiating the solution with respect to 'x', we get,

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

$$\frac{d\psi}{dx} = e^{ikx} \frac{dU_k}{dx} + U_k i k e^{ikx} \quad \text{and}$$

$$\frac{d^2\psi}{dx^2} = -k^2 e^{ikx} U_k + 2ike^{ikx} \frac{dU_k}{dx} + e^{ikx} \frac{d^2U_k}{dx^2}$$

Substituting these values in (8) and (9), we get,

$$\frac{d^2U_1}{dx^2} + 2ik \frac{dU_1}{dx} + (\alpha^2 - k^2)U_1 = 0, \text{ for } 0 < x < a \quad \rightarrow (10)$$

$$\frac{d^2U_2}{dx^2} + 2ik \frac{dU_2}{dx} - (\beta^2 + k^2)U_2 = 0, \text{ for } -b < x < 0 \quad (11)$$

Where  $U_1 = U_k(x)$  in  $0 < x < a$  and  $U_2 = U_k(x)$  in  $-b < x < 0$ .

The solution of the equation (10) is given by,

$$U_1 = A e^{i(\alpha-k)x} + B e^{-i(\alpha+k)x} \quad \rightarrow (12), A \& B \text{ are constants}$$

Similarly, for the equation (11), the general solution is,

$$U_2 = C e^{(\beta-ik)x} + D e^{-(\beta+ik)x} \quad \rightarrow (13), C \& D \text{ are constants}$$

The values of A, B, C, D can be obtained by applying the boundary conditions. They are as follows;

$$\text{Continuity condition: } [U_1(x)]_{x=0} = [U_2(x)]_{x=0}; \left[ \frac{dU_1(x)}{dx} \right]_{x=0} = \left[ \frac{dU_2(x)}{dx} \right]_{x=0}$$

$$\text{Periodicity condition: } [U_1(x)]_{x=a} = [U_2(x)]_{x=-b}; \left[ \frac{dU_1(x)}{dx} \right]_{x=a} = \left[ \frac{dU_2(x)}{dx} \right]_{x=-b}$$

Applying the conditions, we get,

$$(A + B) = (C + D) \quad \rightarrow (14)$$

$$i(\alpha - k)A - i(\alpha + k)B = (\beta - ik)C - (\beta + ik)D \quad \rightarrow (15)$$

$$A e^{i(\alpha-k)a} + B e^{-i(\alpha+k)a} = C e^{-(\beta-ik)b} + D e^{(\beta+ik)b} \quad \rightarrow (16)$$

$$\begin{aligned} & Ai(\alpha - k) e^{i(\alpha-k)a} - B i(\alpha + k) e^{-i(\alpha+k)a} \\ & = C(\beta - ik) e^{-(\beta-ik)b} - D(\beta + ik) e^{(\beta+ik)b} \end{aligned} \quad \rightarrow (17)$$

Equations (14), (15), (16), (17) will have non-vanishing solutions if and only if the determinant of the coefficients of A, B, C, D vanish.

i.e.

$$\begin{vmatrix} 1 & 1 & 1 & 1 \\ i(\alpha - k) & -i(\alpha + k) & (\beta - ik) & -(\beta + ik) \\ e^{i(\alpha-k)a} & e^{-i(\alpha+k)a} & e^{-(\beta-ik)b} & e^{(\beta+ik)b} \\ i(\alpha - k) e^{i(\alpha-k)a} & -i(\alpha + k) e^{-i(\alpha+k)a} & (\beta - ik) e^{-(\beta-ik)b} & -(\beta + ik) e^{(\beta+ik)b} \end{vmatrix} = 0$$

Simplifying the above equation, we get

$$\frac{mV_0ab}{\hbar^2} \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

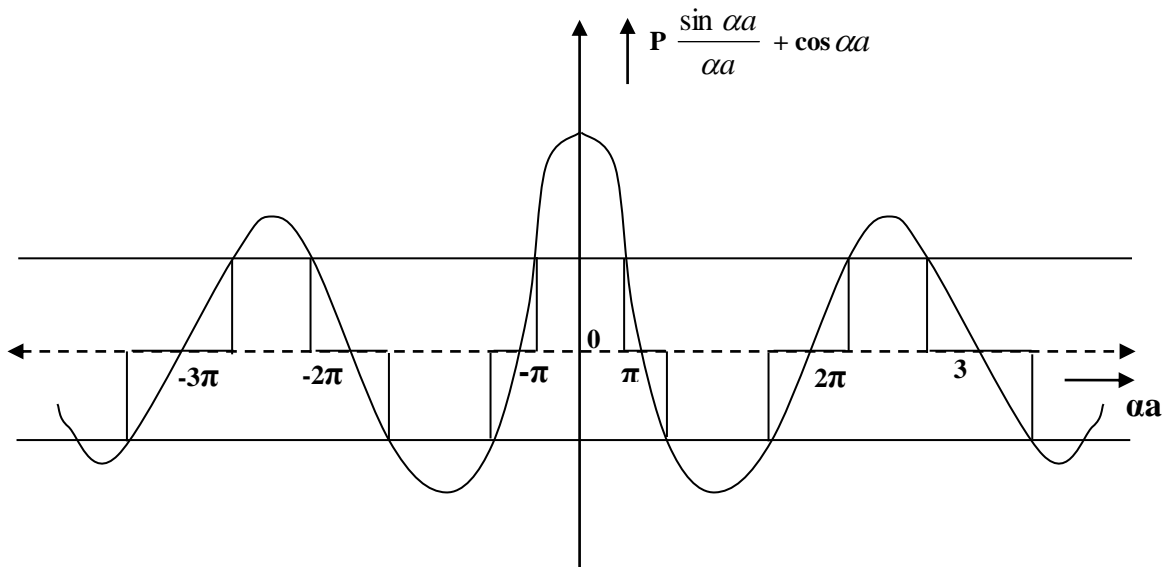
$$\boxed{P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka} \longrightarrow (18)$$

Where  $P = \frac{mV_0ab}{\hbar^2}$ . The term  $V_0b$  is called the barrier strength. The term  $P$  is referred to as scattering power of the potential barrier. It is a measure of the strength with which electrons in a crystal are attracted to the ions on the crystal lattice sites.

$$\text{Also, } \alpha^2 = \frac{8\pi^2mE}{\hbar^2} \text{ or } E = \frac{\alpha^2\hbar^2}{8\pi^2m} \text{ and } k = \frac{2\pi}{\lambda}$$

Equation (18) is a condition for the existence of a solution for the electron wave function. The RHS of the equation (18) is bounded since it can assume values between -1 & +1. If we plot the LHS of this equation against, it is possible to determine those values of  $\alpha$  and energy which are permissible i.e. those values of  $P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$  which lie between -1 & +1 are permissible.

When each of these values is set equal to  $\cos ka$ ,  $k$  is determined. This gives the value of  $\alpha$  from equation (10). The permissible  $\alpha$  values obviously result in permissible energy values, since  $\alpha^2 = \frac{8\pi^2mE}{\hbar^2}$ . Figure shows the plot for an arbitrary value of  $P = \frac{3\pi}{2}$ .



Following inferences can be drawn from the figure.

The allowed ranges of  $\alpha a$ , which permit a wave mechanical solution to exist are bands of allowed energy separated by forbidden regions.

As  $\alpha a$  increases, the width of the energy bands increases and the width of the forbidden bands decreases.

Let us now consider the varying effect of P

If P is large, i.e. if  $P \rightarrow \infty$ , the function described by the LHS of the equation (18) crosses +1 & -1 region at a steeper angle. This widens the forbidden bands and reduces the width of allowed bands.

