

UNIT-I

WAVE OPTICS

WAVE OPTICS

Interference:

Introduction: Wave theory of light attempts to understand the various optical phenomena exhibited by light waves. Interference constitutes the first proof of the wave nature of light. Thomas Young first experimentally demonstrated interference of light waves.

Principle of Superposition:

"when two or more light waves superimpose in the medium, the resultant displacement at any point is equal to the algebraic sum of the displacements due to individual waves".

If y_1 and y_2 are the displacements of two light waves. The resultant wave is given by

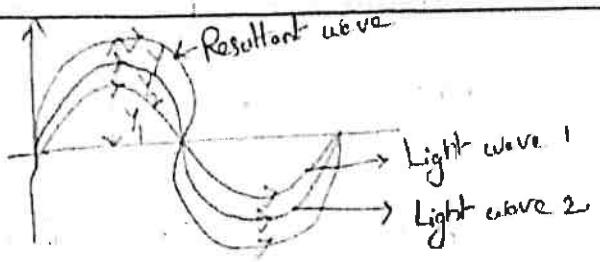
$$y = y_1 + y_2$$

Interference of light:

"when two or more light waves are superimposed. The resultant wave intensity is modified. This modification in the distribution of intensity in the region of superposition principle is known as Interference."

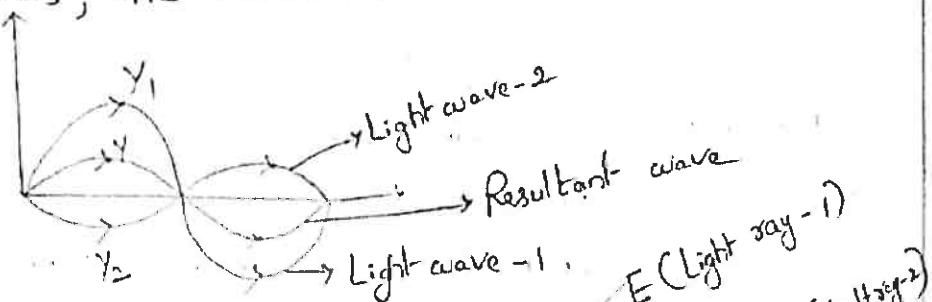
Constructive Interference:

"The resultant amplitude is the sum of the amplitudes due to two light waves. The interference is Constructive Interference."

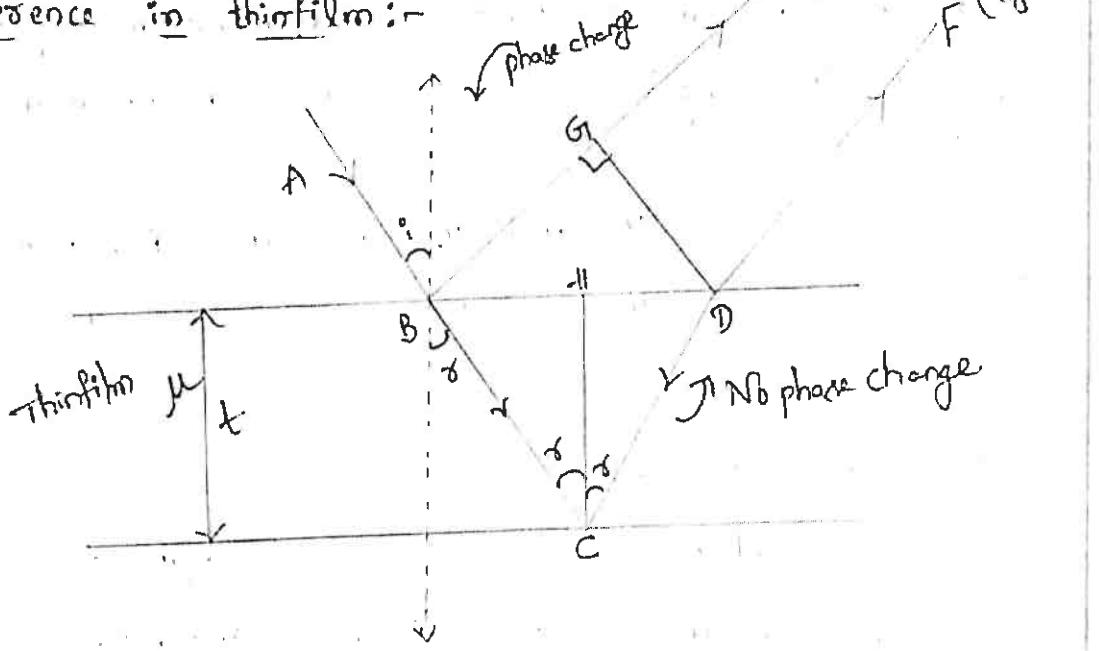


Destructive Interference :-

"If the resultant amplitude is equal to the difference of two amplitudes, the interference is called Destructive Interference."



Interference in thin film :-



When light is incident on a plane parallel thin film, some portion gets reflected from the upper surface and the remaining portion is transmitted into the film.

Again some portion of the transmitted light is reflected back into the film by lower surface and emerges through the upper surface. These reflected light superimpose and forms the interference pattern.

(2)

Consider a transparent plane parallel thin film of thickness 't' with refractive index ' μ '. AB be incident at an angle of incidence of ' i ' on the upper surface of the film. BE & BC are the reflected and transmitted light rays. Let the angle of refraction is ' r '. The ray BC will be reflected in to the film and emerge through the film in the form of the light ray DF. These two light rays superimpose and depending upon path difference between them, they produce interference pattern.

To know the path difference, let us draw the normal DG to BE. From the points D & G onwards, the light rays travel equal distances. By the time the light ray travels from B to G, the transmitted light ray has to travel from B to C & C to D.

The path difference between light rays (1) & (2) is

$$\text{path difference} = \mu(BC + CD) \text{ in film} - BG \text{ in air} \quad \text{--- (1)}$$

Consider $\triangle ABC$, $\cos r = \frac{HC}{BC}$



$$BC = \frac{HC}{\cos r} = \frac{t}{\cos r}$$

By form $\triangle DCB$, $CD = \frac{t}{\cos r}$.

$$BC = CD = \frac{t}{\cos r} \rightarrow \text{--- (2)}$$

To calculate BG , first BD which is equal to $(BH + HD)$ has to be obtained.

form $\triangle BHC$, $\tan r = \frac{BH}{CH} = \frac{BH}{t}$

$$BH = t \tan r$$

$$\text{By } BD = t \tan \alpha.$$

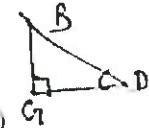
$$BD = BI + HD = at \tan \alpha \quad (\because BI = HD) \rightarrow (3)$$

$$\text{From } \triangle ABG, \sin i = \frac{BG}{BD}$$

$$BG = BD \sin i = at \tan \alpha \sin i$$

$$\text{from Snell's law, } \sin i = \mu \sin r$$

$$BG = at \tan \alpha \sin r \rightarrow (4)$$



Sub the above values in eqn (1)

$$\text{path difference} = \frac{at\mu}{\cos \alpha} - at \tan \alpha \sin r$$

$$= \frac{at\mu}{\cos \alpha} - \frac{at \tan \alpha \sin^2 r}{\cos \alpha}$$

$$= \frac{at\mu}{\cos \alpha} (1 - \sin^2 r)$$

$$= \frac{at\mu}{\cos \alpha} \times \cos^2 r$$

$$\text{path difference} = at \mu \cos^2 r$$

At the point B, reflection occurs from the upper surface of the thin-film. Light ray (1) undergoes an additional phase change of π or an additional path difference of $\frac{\lambda}{2}$

$$\text{total path difference} = at \mu \cos^2 r + \frac{\lambda}{2}$$

when the path difference is equal to the integral multiples of λ then the rays (1) & (2) meet in phase & undergo constructive interference.

The condition for bright fringe is

$$at \mu \cos^2 r + \frac{\lambda}{2} = n\lambda$$

$$at \mu \cos^2 r = (2n-1) \frac{\lambda}{2}, \text{ where } n=0, 1, 2, \dots \rightarrow (5)$$

Applications of Interference:-

- In optical testing, interference is used in testing surface.
- In space applications Interference is used to measuring light intensity.
- In hologram Interference pattern is used.
- In Anti-reflecting Coating Interference is used.

Colors in Thinfilm:

- When a thin-film is exposed to white light from an extended source, it shows beautiful colors in the reflected system.
- Light is reflected from the top and bottom surfaces of a thinfilm and the reflected rays interfere.
- Colors in thinfilms are because of thinfilms such as Soap bubble or a thin layer of oil on water show beautiful colors when illuminated by white light.
- It happens due to the interference of light reflected from the upper surface of the thinfilm.

Newton's Rings:-

When a plano Convex-lens with its Convex surface is placed on a plane glass plate, an air film of increasing thickness is formed b/w the two. The thickness of the film at the point of contact is zero. If monochromatic light is allowed to fall normally, alternate dark and bright fringes Concentric around the point of contact b/w the lens and glass plate are seen. These circular rings were discovered by Newton and are called Newton's rings.

Experimental Arrangement :-

The Experimental arrangement is as shown in fig.

The plano convex lens of large radius of curvature is placed with its convex surface on a plane glass plate (P).

The Contact d. lens and plate is 0. The monochromatic light is falls on a glass plate G held at angle of 45° with the vertical. The glass plate G reflects normally a part of the light towards the air film enclosed by the lens L and plate P.

A part of the light 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 reflected rays interfere and give rise to an interference pattern in the form of circular rings. These are seen near the upper surface of the air through the microscope.