When  $\alpha a = \pm n\pi$ ,  $\cos \alpha a = \cos ka$ . Then,  $ka = \pm n\pi \Rightarrow k = \pm \frac{n\pi}{a}$

These values of 'k' are points of discontinuity in the E-k curve for the electrons in the crystal.

$P \rightarrow \infty$  means that  $\sin \alpha a = 0 \Rightarrow \alpha a = \pm n\pi$

$$\Rightarrow \alpha^2 = \frac{n^2 \pi^2}{a^2} \text{ but, } \alpha^2 = \frac{8\pi^2 mE}{h^2}$$

$$\therefore \frac{n^2 \pi^2}{a^2} = \frac{8\pi^2 mE}{h^2}$$

$$\text{i.e. } \boxed{E = \frac{n^2 h^2}{8ma^2}} \rightarrow (19)$$

i.e. we get reduced to quantum case. Here E is independent of k. the energy levels are discrete similar to the energy levels of a particle in constant potential box.

The other extreme case is  $P \rightarrow 0$

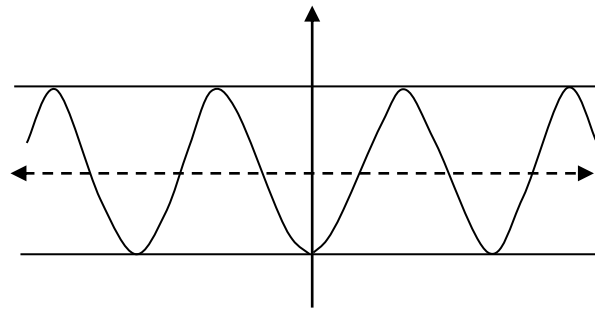
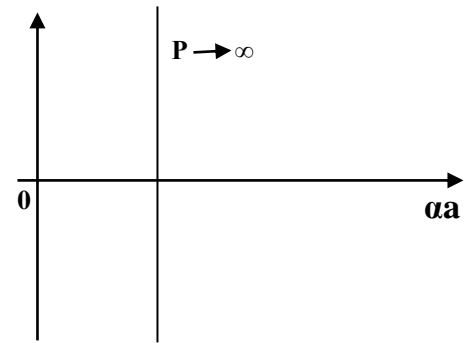
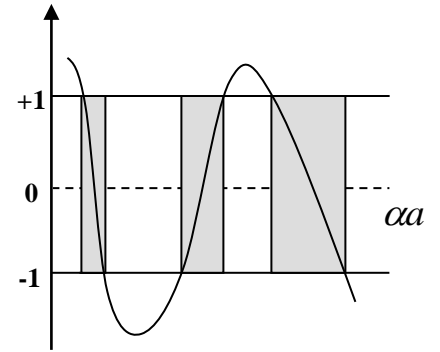
Here,  $\cos \alpha a = \cos ka \Rightarrow \alpha = k$

$$\text{and } \alpha^2 = k^2$$

$$\text{Thus, } k^2 = \frac{8\pi^2 mE}{h^2}$$

$$\therefore E = \frac{h^2}{8\pi^2 m} \left( \frac{2\pi}{\lambda} \right)^2 = \frac{h^2}{2m} \left( \frac{p}{h} \right)^2 = \frac{p^2}{2m}$$

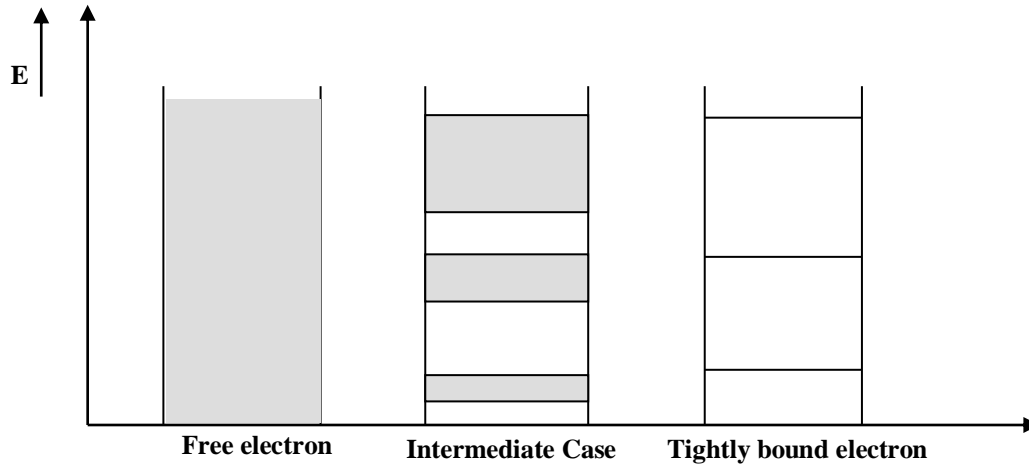
$$\therefore \boxed{E = \frac{1}{2} m v^2} \rightarrow (20)$$





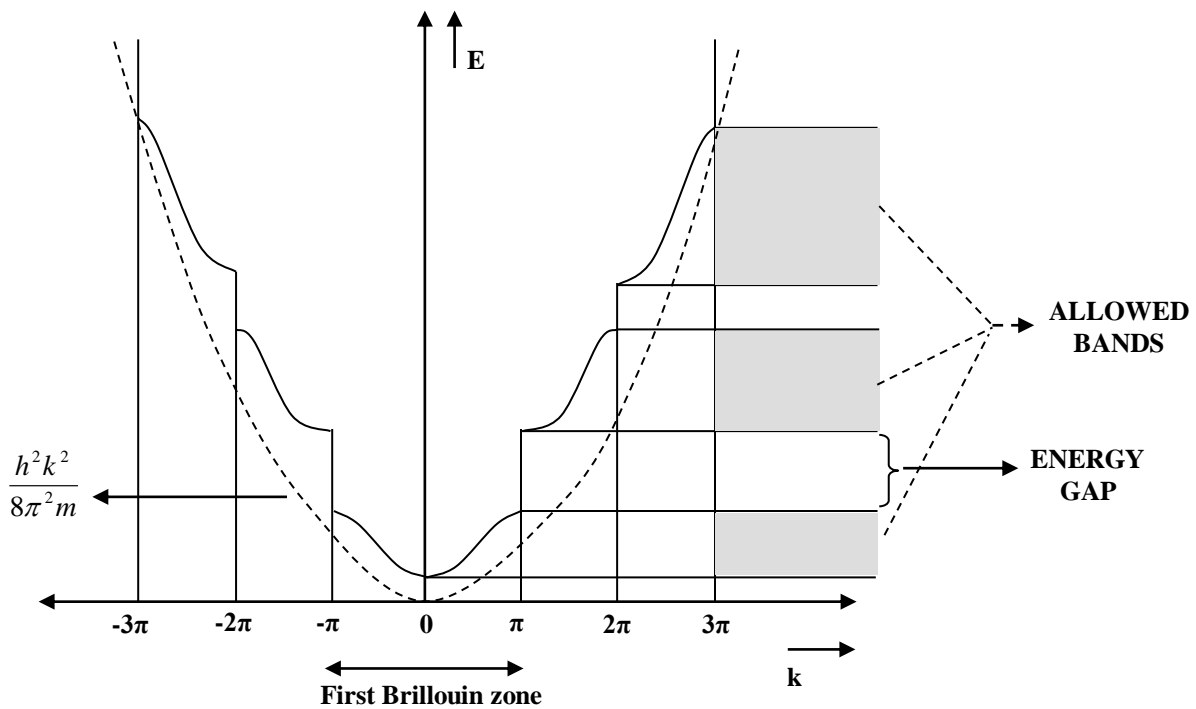
Hence, in this case all the energy values are allowed to the electron i.e. the electron is very free.

Thus, by varying P from zero to infinity, we can cover the whole range, from completely free electron to completely bound electron.



### BRILLOUIN ZONES

The electron moving in a periodic potential lattice can have energy values only between allowed regions or zones. With the help of equation (18), it is possible to plot the total energy E of the electron versus wave number 'k'.



The RHS of the equation (18) becomes  $\pm 1$  for values  $k = \pm \frac{n\pi}{a}$  and hence, discontinuities in E vs. k graph occur at  $k = \frac{n\pi}{a}$ , where  $n = \pm 1, \pm 2, \pm 3, \dots$

The dotted curve shows the free electron parabola,  $\frac{\hbar^2 k^2}{2m}$ . We see that the electron has allowed energy values in the region or zone extending from  $k = -\frac{\pi}{a}$  to  $k = +\frac{\pi}{a}$ . This zone is called the first Brillouin zone.

After a break in the energy values, called forbidden region, we get another zone of allowed values in the region extending from  $k = -\frac{2\pi}{a}$  to  $-\frac{\pi}{a}$  and  $k = +\frac{\pi}{a}$  to  $+\frac{2\pi}{a}$ . This is called the second Brillouin zone. Similarly, the other higher order Brillouin zones can also be defined.

## MOTION OF ELECTRONS IN A 1-D PERIODIC POTENTIAL

### Velocity

According to the de-Broglie hypothesis, electron moving in a periodic potential is associated with a matter wave. Now, we analyze the motion of the electron in a periodic potential, quantum mechanically. Accordingly, the velocity of the electron is equal to the group velocity of the wave packet associated with the electron.

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

Here,  $\omega$  is the angular frequency of the de-Broglie's wave and can be expressed as,  $E = \hbar\omega$

$$\text{Now, } \frac{dE}{dk} = \hbar \frac{d\omega}{dk}$$

Substituting in (1), we get

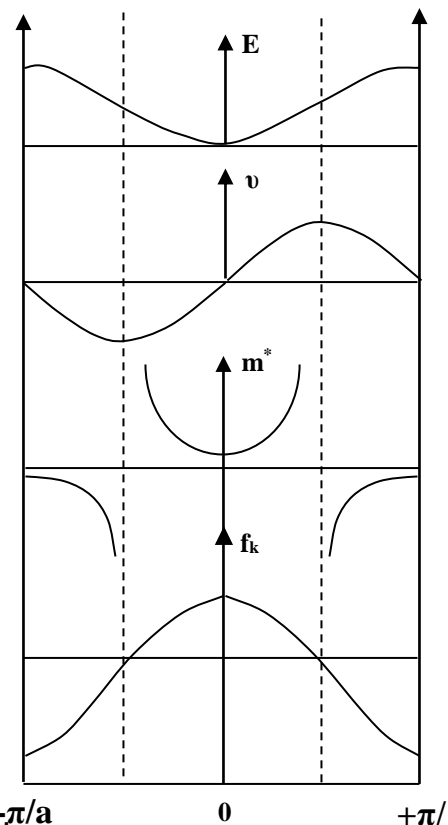
$$v = \frac{1}{\hbar} \left( \frac{dE}{dk} \right) \rightarrow (2)$$

$$\text{For free electrons, } E = \frac{\hbar^2 k^2}{2m}$$

$$\text{i.e. } \left( \frac{dE}{dk} \right) = \frac{\hbar^2}{2m} \times 2k = \frac{\hbar^2 k}{m}$$

Thus, equation (2) becomes,

$$v = \frac{1}{\hbar} \left( \frac{\hbar^2 k}{m} \right) = \frac{\hbar}{m} \left( \frac{2\pi}{\lambda} \right) = \frac{\hbar}{m} \left( \frac{2\pi p}{h} \right) = \frac{p}{m}$$



$$\therefore v = \frac{p}{m} \rightarrow (3)$$

Equation (3) shows that  $v$  varies linearly with 'k'. In band theory,  $E$  is not proportional to  $k^2$ . Using equation (2),  $v$  can be calculated. But, the velocity curve is found to be strange.

At the bottom of the energy band ( $k=0$ ), the velocity is zero and as  $k$  increases, the velocity increases and reaches its maximum at  $k = k_0$ .

Beyond this point, the velocity decreases and finally assumes zero value at  $k = \frac{\pi}{a}$ , which is the top of the band.

### EFFECTIVE MASS OF THE ELECTRON

The mass of the electron moving under a periodic potential inside a crystal appears different from the free electron mass. Such apparent mass is referred to as the effective mass.

The velocity of the electron in a 1-D lattice is,

$$v = \frac{2\pi}{h} \left( \frac{dE}{dk} \right) \rightarrow (4)$$

The acceleration is given by,

$$a = \frac{2\pi}{h} \frac{d}{dt} \left( \frac{dE}{dk} \right)$$

$$\Rightarrow a = \frac{2\pi}{h} \frac{d^2E}{dk^2} \left( \frac{dk}{dt} \right) \rightarrow (5)$$

Since we can know the value  $\frac{d^2E}{dk^2}$  from  $E$  &  $k$  relation, all we have to find is,  $\frac{dk}{dt}$  under the influence of the applied field  $E$ .

Let an electron be subjected to the influence of an external field of strength  $E$  for a time  $dt$ . If the velocity of the electron is  $v$ , the distance traveled in the time  $dt$  is,  $vdt$ .

Hence,  $dE = e E v dt$ .

Substituting the value of  $v$  from the equation (4) in the above relation, we get

$$dE = e\mathcal{E} \left( \frac{2\pi}{h} \right) \left( \frac{dE}{dk} \right) dt$$

$$\text{Thus, } \frac{dk}{dt} = \frac{2\pi e\mathcal{E}}{h} \rightarrow (6)$$

Now the acceleration 'a' can be written as,

$$\Rightarrow a = \frac{2\pi}{h} \frac{d^2E}{dk^2} \left( \frac{2\pi e\mathcal{E}}{h} \right)$$

$$\Rightarrow a = \left( \frac{4\pi^2}{h^2} \right) e\mathcal{E} \frac{d^2 E}{dk^2} \quad \longrightarrow \quad (7)$$

Comparing this formula with that of a free classical particle,

$$m \frac{dv}{dt} = e\mathcal{E}$$

$$\text{or } \frac{dv}{dt} = a = \frac{e\mathcal{E}}{m} \quad \longrightarrow \quad (8)$$

Equations (7) & (8) are identical in form, if we define a new quantity  $m^*$  such that,

$$m^* = \left( \frac{h^2}{4\pi^2} \right) \left( \frac{d^2 E}{dk^2} \right)^{-1}$$

This  $m^*$  is called the **effective mass**, and is determined by  $\frac{d^2 E}{dk^2}$ .

For a free electron,  $E = \frac{\hbar^2 k^2}{2m}$  &  $\frac{d^2 E}{dk^2} = \frac{\hbar^2}{m}$

$$\therefore m^* = m$$

Thus, for an electron moving in a periodic potential,  $m^* \neq m$  and  $E = \frac{\hbar^2 k^2}{2m^*}$

This is known as the effective mass approximation.

We introduce another parameter called the degree of freedom of the electron, given by

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

Where,  $f_k$  is the measure of the extent to which an electron in a state 'k' is free. If  $m^*$  is large,  $f_k$  is small i.e. the particle behaves as a heavy particle. When  $f_k = 1$ , the electron behaves as a free electron.  $f_k$  is positive in the lower half of the band, and negative in the upper half.