Condition for Bright ring:-

$$\text{Condition} - \text{For Bright ring is } 2n \cos \theta = (2n-1) \frac{\lambda}{2}$$

But $\mu = 1$ (For air medium)

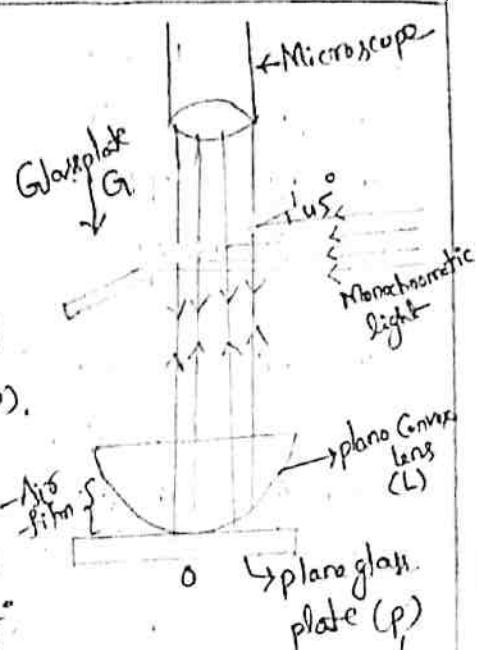
$$\theta = 0$$

Hence $2t = (2n-1) \frac{\lambda}{2}$ where $n = 1, 2, 3, \dots$

Condition for Dark ring:-

$$2t \cos \theta = n\lambda$$

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



Theory of Newton's Rings:-

To find - the Diameters of dark and bright rings. Let 'L' be a lens placed on a glass plate 'P'. The Convex Surface of the lens is the part of spherical surface with centre at 'C'. Let 'R' be the radius of curvature and 'n' be the refractive index corresponding to the film of thickness 't'.

From the property of a circle, $N_A \times N_B = N_0 \times N_D$.

$$\text{Sub the values, } n_A \cdot n_D = t(2R-t)$$

$$n^2 = 2Rt - t^2$$

As 't' is small, t^2 will be negligible, $n^2 = 2Rt$

$$t = \frac{n^2}{2R}$$

For Bright ring, the condition is

$$\alpha t = (\alpha n - 1) \frac{\lambda}{2}$$

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

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

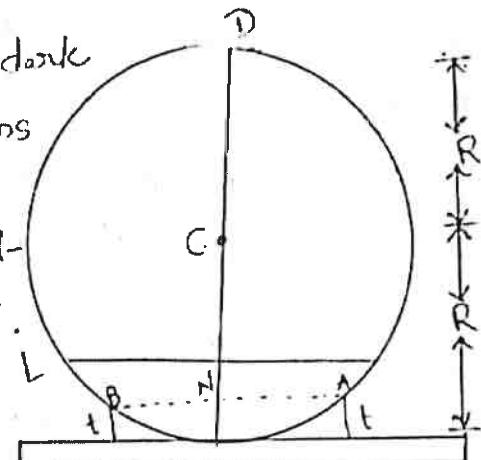
Replacing α by $\frac{D}{\alpha}$, the Diameter of n^{th} bright ring will be

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

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

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

$$D \propto \sqrt{\text{odd Natural Numbers}}$$



(4)

thus the diameter of the bright rings are proportional to the square root of odd natural numbers.

for dark ring, the condition is

$$d\lambda = n\lambda$$

$$d \cdot \frac{\pi^2}{dR} = n\lambda$$

$$\pi^2 = n\lambda R$$

$$D^2 = 4n\lambda R$$

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

$$D \propto \sqrt{n}$$

$D \propto \sqrt{\text{natural numbers}}$
thus, the diameters of dark rings are proportional to the square root of natural numbers
with increase in order(n), the rings get closer & the fringe width decreases as shown in fig.

Determination of wavelength of a light source:-
the wavelength of a light source can be calculated by measuring the diameters of the various rings & knowing the radius of curvature of the plane convex lens.

let R be radius of curvature of a plane convex lens & λ be the wavelength of light used. D_m & D_n are the diameters of m^{th} & n^{th} dark rings respectively

$$\text{then, } D_m^2 = 4m\lambda R$$

$$D_n^2 = 4n\lambda R$$

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

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

using the above formula, λ can be calculated.

fig: Newton's rings pattern

Diffraction

Introduction:

- The wave nature of light is further confirmed by the optical phenomenon of diffraction.
- The word diffraction is derived from the Latin word diffractus which means to "break to pieces".
- Diffraction was first observed by "Grimaldi".
- When light falls on an obstacle whose size is comparable with the wavelength of light then light bends around the edges or corners of an obstacle and entering into the geometric shadow. This bending of light is known as diffraction.

Diffraction divided into two types.

1. Fresnel Diffraction

2. Fraunhofer Diffraction

Fresnel Diffraction:-

- To occur Fresnel diffraction, the light source and screen are at finite distance from the obstacle.
- No lenses are necessary to study the diffraction.

- Study of this diffraction is complicated.
- This Diffraction can be studied only in the direction of propagation of light.
- In this diffraction incident wavefronts are either spherical or cylindrical.

Fraunhofer Diffraction:-

- To occur this diffraction the light source and Screen are at infinite distance from the obstacle.
- To study this diffraction lenses are necessary.
- The study of this diffraction is easy.
- This diffraction can be studied in any direction of propagation of light.
- In this diffraction wavefronts are plane.

Interference

- ① Interference is due to superposition of two sources different wavefronts originating from two point sources.
- ② Bands are of equal width.
- ③ All the bright fringes are of same intensity.
- ④ All the dark fringes have zero intensity.

Diffraction

- ① It is due to superposition of secondary wavelets originating from different parts of wavefront.
- ② Band's width decreases when order increases.
- ③ All Bright fringes are of varying intensity.
- ④ Dark fringes Intensity is zero.

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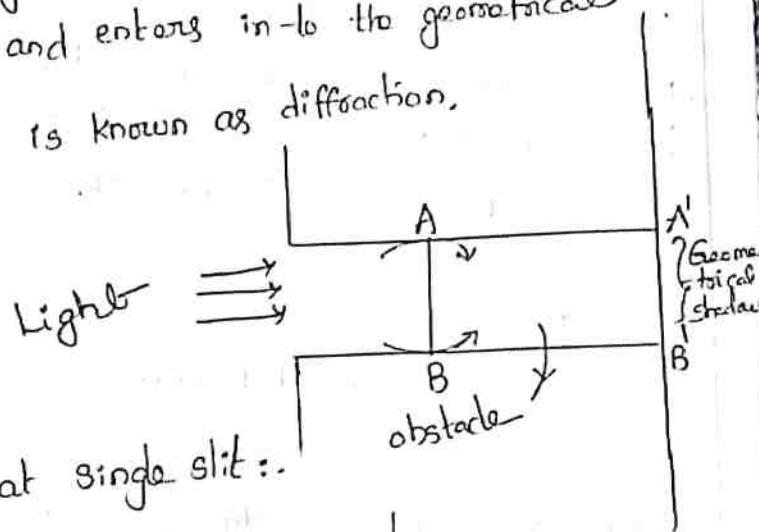
Diffraction :-

→ The wave nature of light is confirmed by optical phenomenon of diffraction.

→ Diffraction was first observed by "Grenmoldy".

when light falls on obstacle whose size is comparable with the wavelength of light then light bends around the edges or corners of an obstacle and enters into the geometrical shadow.

→ This bending of light is known as diffraction.



Fraunhofer Diffraction at single slit :-

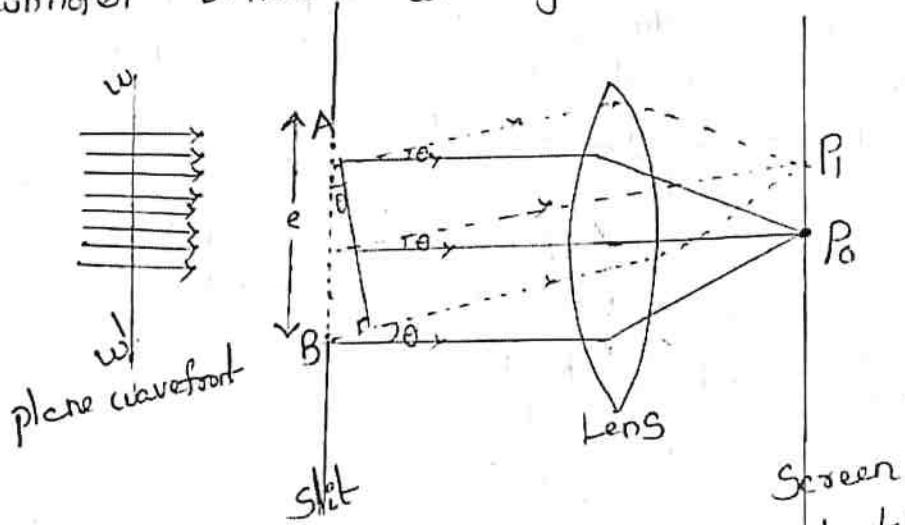


Fig: Fraunhofer Diffraction - Single slit

Consider a slit AB of width 'e'. Let a plane wavefront w of monochromatic light of wavelength λ propagating normally towards the slit incident on it. The diffracted light through the slit is focused by means of a convex lens on a screen placed in the focal plane of the lens. According to Fresnel, every point on the wavefront in the plane of the slit is a source of

Secondary wavelets which spread out to the right in all directions. Those wavelets travelling normal to the slit i.e., along the direction α_0 are brought to focus at P_0 by the lens. Thus P_0 is a bright central image. The secondary wavelets travelling at an angle θ with the normal are focused at a point P_1 on the screen. Depending on path difference the point P_1 may have maximum or minimum intensities. To find intensity at P_1 let us draw the normal AC from A to the light ray at B . The path difference b/w the wavelets from A & B in the direction θ is given by

$$\text{path difference} = BC = AB \sin\theta = e \sin\theta.$$

$$\text{Corresponding phase difference} = \frac{\partial \pi}{\lambda} \times \text{path difference}$$

$$= \frac{\partial \pi}{\lambda} e \sin\theta$$

Let the width of the slit be divided into 'n' equal parts & the amplitude of the wave from each part is 'a'. Then the phase difference b/w any two successive waves from these parts would be

$$\frac{1}{n} [\text{Total phase}] = \frac{1}{n} \left[\frac{\partial \pi}{\lambda} e \sin\theta \right] = d \text{ (say)}$$

Using the method of vector addition of amplitudes the resultant amplitude 'R' is given by

$$R = a \frac{\sin n d}{\sin d}$$

$$= \frac{a \sin \left(\pi e \frac{\sin\theta}{\lambda} \right)}{\sin \left(\pi e \frac{\sin\theta}{\lambda} \right)}$$

$$= a \frac{\sin \alpha}{\sin \alpha/n} \quad \text{where } \alpha = \pi e \frac{\sin\theta}{\lambda}.$$

$$= a \frac{\sin \alpha}{\alpha/n} \quad \left(\because \frac{\alpha}{n} \text{ is very small} \right)$$

$$R = \frac{n a \sin \alpha}{\alpha} \quad \left(\because n a = A \right)$$

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

$$\text{Intensity } I = R^2 = A^2 \left(\frac{\sin \alpha}{\alpha} \right)^2 \quad \rightarrow \textcircled{1}$$

Principal Maximum:-

The resultant amplitude R can be written in ascending powers of ' α ' as

$$R = \frac{A}{\alpha} \left[\alpha - \frac{\alpha^3}{3!} + \frac{\alpha^5}{5!} - \frac{\alpha^7}{7!} + \dots \right]$$

$$R = A \left[1 - \frac{\alpha^2}{3!} + \frac{\alpha^4}{5!} - \frac{\alpha^6}{7!} + \dots \right]$$

I will be maximum, when the value of R is maximum.