## UNIT-VI

### SEMICONDUCTORS

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#### INTRODUCTION

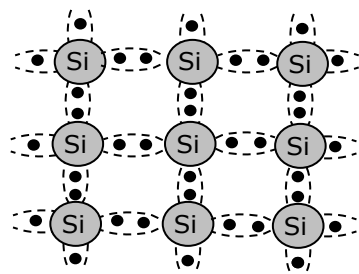
Semiconductors are those materials whose electronic properties are intermediate between those of metals and insulators. These intermediate properties are determined by the crystal structure, bonding characteristics, and electronic energy bands and also by the fact, unlike metals, a semiconductor has both positive and negative carriers of electricity whose densities can be controlled by doping the pure semiconductor with chemical impurities during crystal growth.

In this chapter we shall see the physics of semiconductors and the phenomenon that takes place in these solids.

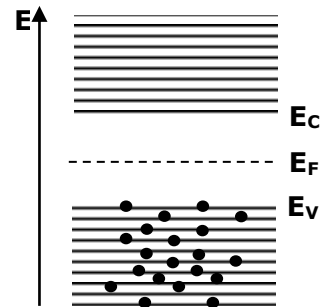
#### **INTRINSIC SEMICONDUCTORS AND CARRIER CONCENTRATION**

Chemically pure semiconductors in which the electrons and holes are produced by the **thermal activation** are called **intrinsic semiconductors**. Silicon and germanium serve as good

examples for intrinsic semiconductors. At 0K, all the valence electrons are strongly bound to their atoms and they spend most of the time between the neighboring atoms. Since all the valence electrons are engaged in covalent bonds, the bonds are **complete**. Free electrons do not exist in the solid. **Thus, a semiconductor at 0K cannot conduct and acts as a perfect insulator.**



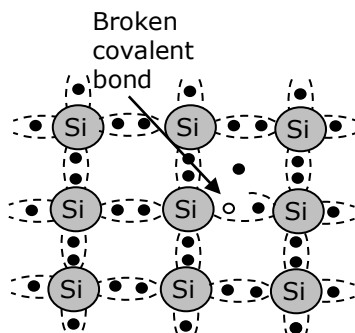
At T = 0 K



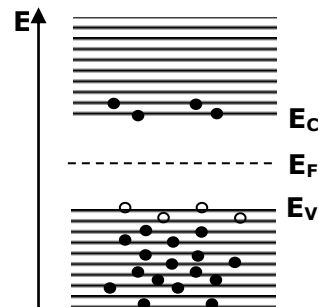
FILLED VALENCE BAND AND EMPTY CONDUCTION BAND AT 0K

At higher temperatures, the finite thermal energy causes each atom in the crystal to vibrate about its mean position. When the vibrations grow large, some of the electrons acquire sufficient energy and break away from the covalent bonds. The electrons liberated from the bonds become **free electrons** which move randomly in the empty spaces that exist for them between the fixed positions of the atoms.

From an energy band point of view, it means that some electrons which receive the energy equal to or more than band gap energy, are excited from the valence band to the conduction band. This band gap energy is a characteristic of the material. Thus, **the band gap energy is the minimum amount of energy required to excite an electron from valence band to the conduction band.** The number of electrons excited into the conduction band depends upon the thermal energy received by the crystal.



At T > 0 K



The motion of the electrons in the valence band is described in terms of a fictitious particle called **hole** which is bequeathed with a positive charge and a mass  $m_h$ .

### CARRIER CONCENTRATION IN INTRINSIC SEMICONDUCTORS

At equilibrium, the number of electrons present per unit volume ( $n$ ) in the conduction band is equal to the number of holes per unit volume ( $p$ ) in the valence band.

In order to calculate the intrinsic carrier concentration, we first calculate the number of electrons excited into the conduction band at any temperature  $T$  K and also the number of holes created in the valence band.

Under equilibrium, the no. of electrons per unit volume having energies in between  $E$  and  $E + dE$  is given by,

$$n(E)dE = Z_c(E)dE.F_n(E) \longrightarrow (1)$$

where  $F_n(E)$  is the Fermi distribution function for the electrons and  $Z_c(E)$  is the density of states factor.

$$Z_c(E) = \frac{\pi}{2} \left( \frac{8m_e^*}{h^2} \right)^{\frac{3}{2}} E^{\frac{1}{2}} \text{ and } F_n(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{K_B T}\right)} \longrightarrow (2)$$

In the above equation,  $E$  starts from the bottom of the conduction band. Hence,

$$Z_c(E) = \frac{\pi}{2} \left( \frac{8m_e^*}{h^2} \right)^{\frac{3}{2}} (E - E_c)^{\frac{1}{2}} \longrightarrow (3)$$

where  $m_e^*$  is the effective mass the electron. And  $F_n(E)$  in this case can be reduced to

$$F_n(E) = \frac{1}{\exp\left(\frac{E - E_F}{K_B T}\right)} = \exp\left(\frac{E_F - E}{K_B T}\right)$$

This is because at all temperatures of interest  $\exp\left(\frac{E_F - E}{K_B T}\right) \gg 1$ .

Hence, the total number of electrons per unit volume in the conduction band is given by,

$$\int n(E)dE = \int_{E_c}^{\infty} Z_c(E)F_n(E)dE$$

$$n = \frac{\pi}{2} \left( \frac{8m_e^*}{h^2} \right)^{\frac{3}{2}} \int_{E_c}^{\infty} (E - E_c)^{\frac{1}{2}} \exp\left(\frac{E_F - E}{K_B T}\right) dE$$

Now, let us write  $E - E_C = \varepsilon \Rightarrow dE = d\varepsilon$ . Hence, the quantity  $\varepsilon$  varies from 0 to  $\infty$ .

$$\begin{aligned} n &= \frac{\pi}{2} \left( \frac{8m_e^*}{h^2} \right)^{\frac{3}{2}} \exp\left(\frac{E_F}{K_B T}\right) \int_0^{\infty} (\varepsilon)^{\frac{1}{2}} \exp\left(-\frac{(\varepsilon + E_C)}{K_B T}\right) d\varepsilon \\ &= \frac{\pi}{2} \left( \frac{8m_e^*}{h^2} \right)^{\frac{3}{2}} \exp\left(\frac{E_F - E_C}{K_B T}\right) \int_0^{\infty} (\varepsilon)^{\frac{1}{2}} \exp\left(-\frac{\varepsilon}{K_B T}\right) d\varepsilon \longrightarrow (4) \end{aligned}$$

The integral  $\int_0^{\infty} (\varepsilon)^{\frac{1}{2}} \exp\left(-\frac{\varepsilon}{K_B T}\right) d\varepsilon$  is in the form  $\int_0^{\infty} (x)^{\frac{1}{2}} \exp(-ax) dx$  which has a solution  $\frac{\sqrt{\pi}}{2a\sqrt{a}}$ .

$$\begin{aligned} \text{Hence, } \int_0^{\infty} (\varepsilon)^{\frac{1}{2}} \exp\left(-\frac{\varepsilon}{K_B T}\right) d\varepsilon &= \frac{\sqrt{\pi}}{2} (K_B T)^{\frac{3}{2}} \\ \therefore n &= \frac{\pi}{2} \left( \frac{8m_e^*}{h^2} \right)^{\frac{3}{2}} \exp\left(\frac{E_F - E_C}{K_B T}\right) \frac{\sqrt{\pi}}{2} (K_B T)^{\frac{3}{2}} \\ &= 2 \left( \frac{2\pi m_e^* K_B T}{h^2} \right)^{\frac{3}{2}} \exp\left(\frac{E_F - E_C}{K_B T}\right) \longrightarrow (5) \end{aligned}$$

The term  $2 \left( \frac{2\pi m_e^* K_B T}{h^2} \right)^{\frac{3}{2}}$  is almost constant compared with the exponential term and so it is called pseudo constant and is denoted by the symbol  $N_C$ .

$$n = N_C \exp\left[-\left(\frac{E_C - E_F}{K_B T}\right)\right] \longrightarrow (6)$$

This is the expression for the density of electrons in conduction band. The number of holes per unit volume can be found in the similar model.