For maximum value of R , the negative terms must vanish.
i.e., $\alpha = 0$

$$\frac{\text{d}I}{\text{d}\theta} = 0$$

$$\sin \theta = 0$$

$$\theta = 0$$

$$R = A \quad \rightarrow \textcircled{2}$$

$$\text{then } I_{\max} = R^2 = A^2 \quad \rightarrow \textcircled{3}$$

The condition $\theta = 0$ means that the maximum intensity is formed at P_0 & is known as principal maximum.

Minimum Intensity positions:-

I will be minimum, when $\sin \alpha = 0$

$$\alpha = \pm \pi, \pm 2\pi, \pm 3\pi$$

$$\alpha = \pm m\pi$$

$$\frac{\text{d}I}{\text{d}\theta} = \pm m\pi$$

$$\sin \theta = \pm m\lambda, \quad m = 1, 2, 3, \dots$$

Thus, we obtain the points of minimum Intensity on either side of the principal maximum. For $m=0$, $\sin \theta = 0$, which corresponds to principal maximum.

Secondary maxima:-

In b/w these minima, we get secondary maxima. The position can be obtained by differentiating the expression of I w.r.t. α & equating to zero. We get

$$\frac{dI}{d\alpha} = \frac{d}{d\alpha} \left[A^2 - \left(\frac{\sin \alpha}{\alpha} \right)^2 \right] = 0$$

$$A^2 \cdot \frac{2 \sin \alpha}{\alpha} \cdot \frac{\alpha \cos \alpha - \sin \alpha}{\alpha^2} = 0$$

or for α

$$\sin \alpha = 0 \quad \text{or} \quad \alpha \cos \alpha - \sin \alpha = 0$$

$\sin \alpha = 0$ gives position of minima
Hence the positions of secondary maxima are given by

$$\alpha \cos \alpha - \sin \alpha = 0$$

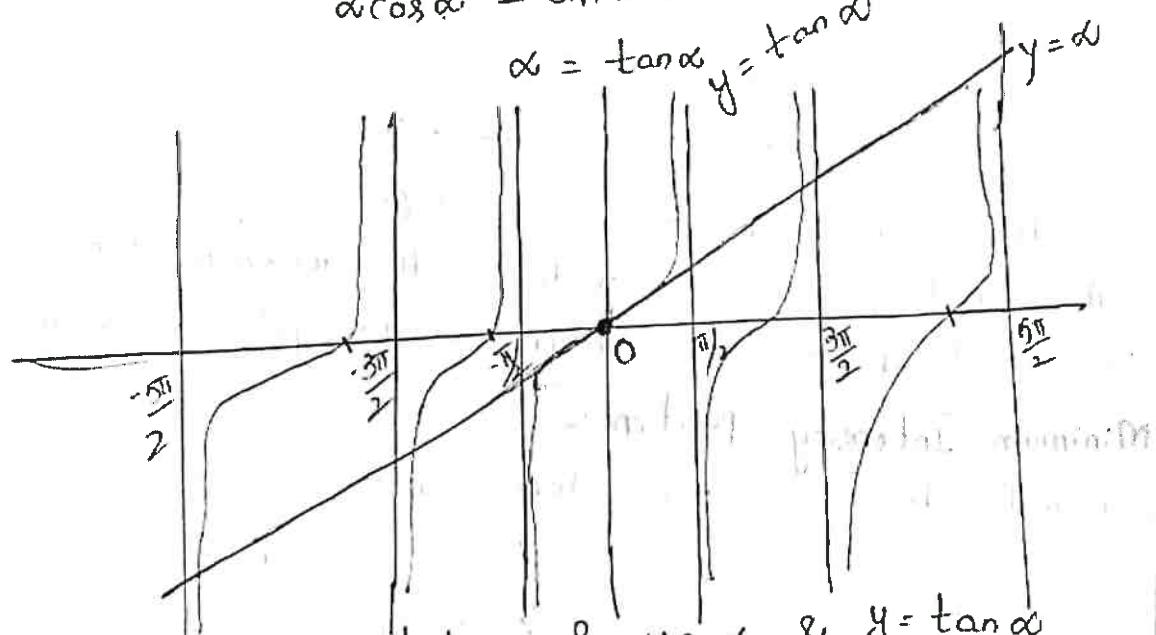


fig: plots of $y = \alpha$ & $y = \tan \alpha$

The values of α satisfying the above equation are obtained graphically by plotting the curves $y = \alpha$ & $y = \tan \alpha$ on the same graph. The points of intersection of the two curves give the values of α which satisfy the above equation. The plots of $y = \alpha$ & $y = \tan \alpha$ are shown in fig.

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The points of intersections are

$$\alpha = 0, \pm \frac{3\pi}{2}, \pm \frac{5\pi}{2}, \dots$$

Sub -the above values in eqn (1), we get -the intensities in Various maxima.

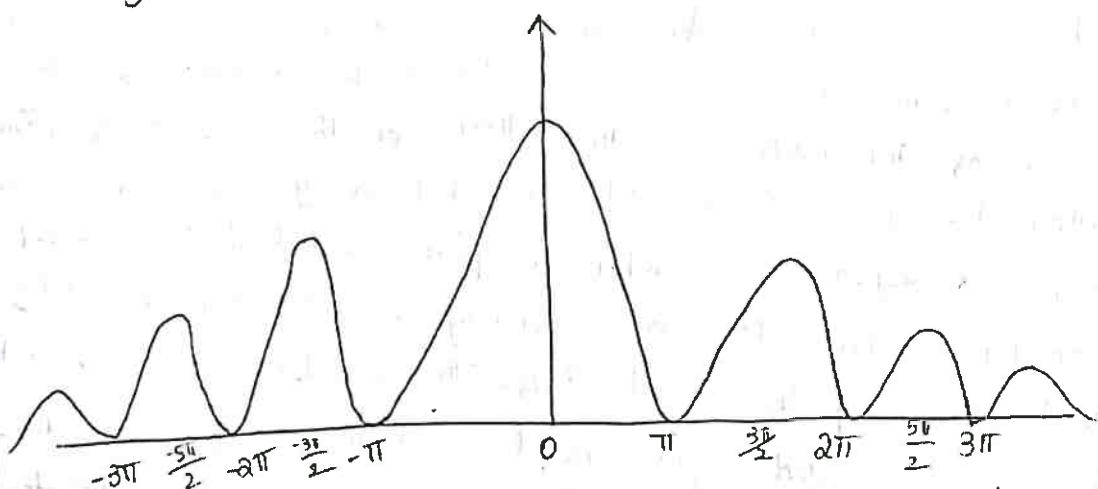
$$\alpha = 0, I_0 = A^2 \text{ (principal maximum)}$$

$$\alpha = \frac{3\pi}{2}, I_1 = A^2 \left[\frac{\sin \left(\frac{3\pi}{2} \right)^2}{\frac{3\pi}{2}} \right]^2 \approx \frac{A^2}{22} \text{ (1st Secondary maximum)}$$

$$\alpha = \frac{5\pi}{2}, I_2 = A^2 \left[\frac{\sin \left(\frac{5\pi}{2} \right)^2}{\left(\frac{5\pi}{2} \right)} \right]^2 \approx \frac{A^2}{62} \text{ (2nd Secondary maximum)}$$

From the above expressions, it is evident -that most of -the incident light is concentrated in the principal maximum and -the rest is distributed in -to -the Secondary maxima.

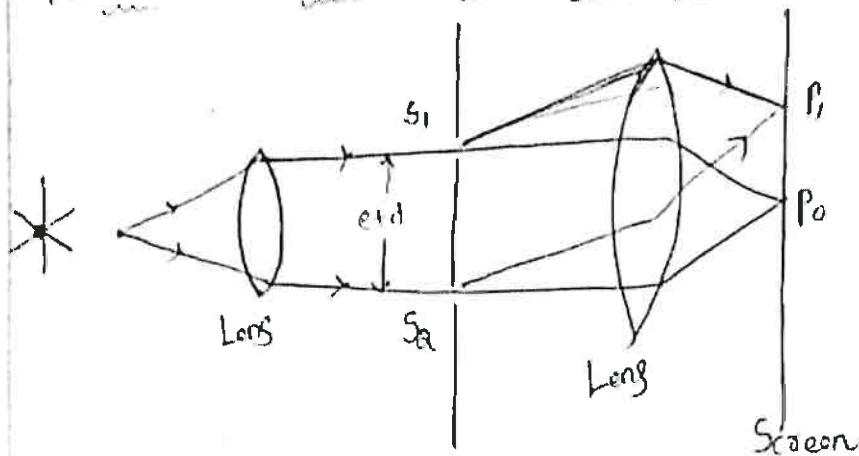
Intensity Distribution :



The variation of I w.r.t α is shown in fig.

The diffraction pattern consists of a central principal maximum -for $\alpha = 0$. There are Secondary maxima of decreasing intensity on either sides of it at positions $\alpha = \pm \frac{3\pi}{2}, \pm \frac{5\pi}{2}$ between Secondary maxima, there are minima at positions $\alpha = \pm \pi, \pm 2\pi, \pm 3\pi$.

Fraunhofer Diffraction at Double slit :-



Double slit

fig :- Fraunhofer Diffraction - Double slit
 Let S_1 & S_2 be the double slits of equal widths e &
 Separated by a distance d . The distance between the middle points of
 the two slits is $(e+d)$. A monochromatic light of wavelength λ is
 incident normally on the two slits. The light diffracted from these
 slits is focussed by a lens on the screen placed in the focal plane
 of the 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 superimposed. When a plane wavefront is incident
 normally on two slits, the secondary wavelets from the slits
 travel uniformly in all directions. The wavelets travelling in the
 direction of incident light come to a focus at P_0 while the
 wavelets travelling in a direction making an angle θ , come to
 focus at P_1 .

From the study of diffraction due to single slit, the resultant
 amplitude = $\frac{A \sin \alpha}{\alpha}$ where $\alpha = \frac{\pi e \sin \theta}{\lambda}$

Since we use double slit, from each slit we
 get a wavelet of amplitude $\frac{A \sin \alpha}{\alpha}$ in a direction θ .

These two wavelets interfere and meet at a point P_1 on the screen. To calculate the path difference b/w the wavelets.

Let us draw a normal $S_1 K$ to the wavelet through S_2

$$\text{path difference} = S_2 K$$

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

$$\text{phase difference } \delta = \frac{2\pi}{\lambda} (e+d) \sin \theta \rightarrow ⑥^{\circ}$$

To find the resultant amplitude at P_1 we use vector addition method in which the two sides of a triangle are represented by the amplitude through S_1 & S_2 . The third side gives the resultant amplitude. From fig.,

$$(OG)^2 = (OG)^2 + (GII)^2 + 2(OG)(GII) \cos \delta$$

$$= \left(\frac{A \sin d}{\alpha}\right)^2 + \left(\frac{A \sin e}{\alpha}\right)^2 + 2 \cdot \left(\frac{A \sin d}{\alpha}\right) \left(\frac{A \sin e}{\alpha}\right) \cos \delta$$

$$= \frac{A^2 \sin^2 \alpha}{\alpha^2} (2 + 2 \cos \delta)$$

$$= 2 \left(\frac{A \sin d}{\alpha}\right)^2 (1 + \cos \delta)$$

$$= 2 \left(\frac{A \sin d}{\alpha}\right)^2 (1 + 2 \cos^2 \frac{\delta}{2} - 1)$$

$$R^2 = 4 A^2 \cos^2 \frac{\delta}{2} \cdot \left(\frac{A \sin d}{\alpha}\right)^2$$

$$R^2 = 4 A^2 \cos^2 \left(\frac{\pi(e+d) \sin \theta}{\lambda}\right) \left(\frac{A \sin d}{\alpha}\right)^2$$

$$\text{Let } \beta = \frac{\pi(e+d) \sin \theta}{\lambda}$$

$$R^2 = 4 A^2 \left(\frac{A \sin d}{\alpha}\right)^2 \cos^2 \beta$$

The resultant intensity $I = R^2 = 4 A^2 \left(\frac{A \sin d}{\alpha}\right)^2 \cos^2 \beta$
From the above expression, it is clear the resultant intensity is the product of two factors i.e.,

1. $A^2 \left(\frac{\sin \alpha}{\alpha}\right)^2$ which represents the diffraction pattern due to single slit.
 2. $\cos^2 \beta$ which gives the interference pattern due to waves from double slit.
- The resultant intensity is due to both Diffraction & interference effects.

Diffraction effect:-

The diffraction term $A^2 \left(\frac{\sin \alpha}{\alpha}\right)^2$ gives the principal maximum at the centre of the screen with alternate minima and secondary maxima of decreasing intensity. we get principal maximum for $\theta = 0$. we get minima for $\sin \alpha = 0$

$$\alpha = \pm m\pi, \text{ where } m = 1, 2, 3, \dots$$

$$\frac{\pi e \sin \theta}{\lambda} = \pm m\pi$$

The positions of secondary maxima occurs for

$$\alpha = \pm \frac{3\pi}{2}, \pm \frac{5\pi}{2}, \pm \frac{7\pi}{2}, \dots$$

Interference effect:-

The interference term $\cos^2 \beta$ gives the equidistant bright & dark fringes.

The maxima will occur for $\cos^2 \beta = 1$

$$\beta = \pm n\pi, \text{ where } n = 0, 1, 2, 3, \dots$$

$$\beta = 0, \pm \pi, \pm 2\pi, \pm 3\pi, \dots$$

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

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

The minima will occur for $\cos^2 \beta = 0$

$$\beta = \pm (2n+1) \frac{\pi}{2}, \text{ where } n = 0, 1, 2, 3, \dots$$

$$(e+d) \sin \theta = \pm (2n+1) \frac{\lambda}{2}$$

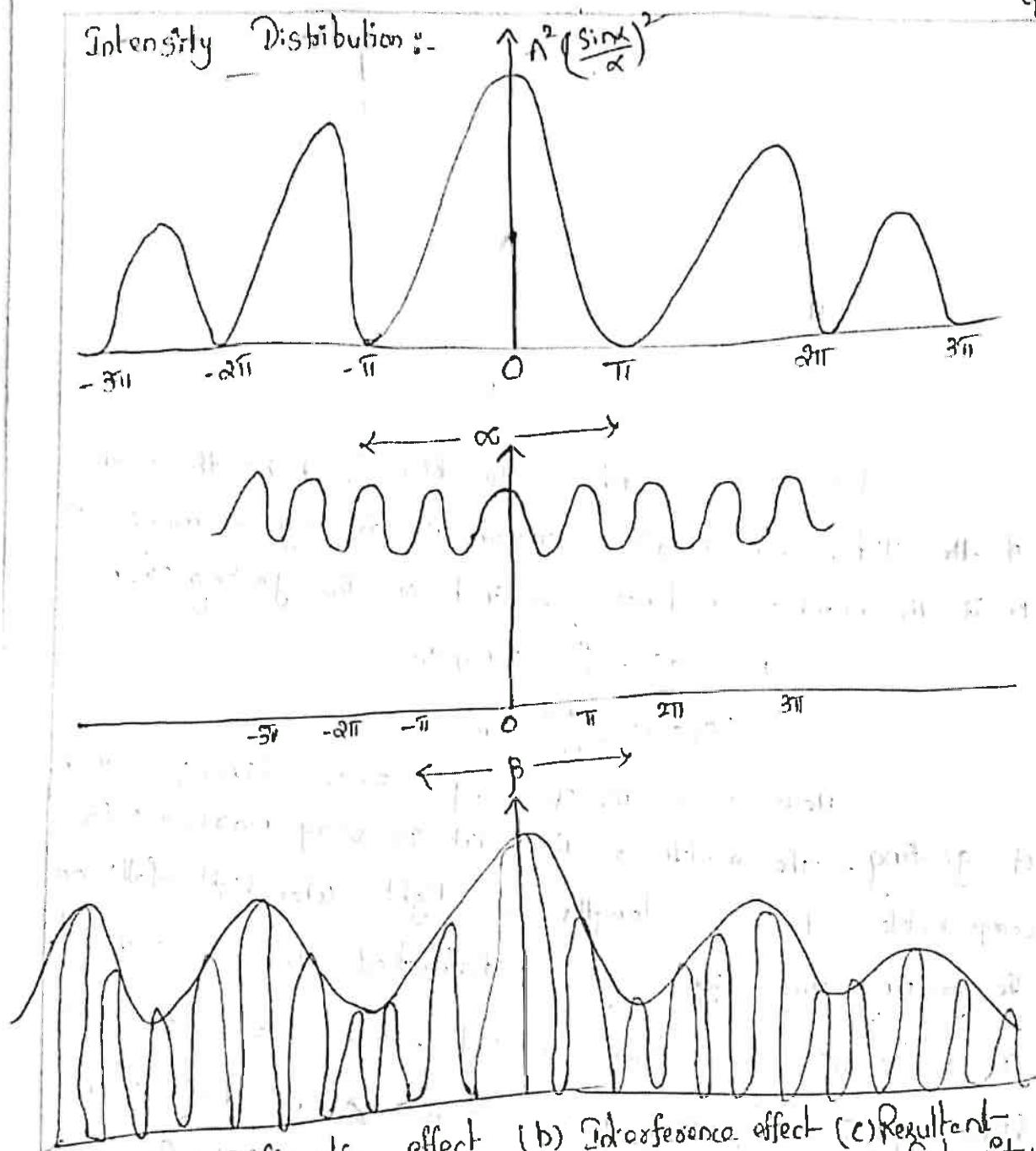


fig: (a) : Diffraction effect (b) Interference effect (c) Resultant Intensity

Diffraction Grating:-

An arrangement which consist of a large number of parallel slits of the same width and separated by equal opaque space is known as "Diffraction Grating".

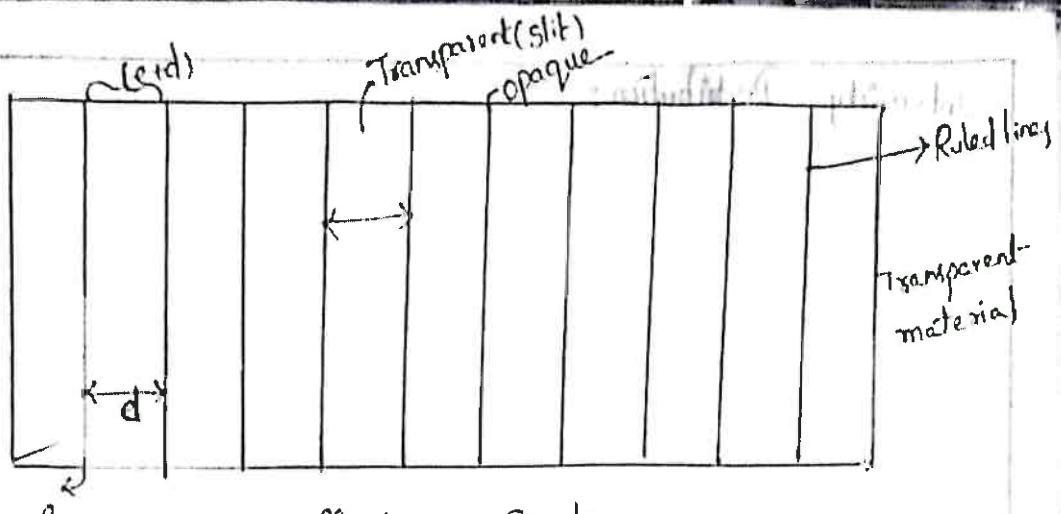


Fig: Diffraction Grating

Let 'e' be width of the slit & 'd' be the width of the slit. Then $(e+d)$ is known as Grating element. If N is the number of lines per inch on the grating, then

$$N(e+d) : " = 2.54 \text{ cm}$$

$$(e+d) = \frac{2.54}{N} \text{ cm}$$

There will be nearly 30,000 lines per inch of grating. The width of the slit is very narrow & is comparable to wavelengths of light. When light falls on the grating, the light gets diffracted through each slit. As a result diffraction & interference of diffracted light gets enhanced and forms a diffraction pattern. This pattern is known as diffraction spectrum.