The number of holes present in the valence band in the energy range  $dE$  is given by,

$$\rho(E)dE = Z_v(E)dE F_p(E) \longrightarrow (7)$$

Where  $Z_c(E)$  is the density of the states factor for the hole given by,



$$Z_V(E) = \frac{\pi}{2} \left( \frac{8m_p^*}{h^2} \right)^{\frac{3}{2}} (E_V - E)^{\frac{1}{2}} \longrightarrow (8)$$

And  $F_P(E)$  is the probability of occupation of a hole in the state  $E$  which is given by,

$$\therefore F_P(E) = 1 - F_n(E)$$

$$\begin{aligned} \therefore F_P(E) &= 1 - \frac{1}{1 + \exp\left(\frac{E - E_F}{K_B T}\right)} = \frac{\exp\left(\frac{E - E_F}{K_B T}\right)}{1 + \exp\left(\frac{E - E_F}{K_B T}\right)} \\ &= \frac{1}{\exp\left(\frac{E_F - E}{K_B T}\right) + 1} = \exp\left(\frac{E - E_F}{K_B T}\right) \longrightarrow (9) \end{aligned}$$

Using equations (7), (8) & (9) we can write,

$$p(E)dE = \frac{\pi}{2} \left( \frac{8m_p^*}{h^2} \right)^{\frac{3}{2}} (E_V - E)^{\frac{1}{2}} \exp\left(\frac{E - E_F}{K_B T}\right)$$

$$\therefore p(E) = \int p(E)dE = \int_{-\infty}^{E_V} Z_V(E) F_P(E) dE$$

$$\therefore p = \frac{\pi}{2} \left( \frac{8m_p^*}{h^2} \right)^{\frac{3}{2}} \int_{-\infty}^{E_V} (E_V - E)^{\frac{1}{2}} \exp\left(\frac{E - E_F}{K_B T}\right) dE$$

Now, let us write  $E_V - E = \varepsilon \Rightarrow dE = -d\varepsilon$ . Hence, the quantity  $\varepsilon$  varies from  $\infty$  to 0.

$$\text{Thus, } p = \frac{\pi}{2} \left( \frac{8m_p^*}{h^2} \right)^{\frac{3}{2}} \exp\left(\frac{E_V - E_F}{K_B T}\right) \int_0^{\infty} (\varepsilon)^{\frac{1}{2}} \exp\left(-\frac{\varepsilon}{K_B T}\right) d\varepsilon$$

$$\therefore p = \frac{\pi}{2} \left( \frac{8m_p^*}{h^2} \right)^{\frac{3}{2}} \exp\left(\frac{E_V - E_F}{K_B T}\right) \frac{\sqrt{\pi}}{2} (K_B T)^{\frac{3}{2}}$$

$$= 2 \left( \frac{2\pi m_p^* K_B T}{h^2} \right)^{\frac{3}{2}} \exp\left(\frac{E_V - E_F}{K_B T}\right)$$

Again we have a pseudo constant and we denote this here as  $N_V$ .

$$p = N_V \exp\left[-\left(\frac{E_F - E_V}{K_B T}\right)\right] \longrightarrow (10)$$

### Position of the Fermi level in intrinsic semiconductors

For intrinsic semiconductors, the density of electrons is equal to the density of holes.

$$\text{Thus, we can write, } N_C \exp\left(\frac{E_F - E_C}{K_B T}\right) = N_V \exp\left(\frac{E_V - E_F}{K_B T}\right)$$

$$\exp\left(\frac{E_F - E_C - E_V + E_F}{K_B T}\right) = \frac{N_V}{N_C}$$

$$\therefore E_F = \frac{E_C + E_V}{2} + \frac{K_B T}{2} \ln \frac{N_V}{N_C}$$

$$\therefore E_F = \frac{E_C + E_V}{2} + \frac{3K_B T}{4} \ln\left(\frac{m_p^*}{m_v^*}\right) \longrightarrow (11)$$

If it happens that  $m_p^* = m_e^*$  then, the above equation takes the below form

$$\therefore E_F = \frac{E_C + E_V}{2}$$

i.e. the Fermi level lies in the midway between the valence band and the conduction band in an intrinsic semiconductor.

### Law of mass-action

For a given semi conducting substance, the effective mass and the energy gap are fixed. Hence the product  $np$  in a given material must be a function of temperature only. This is known as law of mass action governing the relative concentrations of holes and electrons.

$$n_i^2 = n \times p = N_C N_V \exp\left(\frac{-E_g}{K_B T}\right)$$

$$n_i = (N_C N_V)^{\frac{1}{2}} \exp\left(\frac{-E_g}{2K_B T}\right)$$

Substituting the values of  $N_C$  and  $N_V$  and simplifying, we get

$$n_i = 2 \left(\frac{2\pi K_B T}{h^2}\right)^{\frac{3}{2}} (m_e^* m_p^*)^{\frac{3}{4}} \exp\left(\frac{-E_g}{2K_B T}\right)$$

If  $m_p^* = m_e^* = m$ , ( $m$  is the rest mass of the electron) then

$$n_i = 2 \left(\frac{2\pi K_B m T}{h^2}\right)^{\frac{3}{2}} \exp\left(\frac{-E_g}{2K_B T}\right)$$

$$n_i = CT^{\frac{3}{2}} \exp\left(\frac{-E_g}{2K_B T}\right)$$

Where  $C = 2\left(\frac{2\pi K_B m}{h^2}\right)^{\frac{3}{2}} = 4.83 \times 10^{21}$ . At  $T = 300$  K, energy gap of intrinsic semiconductors  $E_g \sim 1\text{eV}$ .

$$\text{Then } n_i = 10^{17} / \text{m}^3$$

since the number of atoms per  $\text{m}^3$  may be of the order of  $10^{28}$ , only a small fraction of the valence electrons are excited to the conduction band i.e. in case of an intrinsic semiconductor, the conductivity is very small at room temperature.

### **CONDUCTIVITY OF AN INTRINSIC SEMICONDUCTOR**

If an electric field is applied to the intrinsic semiconductor in the X-direction, the electrons receive this energy and there is a drift velocity of electrons in the  $-X$  direction superimposed on their random thermal motion.

This means that a positive current flows in the positive X-direction. The field also imposes a drift velocity in +ve X direction on the random movement of holes. Thus, positive charge is carried by holes in this direction.

Based on the definition of drift velocity, the mobility can be defined as the drift velocity per unit electric field. In an ideal intrinsic semiconductor the mobility is determined by the scattering of electrons by the lattice vibrations. At low enough temperatures, where the mean free path is long, scattering by impurity atoms and defects sets a limit to the mobility attained.

Since there are two types of carriers in the intrinsic semiconductor, i.e. electrons and holes, its specific conductance is sum of the conductivities due to the free electrons and that of the holes.