Grating Spectrum :-

"The principal maxima in the diffraction of grating known as grating spectrum".

The position of the principal maxima is

$$d \sin \theta = m\lambda \quad (m = 0, 1, 2, 3, \dots)$$

In fig. 'xy' represents a plane transmission grating having $(e+d)$ as grating element and N lines per unit width of grating. A light beam having two slightly different wavelengths λ & $\lambda + d\lambda$ is incident normally on the surface of grating. SS, is the Screen. primary maximum spectral line of wavelength λ diffracted at an angle θ_0 . If P_2 represents the position of n^{th} order primary maximum spectral line of wavelength $\lambda + d\lambda$, diffracted at angle $\theta_0 + d\theta$. Then n^{th} order maxima lines can be resolved if P_2 corresponds to the minimum of wavelength λ .

The principal maximum for wavelength ' λ ' at the direction (diffracted) angle θ_0 is $(e+d) \sin \theta_0 = n\lambda \rightarrow (1)$
 the equation for the first minimum of wavelength λ in the direction ($\theta_0 + d\theta$) is $N(e+d) \sin(\theta_0 + d\theta) = (nN+1)\lambda \rightarrow (2)$
 The n^{th} principal maximum for wavelength $(\lambda + d\lambda)$ in the direction $\theta_0 + d\theta$ is

$$(e+d) \sin(\theta_0 + d\theta) = n(\lambda + d\lambda) \rightarrow (3)$$

Multiply eqn (3) with N , we have

$$N(e+d) \sin(\theta_0 + d\theta) = nN(\lambda + d\lambda) \rightarrow (4)$$

from eqn (2) & (4)

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

$$nN\lambda + nNd\lambda = nN\lambda + \lambda$$

$$\lambda = nNd\lambda \quad (\text{or})$$

$$\frac{\lambda}{d\lambda} = nN$$

The above eq represents the expression for the resolving power of grating

Dispersive Power:

Dispersive power of a prism is defined as the ratio of angular dispersion to mean deviation produced by prism

$$D = \frac{\mu_V - \mu_R}{\mu - 1}$$

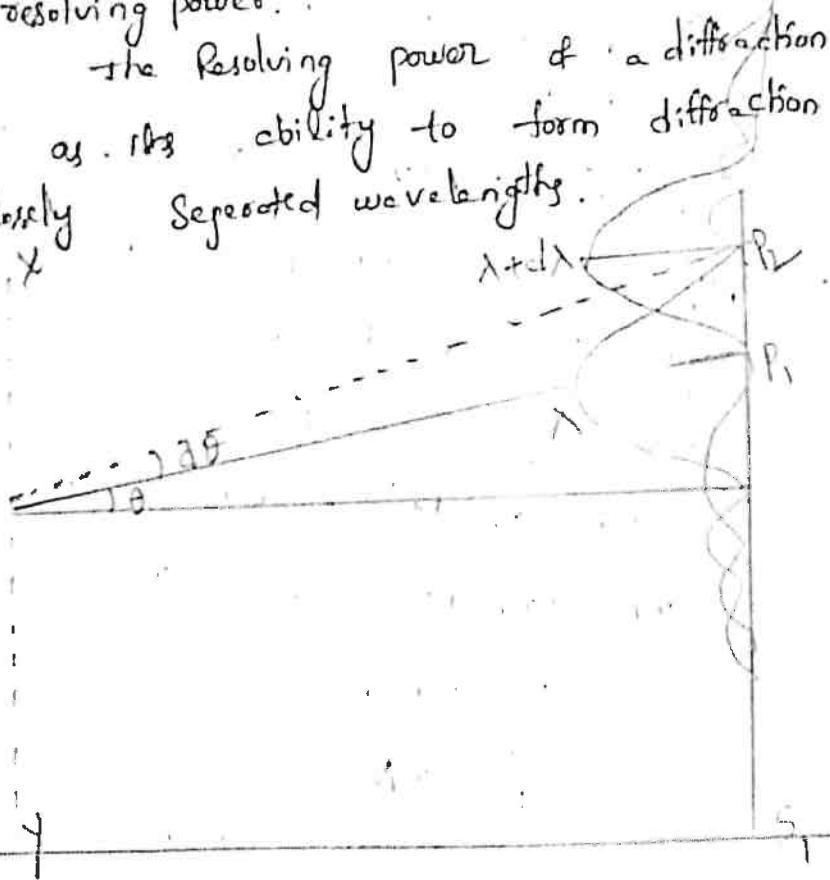
where, μ_V — Refractive index of violet

μ_R — Refractive index of Red

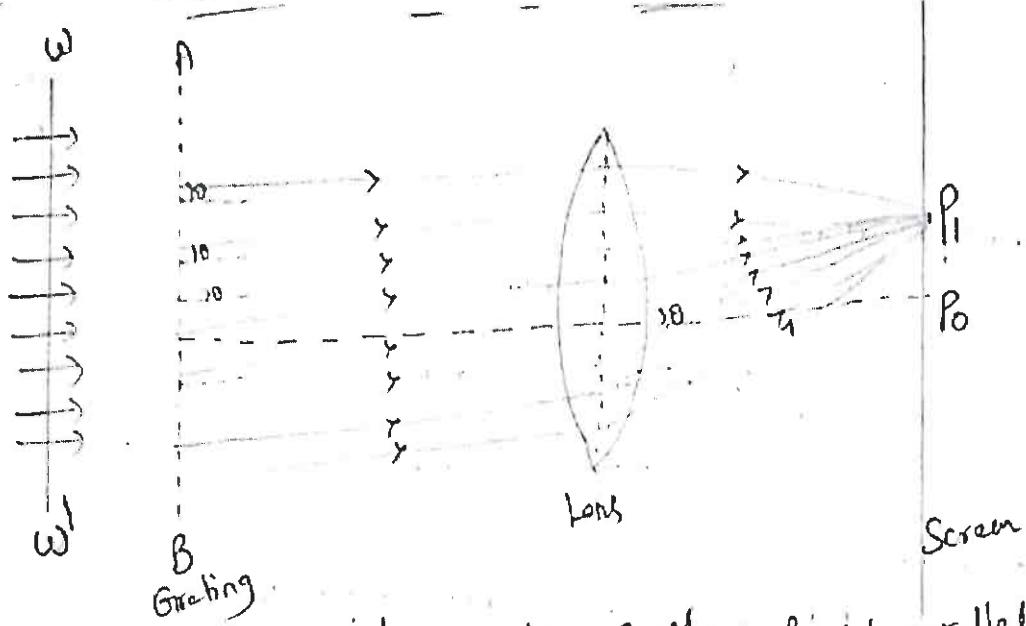
$$\mu = \frac{\mu_V + \mu_R}{2}$$

Resolving power of Grating
The capacity of an optical instrument to show separate images of very closely placed two objects is called resolving power.

The resolving power of a diffraction grating is defined as its ability to form diffraction maxima of two closely separated wavelengths.



Fraunhofer Diffraction due to N-Slits:



Consider a grating AB consists of N parallel slits with grating element ($e+d$).

Let a plane wavefront WW' of monochromatic light of wavelength λ be incident normally on the grating. The diffracted light through the N parallel slits is focussed by means of Convex lens on a Screen placed in the focal plane of the lens. The Secondary wavelets at an angle θ with the direction of the incident light are focused at a point P_1 on the screen.

The path difference b/w the wavelets emerging through the successive slits = $(e+d) \sin\theta$

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

$$\text{resultant Intensity } I = R^2 = \left(\frac{-1 \sin\alpha}{\alpha} \right)^2 \left(\frac{\sin N\beta}{\sin\beta} \right)^2$$

$\left(\frac{\sin \alpha}{\alpha}\right)^2 \rightarrow$ diffraction effect

$\left(\frac{\sin N\beta}{N\beta}\right)^2 \rightarrow$ Combination of Interference and diffraction.

Principal Maxima :-

for $\beta = \pm n\pi$

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

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

Minima :-

when $\sin N\beta = 0$, but $\sin \beta \neq 0$

$$N\beta = \pm m\pi$$

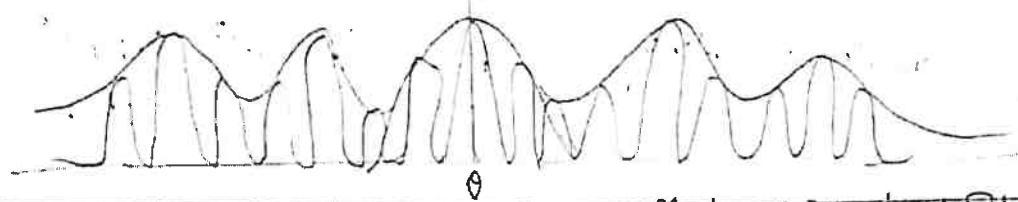
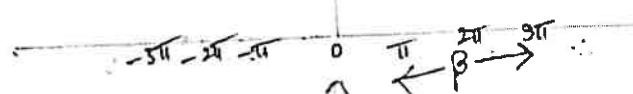
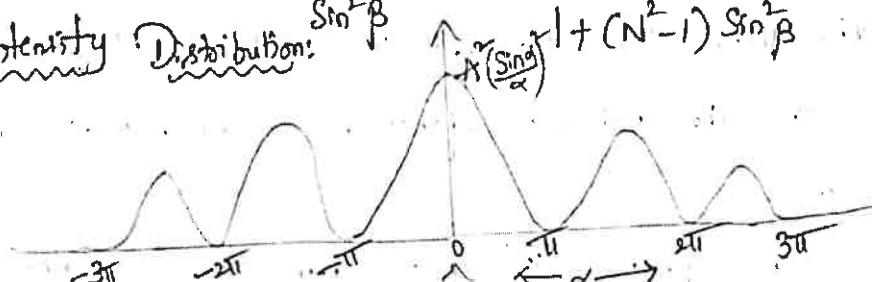
$$N \cdot \frac{\pi}{\lambda} (e+d) \sin \theta = \pm m\pi$$

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

Secondary Maxima :-

$$\frac{\sin^2 N\beta}{\sin^2 \beta} = 1$$

Intensity Distribution: $\frac{\sin^2 \beta}{1 + (N^2 - 1) \sin^2 \beta}$



(a) Diffraction Effect (b) Interference Effect (c) Resultant Intensity

Polarization

Introduction:

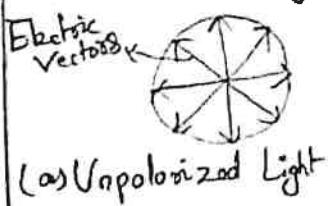
- the phenomenon of Interference and diffraction shows that light has wave nature.
- the phenomenon of polarization shows the transverse nature of light rays.
- Light is made up of electric and magnetic field vectors.
- These field vectors are perpendicular to the direction of propagation of light rays.
- The electric field vector \vec{E} and magnetic field vector \vec{B} are perpendicular to each other.

Representations of polarized and unpolarized light:-

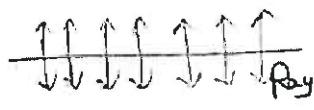
"Polarization is the process of converting non-polarized light into polarized light".

"Light in which the electric field vectors vibrate in a specific plane or direction of polarized light".

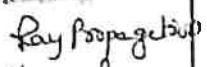
"The light wave in which the electric field vectors vibrate in all possible directions perpendicular to the direction of propagation of the light is called Unpolarized light".



(a) Unpolarized Light



(b) Vertically plane polarized light



(c) Horizontally plane polarized light



(d) Unpolarized Light

Type of polarization:-

Following are the three types of polarization depending on how the electric field is oriented:

(i) Linear polarization

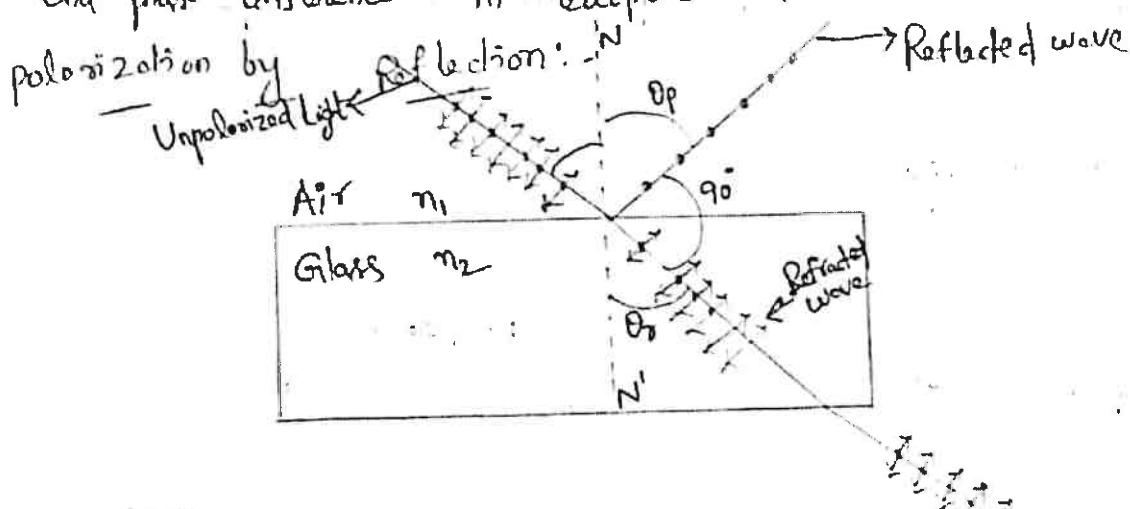
(ii) Circular polarization

(iii) Elliptical polarization

(i) Linear polarization: In linear polarization, the electric field of light is limited to a single plane along the direction of propagation.

(ii) Circular polarization: In circular polarization, the electric field of light has two linear components that are perpendicular to each other and have identical amplitude, but the phase difference is $\frac{\pi}{2}$. The electric field that occurs will propagate in a circular motion.

(iii) Elliptical polarization: In this polarization, the electric field of light propagates along an elliptical path. The two linear components do not have the same amplitude and phase difference in elliptical polarization.



In 1809, Malus, a French Scientist discovered that when ordinary light is incident on the surface of a transparent medium like glass or water, then light can be partially or completely polarized on reflection by varying angle of incidence.

For perpendicular angle of incidence ($\theta_i = \theta_p$, θ_p = angle of polarization) the reflected light is completely plane polarized. This angle of incidence is known as Brewster's angle or angle of polarization. Polarization angle varies with material. The Brewster's angle for glass ($\mu = 1.52$) is 57° .

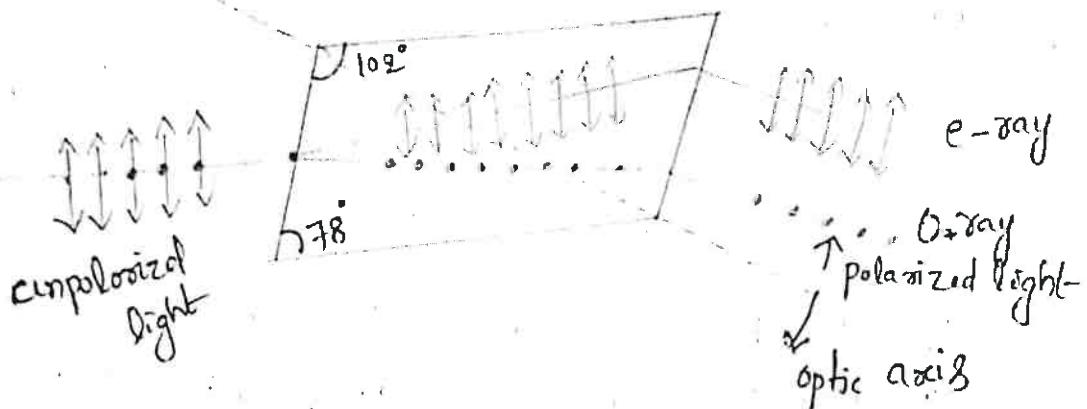
If the incident beam makes Brewster's angle then the reflected light is completely plane polarized while the transmitted light is partially plane polarized. In reflected light the vibrations of the electric vectors are perpendicular to the plane of incidence.

The intensity of reflected light is less compared to the intensity of incident beam. But it is large for transmitted beam. By using a large number of thin parallel glass plate instead of single, the intensity of reflected waves enhanced.

Refraction and Double Refraction:-

When a beam of unpolarized light passes through the glass plate some portion of light is reflected, remaining is refracted into the glass plate is called Refraction.

" when a beam of Unpolarized light passes through anisotropic crystal such as quartz or calcite, the beam will split up into two refracted beams. This is known as double refraction or birefringence."



- Double refraction in calcite crystal is shown in figure.
- through the optic axis light may not refracted into two.
- If only one optic axis in crystal is called Un-axial crystal. If it is two is called biaxial crystal.
- when a beam of unpolarized light is passes through the crystal, ray is divided (refracted) into two, one is extraordinary ray (e-ray) and another one is ordinary ray (o-ray).
- Beam is polarized along the direction of optic axis is called e-ray.
- Beam is polarized perpendicular to the direction of optic axis is called (o-ray) ordinary ray.
- Both e-ray and o-ray are polarized light rays.
- the velocity of o-ray is the same in all directions of a crystal, whereas as the extraordinary ray travels with different velocities in different directions.

(3)

→ the velocity of e-ray and o-ray are same along optic axis
 → the velocity of e-ray is less than the o-ray in quartz crystal
 is called positive crystal. the velocity of e-ray is more
 than the o-ray in calcite crystal is called negative
 crystal.

→ Along the optic axis $\mu_e = \mu_o$
 → In quartz crystal $\mu_e > \mu_o$, in calcite crystal $\mu_e < \mu_o$
 → In opposite crystal $v_e > v_o$, $\mu_e > \mu_o$
 → In positive crystal Ellipsoidal wavefront occurs inside
 Spherical wavefront.
 → In negative crystal $v_e > v_o$, $\mu_e < \mu_o$
 → In negative crystal spherical wavefront occurs
 inside the ellipsoid.