Thus, the electrical conductivity of an intrinsic semiconductor is given by,

$$\sigma_i = \sigma_n + \sigma_p = ne\mu_n + pe\mu_p$$

Since for an intrinsic semiconductor,  $n = p = n_i$ , one gets

$$\sigma_i = n_i e (\mu_n + \mu_p) \longrightarrow (1)$$

The mobility depends upon temperature as  $\mu \propto T^{-\frac{3}{2}}$

Hence we can write that  $\mu_n = \alpha T^{-\frac{3}{2}}$  and  $\mu_p = \beta T^{-\frac{3}{2}}$

Thus,  $(\mu_n + \mu_p) = (\alpha + \beta) T^{-\frac{3}{2}} = \gamma T^{-\frac{3}{2}}$ . Then equation (1) will take the form

$$\sigma_i = n_i e \gamma T^{\frac{-3}{2}}$$

$$\therefore \sigma_i = C e \gamma \exp\left(\frac{-E_g}{2K_B T}\right), \text{ since } n_i = C T^{\frac{3}{2}} \exp\left(\frac{-E_g}{2K_B T}\right)$$

$$\Rightarrow \sigma_i = B \exp\left(\frac{-E_g}{2K_B T}\right)$$

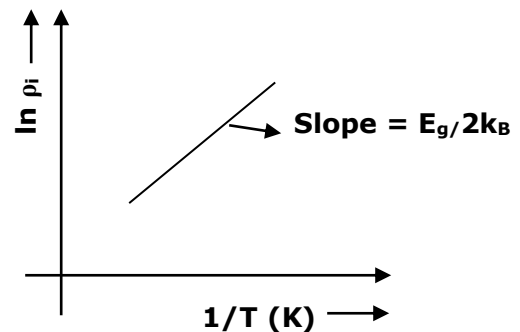
$$\text{Thus, } \Rightarrow \rho_i = \frac{\exp\left(\frac{E_g}{2K_B T}\right)}{B}$$

$$\Rightarrow \rho_i = A \exp\left(\frac{E_g}{2K_B T}\right)$$

Taking logarithm on both the sides, we get

$$\ln \rho_i = \frac{E_g}{2K_B T} + \ln A \longrightarrow \quad (2)$$

This equation suggests a method of determining the energy gap of the semiconductor. If we plot the intrinsic resistivity of the material at different



temperatures, we get a straight line. The slope of this line is  $\frac{E_g}{2K_B}$ . Thus, the energy gap can be determined.

## EXTRINSIC SEMICONDUCTORS

Due to the poor conductivity of intrinsic semiconductors at room temperature, these are not useful as such in the electronic devices. This necessitates the increase in conductivity of the semiconductor.

Without approaching larger temperatures, we can increase the conducting capability by adding some impurities to the intrinsic semiconductor. This process of **controlled addition of impurities to the intrinsic semiconductor is called doping and the impurities added are referred to as dopants. This semiconductor with impurities in it is called an extrinsic semiconductor.**

The amount of impurity added is extremely small; say 1 or 2 impurities for  $10^6$  intrinsic atoms. This doping is done during crystallization process.

Based on the type of impurities added, the extrinsic semiconductors are classified into two types; **p-type and n-type.**

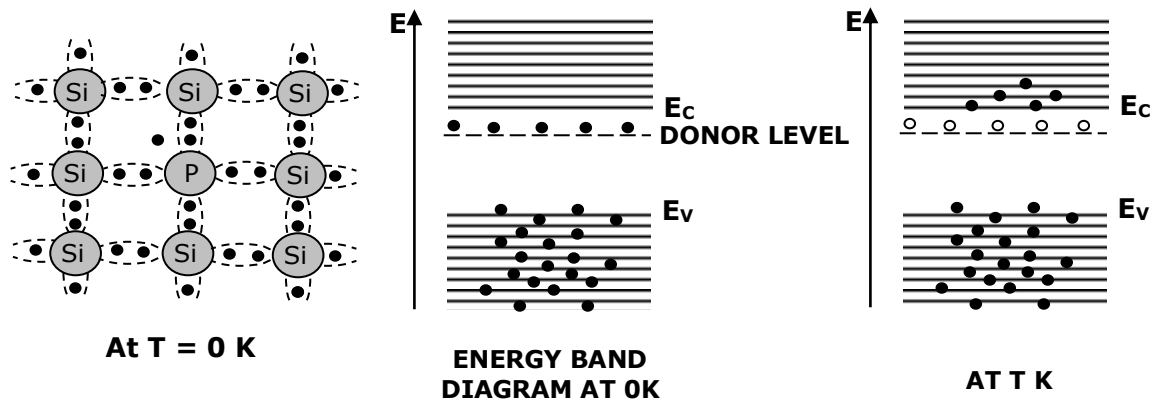
## n-TYPE SEMICONDUCTORS

When some pentavalent (group – V) impurity atoms such as As, Sb, P, Bi, are added to an intrinsic semiconductor (Si or Ge), then we get an n-type semiconductor. These pentavalent impurities donate electrons to the host crystal and hence are referred to as **donor impurities**.

Let us explain the changes in the band structure of an intrinsic semiconductor when doped with a pentavalent impurity with an example.

Silicon has four valence electrons and phosphorus has five valence electrons. When silicon is doped with phosphorus atoms, each phosphorus atom gets locked into the crystal by forming covalent bonds with the surrounding silicon atoms.

The fifth electron of the phosphorus is left alone which is loosely bound to the phosphorus atom at 0K. The ground state energy of this fifth electron lies just below the conduction band of silicon and is called the **donor level**.



The number of states in this level is equal to the number of phosphorus atoms per unit volume of the materials. At 0K, the fifth electron of phosphorus occupies these states. If we raise the temperature of the material slightly, then this fifth electron gets excited easily to the conduction band. Now these electrons will participate in conduction. Thus, every phosphorus atom contributes one conduction electron without any generation of holes in the valence band. As a result of this doping process, the number of electrons in the conduction band far exceeds the number of holes in the valence band of an n-type semiconductor.

Thus, in an n-type semiconductor, the majority carriers are electrons and the minority carriers are holes.

## p-TYPE SEMICONDUCTORS

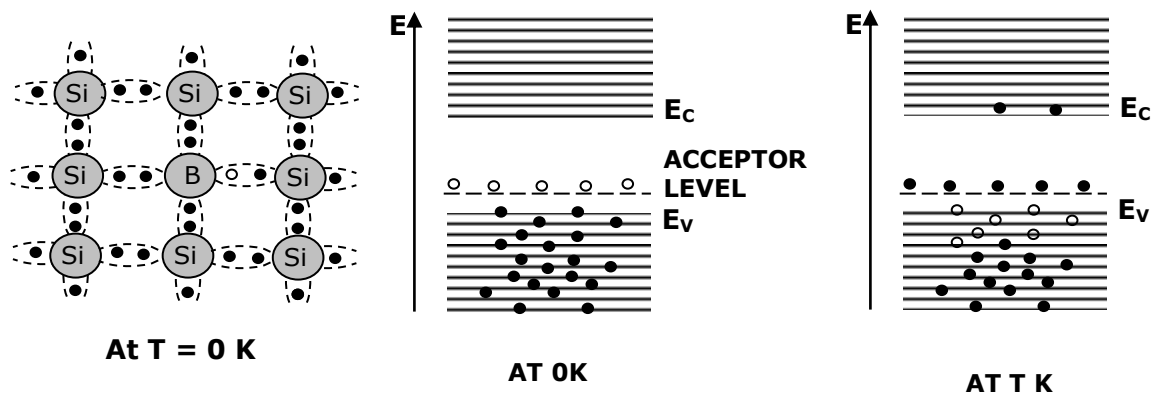
A p-type semiconductor is obtained by doping an intrinsic semiconductor with trivalent impurities such as, B, Al, Ga, In, etc. these trivalent impurities accept electrons from the host crystal and thus are referred to as **acceptor impurities**.