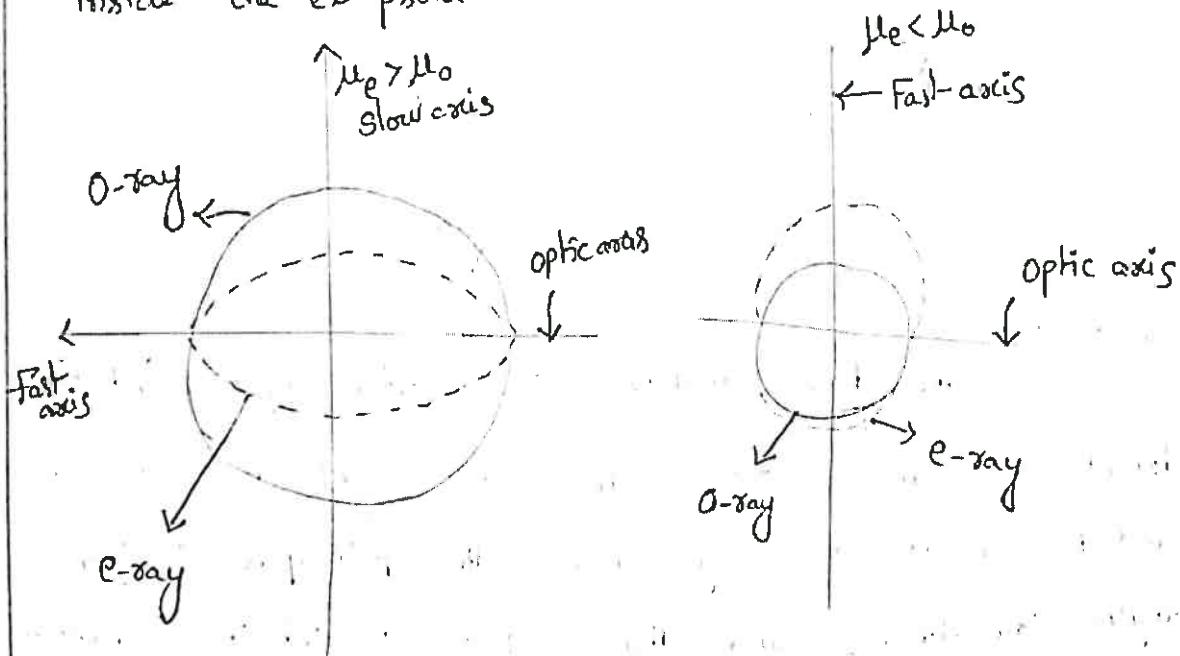


fig: positive crystal

fig: Negative crystal

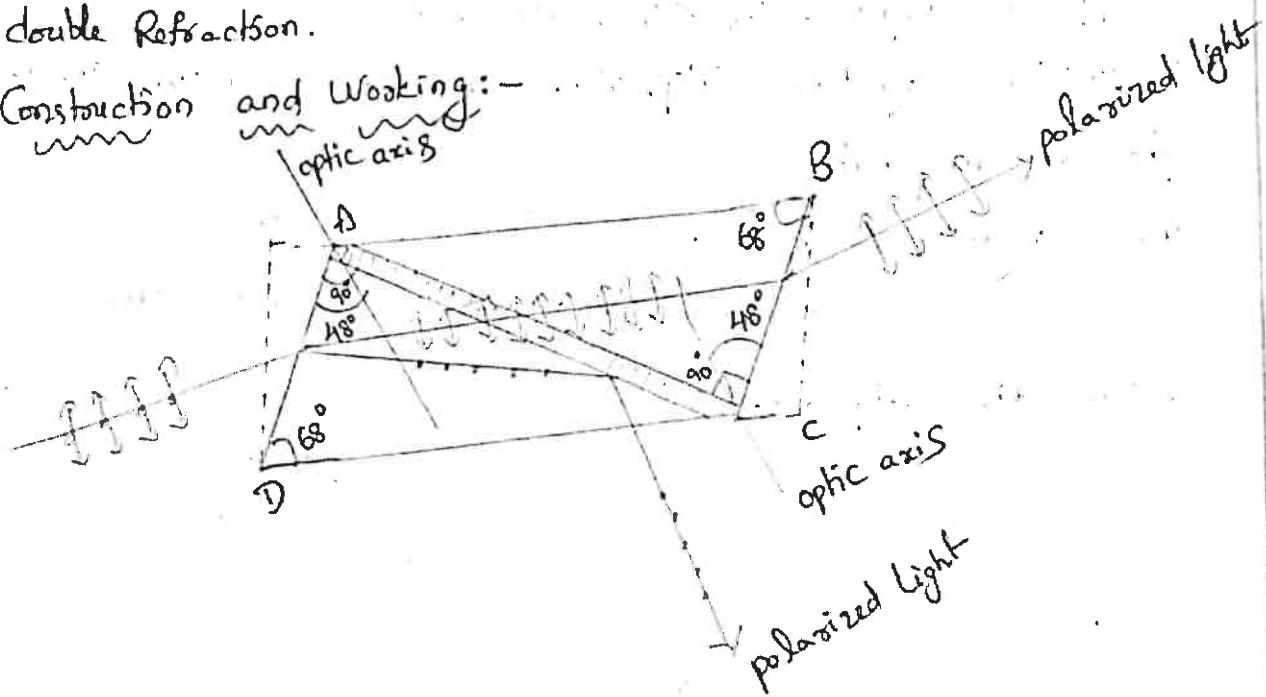
Nicol prism :-

- Nicol prism is an optical device which is used for producing and analysing plane polarized light in practice.
- This was invented by William Nicol in the year 1828.

Principle of Nicol prism:

Nicol prism is based on the phenomenon of double refraction.

Construction and Working:-



Construction:

The base material is calcite crystal (NB_{cD}).
length is three times that of breadth. End faces - AD and BC cut in a way that the principal section angles come to 68° and then, crystal is cut in a diagonal manner generating two parts, surfaces made flat and polished nicely. Polished surfaces are then joined with Canada balsam layer.

working :-

when unpolarized light is passes through the calcite crystal it will be divided into two rays like ordinary and extraordinary rays. Canada balsam acts as a rarer medium for the ordinary ray and acts as a denser medium for extraordinary ray. When the angle of incidence for ordinary ray on the Canada balsam is greater than the critical angle then total internal reflection takes place, while the extraordinary ray gets transmitted through the prism. So polarized light as o-ray is filtered by the Nicol prism.

Nicol prism can be used as an analyser also.

Half wave plate :-

A half wave ($\frac{\lambda}{2}$) plate is a thin double refracting crystal of Calcite or quartz, cut and polished parallel to its optic axis to a thickness 'd' such that it produces a path difference of $\frac{\lambda}{2}$ or phase difference of π b/w o-ray and e-ray.

Consider a calcite crystal of thickness 'd'. The optic axis is parallel to the surface. When a plane polarized light is incident normally on the surface then the light will split up into o-ray and e-ray. These rays travel with different speeds in the crystal.

In calcite crystal the e-ray travel faster than o-ray. Hence the refractive index of o-ray (μ_o) is higher than the refractive index of e-ray (μ_e) of the crystal. The optical path covered by the o-ray as it pass through the crystal of thickness 'd' is $\mu_o d$. Similarly the optical path covered by the e-ray as it pass through the crystal of thickness 'd' is $\mu_e d$.

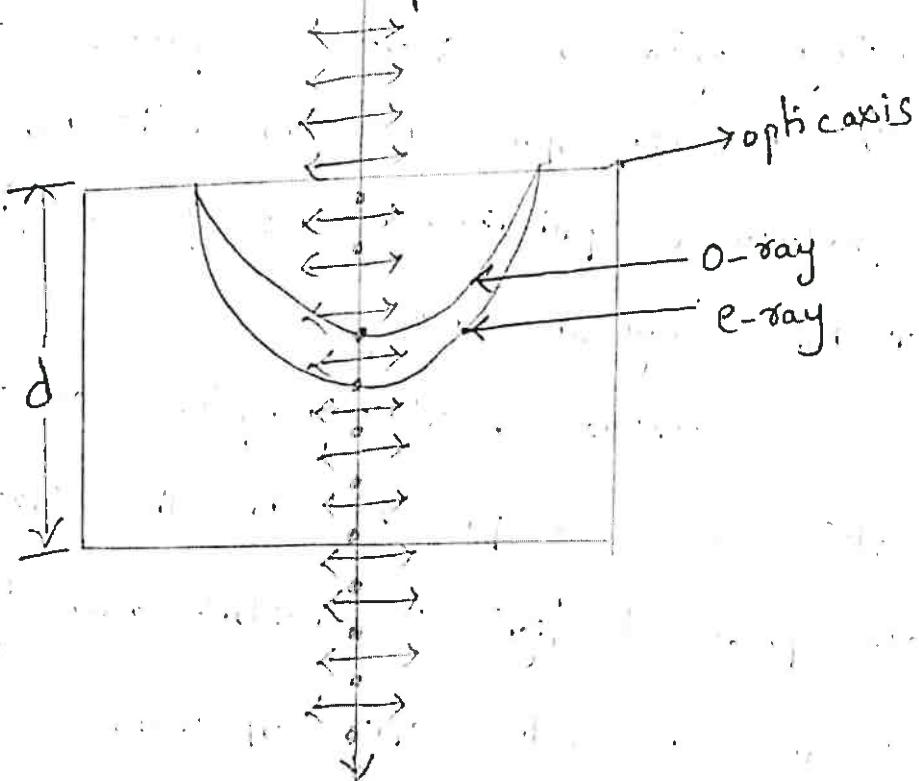
The path difference $\Delta = \mu_o d - \mu_e d = d(\mu_o - \mu_e)$.

$$\frac{\lambda}{2} = d(\mu_o - \mu_e)$$

$$d = \frac{\lambda}{2(\mu_o - \mu_e)} \text{ (For calcite crystal)}$$

$$d = \frac{\lambda}{2(\mu_e - \mu_o)} \text{ (For Quartz crystal)}$$

plane polarized light



Quarter wave plate :-

→ A quarter wave plate is a thin double reflecting crystal of calcite or quartz, cut and polished parallel to its optic axis to a thickness 'd' such that it produces a path difference of $\frac{\lambda}{4}$ or phase difference of b/w o-ray and e-ray.

Consider a calcite crystal of thickness 'd'.
The optic axis is parallel to the surface. When a plane polarized light is incident normally on the surface, then the light will split up into two rays. The optical path covered by the o-ray as it passes through the crystal of thickness d is $\mu_o d$, similarly for e-ray it is $\mu_e d$.

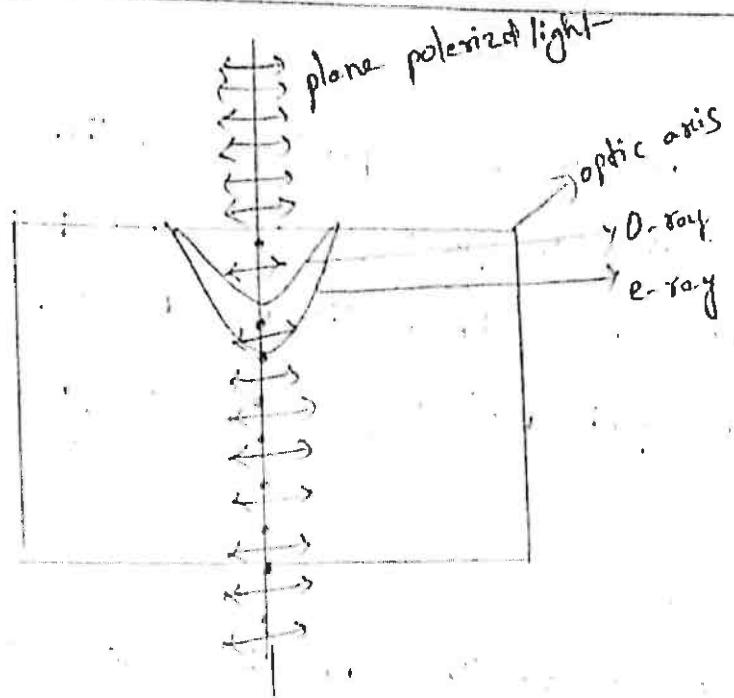
$$\text{path difference } \Delta = \mu_o d - \mu_e d = \frac{\lambda}{4}$$

$$d(\mu_o - \mu_e) = \frac{\lambda}{4}$$

$$d = \frac{\lambda}{4(\mu_e - \mu_o)}$$

(for quartz crystal)

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



UNIT-II
CRYSTALLOGRAPHY
&
X-RAY DIFFRACTION

Crystalllography and X-ray Diffraction.