Let us now discuss the phenomenon that happens when a trivalent impurity is added to an intrinsic semiconductor with a suitable example.

When a trivalent impurity atom substitutes a host silicon atom, its three valence electrons enter the covalent bonds with the neighboring silicon atoms. But, a region of stress exist where the fourth covalent bond is ought to be present. Thus, addition of trivalent impurities produces holes in the semiconductor.

The boron atoms introduce an energy level just above the valence band in the energy gap of the silicon crystal. This energy level is called **acceptor level** since it readily accepts the electrons from the valence band.

Any stray electron in the vicinity can be trapped by this hole and the boron atom thereafter becomes negatively charged. The region from which the electron has come becomes positively charged.



This process will introduce number of holes in the valence band without simultaneous generation of electrons in the conduction band. Thus, in p-type semiconductor, holes are majority carriers and the electrons are minority carriers.

### CARRIER CONCENTRATION IN EXTRINSIC SEMICONDUCTORS

We know that  $n_i^2 = n \times p$ . This equation gives the relationship between the electron and hole concentrations. These densities are further interrelated by the law of electrical neutrality. Now we will discuss about charge neutrality in algebraic form.

Let  $N_D$  be equal to the concentration of donor atoms i.e.  $N_D$  positive charges are contributed by the donor ions. Hence, the total positive charge density is  $N_D + p$ .

Similarly, if  $N_A$  is the concentration of acceptor atoms, then these contribute  $N_A$  negative charges per cubic meter. Then the total negative charge density is  $N_A + n$ .

Since a semiconductor is electrically neutral, the magnitude of the positive charge density must be equal to the negative charge density.

$$\text{i.e. } N_D + p = N_A + n \quad \longrightarrow \quad (1)$$

Here in order to differentiate between the concentrations of n-type and p-type semiconductors, we follow a terminology according to which  $p_n$  &  $n_n$  represent hole and electron

concentrations in an n-type semiconductor and  $p_p$  &  $n_p$  represent the hole and electron concentration in a p-type semiconductor.

Now, if we consider an n-type semiconductor, we have only donor atoms. Thus,  $N_A = 0$ .

Then equation (1) becomes,  $N_D + p_n = n_n \longrightarrow (2)$

In an n-type semiconductor,  $p_n \lll n_n$ . Hence, equation (2) reduces to

$$N_D \sim n_n \longrightarrow (3)$$

Thus, in an n-type material, the free electron concentration is approximately equal to the density of donor atoms. The concentration of holes in n-type semiconductor can be given as,

$$p_n = \frac{n_i^2}{N_D} \longrightarrow (4) \quad (\because np = n_i^2)$$

Similarly for a p-type semiconductor,  $N_D = 0$  and  $p_p \ggg n_p$ .

$$N_A \sim p_p \longrightarrow (5)$$

$$n_p = \frac{n_i^2}{N_A} \longrightarrow (6)$$

### fermi level in extrinsic semiconductors

We know that,  $p = N_V \exp\left(\frac{E_V - E_F}{K_B T}\right)$  and  $n = N_C \exp\left(\frac{E_F - E_C}{K_B T}\right)$ . These relations are valid for both the intrinsic and extrinsic semiconductors.

For n-type semiconductors, we have  $N_D \sim n_n$ . Then we can write

$$N_D = N_C \exp\left(\frac{E_F - E_C}{K_B T}\right)$$

$$\Rightarrow \frac{(E_C - E_F)}{K_B T} = \ln \frac{N_C}{N_D}$$

$$E_F = E_C - K_B T \ln \frac{N_C}{N_D}$$

From the above equation, we can conclude the following points

- In case of n-type semiconductors, the Fermi level is nearer to the conduction band
- As concentration of donor atoms increases the Fermi level raises and moves towards the conduction band.
- As temperature increases, the Fermi level decreases and moves towards the middle.

A similar approach for a p-type semiconductor will lead us to an equation of Fermi level given by,

$$E_F = E_V + K_B T \ln \frac{N_V}{N_A}$$

From this equation we infer the below points

- In case of p-type semiconductors, the Fermi level is nearer to valence band
- As concentration of the acceptor atoms increases, the Fermi level moves towards the valence band
- As temperature increases the Fermi level rises and will move towards the middle of the energy gap.

### CONDUCTIVITY OF EXTRINSIC SEMICONDUCTORS

The mobility of the charge carriers is essentially a measure of the ease with which the carriers move under the influence of the external electric field. This mobility is a function of temperature. With the increase in the temperature, the mobility of the charge carriers reduces due to the frequent scattering of these carriers with lattice cores.

The expression for the conductivity is given by,

$$\sigma = ne\mu$$

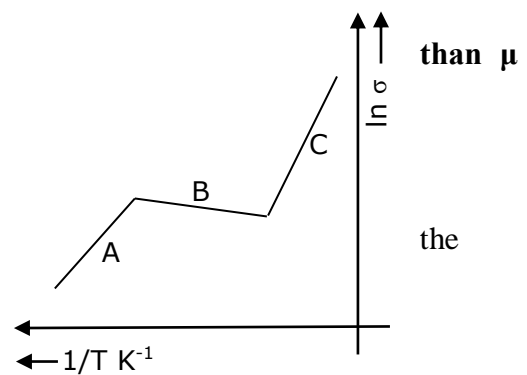
In a metal, the density of the charge carriers is the density of electrons. This number is substantially constant and any variation in the conductivity of the material is due to the variation in the mobility of the charge carriers.

But, conductivity of an extrinsic semiconductor is characterized by the motion of two kinds of charge carriers viz. holes and electrons. Any change in the temperature of the substance not only changes the mobility of these carriers but also influence the number of these carriers.

**When temperature is increased carriers are generated very rapidly such that 'n' increases faster than  $\mu$ . Hence, this rapid generation of new carriers will always increase the value of the conductivity with the increase in the temperature.**

Thus, in contrary to the conductivity of the metal, conductivity of a semiconductor increases with the temperature.

The graph shows qualitatively the temperature dependence of the conductivity of an extrinsic semiconductor.



- In the region A, the impurity atoms are alone ionized and hence  $\sigma$  is low. As the temperature is increasing, the number of atoms ionized will be increasing and thus  $\sigma$  increases. The slow increase is due to large impurity scattering and small amount of carriers. Usually all the impurities are ionized at 200 K. the slope of the line in this region is related to the ionization energy of the impurity.



- In region B, there is no increase in  $\sigma$  due to impurity conduction and the temperature is not high enough to allow very many electrons to jump from the valence band to the conduction band.  $\sigma$  shows a slight downward trend in this region due to the decrease in the mobility because of the predominance of lattice scattering when all the impurities are ionized.
- In the region C, the temperature is high enough to allow carriers to leave valence band and move to the conduction band. Thus, generation of carriers is started here and the semiconductor behaves like an intrinsic semiconductor. The slope of the region is related to the energy gap of the material.

## DRIFT AND DIFFUSION

### Drift

We know that a semiconductor consists of holes and electrons. When it is subjected to an electric field, holes move towards negative terminal and electrons move towards the positive terminal. This movement of charge is called **drift motion** and results in the current flow through the semiconductor. The current which flows under the action of an electric field is called **drift current**.

We know that electric current density is given by,

$$J = nev_d$$

where  $v_d$  is the drift velocity. Again we have  $v_d \propto E$  i.e.  $v_d = \mu E$ , where  $\mu$  is called mobility of the charge carrier within the crystal. **Mobility is defined as the average velocity acquired by a carrier in unit field.**

$$\therefore J = nev_d = ne \mu E$$

In a semiconductor, the current flow would be due to both the electron motion and the hole motion. Correspondingly, the current densities of the electrons and holes are given as,

$$\therefore J_n (\text{drift}) = nev_d = ne \mu_n E$$

$$\text{and } J_p (\text{drift}) = nev_d = pe \mu_p E$$

Though these charge movements are in opposite directions, the total current density is the sum of the two components.

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

$$= ne \mu_n E + pe \mu_p E$$

$$= (ne \mu_n + pe \mu_p) E$$

$$\therefore \sigma = ne \mu_n + pe \mu_p$$

For an intrinsic semiconductor,  $n = p = n_i$ , hence  $\sigma_i = n_i e (\mu_n + \mu_p)$ .

The conductivity is a function of temperature in case of intrinsic semiconductor. When temperature increases, conductivity also increases.

### Diffusion

In addition to the drift motion, the carriers in the semiconductors may move due to diffusion. Diffusion occurs whenever there is a non-uniform concentration of charge carriers at some place of the crystal.

The carrier density in a semiconductor is uniform at equilibrium. Suppose an external agent such as light, or temperature acts momentarily at one end of the semiconductor. This external agent generates additional electron-hole pairs leading to a sudden increase in the concentration of charge carriers at that end. The concentration of the carriers at the other parts of the crystal remains same.

**This difference in the concentration causes migration of carriers from the region of higher concentration to the region of lower concentration in order to restore equilibrium. Such a migration of carriers is called diffusion and the current constituted in the process is called the diffusion current.**

Let us suppose that the concentration  $\Delta n$  of electrons varies with the distance  $x$  in the semiconductor, the concentration gradient being

$$\frac{\partial \Delta n}{\partial x}$$

According to the Fick's law, the rate at which the carriers diffuse is proportional to the density gradient and the movement is in the direction of the negative gradient. The rate of flow of electrons is proportional to

$$-\frac{\partial \Delta n}{\partial x} \longrightarrow (1)$$

$$\text{Hence, the rate of flow across unit area} = -D_n \frac{\partial \Delta n}{\partial x} \longrightarrow (2)$$

Where  $D_n$  is called the *diffusion coefficient* of electrons in that semiconductor. This flow constitutes an electron diffusion current density which is given by,

$$\begin{aligned} J_n (\text{diffusion}) &= -e \times (\text{rate of flow of charge}) \\ &= e D_n \frac{\partial \Delta n}{\partial x} \longrightarrow (3) \end{aligned}$$

Similarly,  $J_p$  (diffusion) =  $e \times$  (rate of flow of charge)

$$= -e D_p \frac{\partial \Delta p}{\partial x} \longrightarrow (4)$$

where  $D_p$  is the hole diffusion coefficient.

If there is an electric field  $E$  and concentration gradient in  $X$  direction, then the total electron current is the sum of the drift and diffusion components,

$$\begin{aligned} J_n &= J_n (\text{drift}) + J_n (\text{diffusion}) \\ \therefore J_n &= ne \mu_n E + e D_n \frac{\partial \Delta n}{\partial x} \end{aligned}$$

Similarly for the holes,

$$\therefore J_p = p e \mu_p E - e D_p \frac{\partial \Delta p}{\partial x}$$

### EINSTEIN'S EQUATIONS

The carrier mobility  $\mu$  gives an indication that how the carrier moves in a semiconductor due to the effect of an electric field. Similarly, carrier diffusion coefficient  $D$  signifies the behavior of the carrier in a semiconductor as a result of concentration gradient. These constants mobility and diffusion coefficients are related according to the Einstein's equation as,

$$\frac{D_n}{\mu_n} = \frac{K_B T}{e} \quad \text{and} \quad \frac{D_p}{\mu_p} = \frac{K_B T}{e}$$

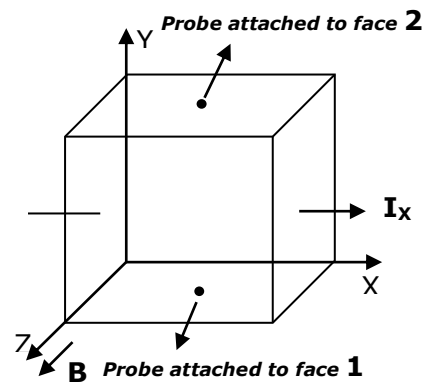
$$\therefore \frac{D_p}{\mu_p} = \frac{D_n}{\mu_n}$$

The above equations are known as Einstein's equations. From these equations we can say that both the mobility and diffusion coefficient are strong functions of the temperature.

### HALL EFFECT

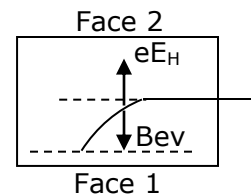
If a piece of conductor (metal or semiconductor) carrying a current is placed in a transverse magnetic field, an electric field is produced inside the conductor in a direction normal to both the current and the magnetic field. This phenomenon is called the **Hall Effect** in the honor of E. H. Hall, the physicist who discovered it in 1879.

Assuming that the material is an n-type semiconductor, the current flow consists of almost electrons moving from right to left. This corresponds to the direction of conventional current from left to right as shown in figure.



If  $v$  is the velocity of electrons at right angles to the magnetic field, there is a downward force on each electron of magnitude  $Bev$ . This causes the electron current to be deflected in downward direction and causes the -ve charges to accumulate on the bottom face of the specimen.

A potential difference is therefore established between the top and bottom faces of the specimen. This potential difference causes a field  $E_H$  -ve Y-direction. Hence, a force equal to  $eE_H$  acts on the electron in upward direction.



A state of equilibrium is reached when

$$eE_H = Bev$$

$$E_H = Bv \quad \longrightarrow \quad (1)$$

If  $J_X$  is the current density in the X-direction, then  $J_X = nev \quad \longrightarrow \quad (2)$

Thus, from the equations (1) and (2),

$$E_H = \frac{BJ_x}{ne}$$

The Hall Effect is described by means of a constant called Hall coefficient  $R_H$ , defined in terms of current density by the relation

$$E_H = R_H J_x B$$
$$\therefore R_H = \frac{E_H}{BJ_x} = \frac{1}{ne}$$

In this case,  $R_H = -\frac{1}{ne}$

Negative sign is used because the field is developed in the  $-Y$  direction. In case of p-type semiconductors,  $R_H = \frac{1}{pe}$

### APPLICATIONS OF HALL EFFECT

- **Determination of semiconductor type:** for an n-type semiconductor, Hall coefficient is –ve whereas for a p-type semiconductor, it is +ve. The sign of Hall Coefficient can be used to determine whether it is p-type or n-type.
- **Calculation of carrier concentration:** the Hall voltage  $V_H$  is measured as usual by placing two probes at the centers of the top and bottom faces of the sample. If the magnetic flux density is known, then  $R_H$  can be calculated.  $R_H$  provides the value of carrier concentration  $n$  since  $R_H = \frac{1}{ne}$
- **Determination of mobility of the charge carriers:** Hall coefficient can be used to determine the mobility of the carriers in the following way,

$$\sigma_n = ne\mu_n$$

$$\Rightarrow \mu_n = \frac{\sigma_n}{ne}$$

$$\therefore \mu_n = \sigma_n R_H$$

Similarly,  $\mu_p = \sigma_p R_H$