Crystalllography:-

- If the atoms or molecules are in a solid are periodical at regular intervals of distances in three-dimensional space, then the solid is known as crystalline solid.
- If the atoms or molecules do not have such a periodicity in a solid, is called amorphous Solid.
- Crystalline solids are anisotropic, Amorphous are isotropic in nature.

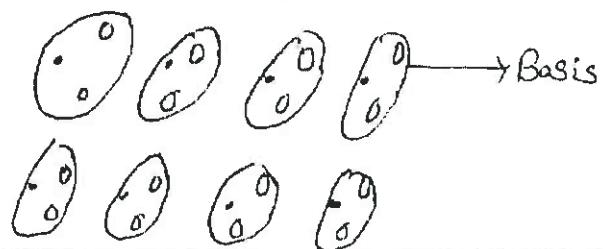
Space lattice :-

- A regular or periodical geometrical arrangement of points in space is called lattice.
- A space lattice represents the geometrical pattern of crystal in which the surroundings of each lattice point is the same.

Fig: Two dimensional Space lattice.

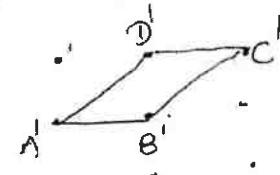
Basis:-

The crystal structure is formed by associating every lattice point with an assembly of atoms or molecules or ions which are identical in composition, arrangement and orientation is called basis.

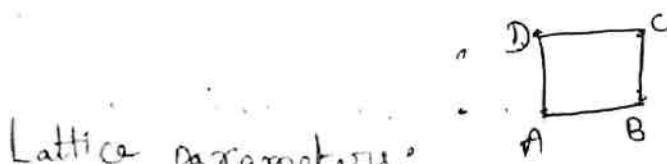


UNIT CELL:-

Unit cell is the smallest geometric figure, which repetition in three-dimensional space, gives the actual crystal structure called a Unit cell.

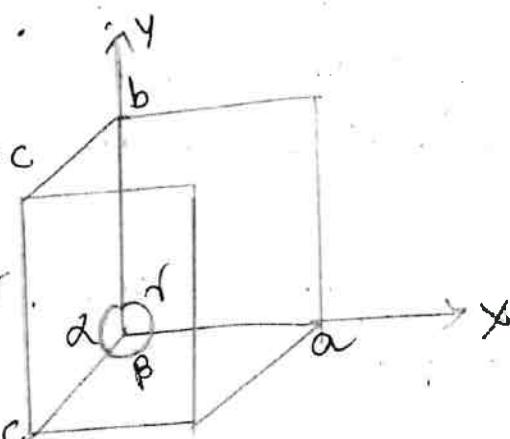


ABCD and $A'B'C'D'$ are Unit cells.



Lattice parameters:

- Consider three crystallographic axes are obtained by the intersection of the three non-coplanar faces of the Unit cell.
- The angles b/w three faces or crystallographic axes are known as interfacial or interaxial angles.
- The angles b/w $y \& z$, $z \& x$ and $x \& y$ are α , β and γ .
- The translational or primitives a, b, c of a Unit cell along x, y, z axes.
- "The combination of translational vectors (a, b, c) and interfacial angles (α, β, γ) are called Lattice parameters".



$$\text{Lattice Parameters} = \text{Interfacial angles} + \text{Translational Vectors.}$$

Bravais Lattices:-

- In 1848, Bravais showed that 14 lattices are sufficient to describe all crystals.
- These 14 lattices are known as Bravais Lattices - and

(2)

are classified into 7 crystal systems based on lattice parameters.

The seven crystal systems are -
 (i) Cubic (ii) Tetragonal (iii) orthorhombic (iv) Monoclinic
 (v) Triclinic (vi) Rhombohedral (vii) Hexagonal.

Crystal Systems (3D):

S.No	Crystal System	Bravais Lattices	No. of Bravais Lattices	Lattice parameters
1	Cubic	P, I, F	3	$a=b=c$ $\alpha=\beta=\gamma=90^\circ$
2	Tetragonal	P, I	2	$a=b \neq c$ $\alpha=\beta=\gamma=90^\circ$
3	orthorhombic	P, I, F, C	4	$a \neq b \neq c$ $\alpha=\beta=\gamma=90^\circ$
4	Monoclinic	P, C	2	$a \neq b \neq c$ $\alpha=\beta=90^\circ \neq \gamma$
5	Triclinic	P	1	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$
6	Rhombohedral (Trigonal)	P	1	$a=b=c$ $\alpha=\beta=\gamma \neq 90^\circ$
7	Hexagonal	P	1	$a=b \neq c$ $\alpha=\beta=90^\circ, \gamma=180^\circ$

(i) Cubic Crystal System :-

primitive (or) Simple Cubic Lattice (P):

In Simple Cubic Lattice, lattice points are present at the corners of the cube.

Body centred Cubic Lattice (I):

In body-centred cube, atoms are present at the corners and one atom is completely at the centre of the cube.

Face centred cube (F):

In Face-Centred Cube atoms are present at corners and at the centres of all faces of cube.

Base-Centred lattice :-

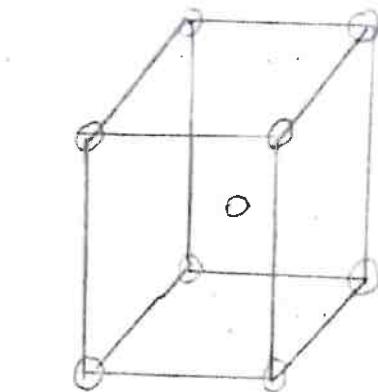
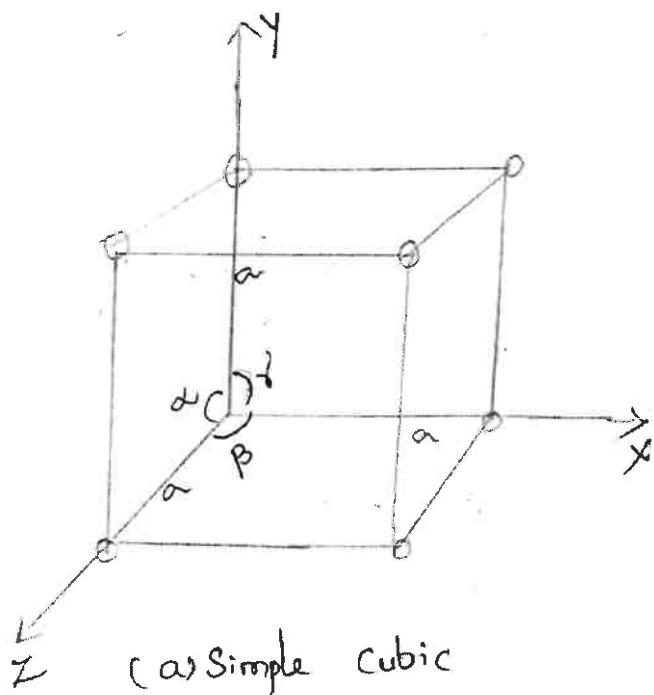
In base centred lattice atoms are present at corners and top and bottom faces has one atom.

(i) Cubic Crystal System :-

In this crystal all unit cell edge lengths are equal and at right angles to one another. i.e.

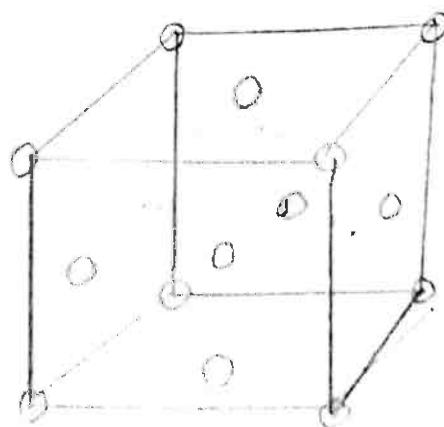
$$a = b = c, \alpha = \beta = \gamma = 90^\circ$$

It has three bravais lattices P, I and F.



(b) Body-Centred cubic

(a) Simple cubic



(c) Face-Centred cubic

(ii) Tetragonal crystal System:-

In this crystal $a = b \neq c$, and $\alpha = \beta = \gamma = 90^\circ$
It has two Bravais Lattices. They are Simple
and Body-centred shown figures.

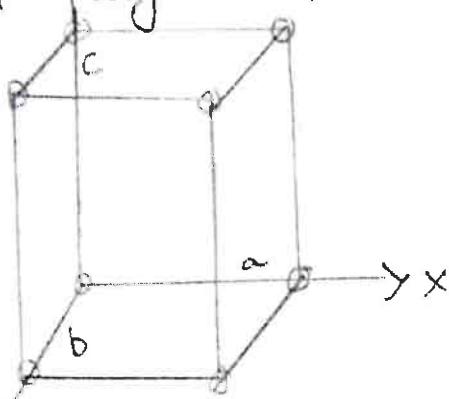


fig: Simple lattice

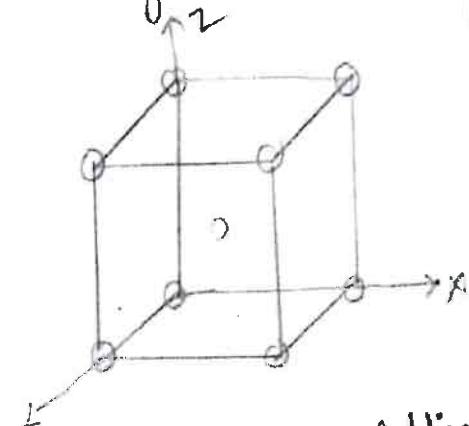
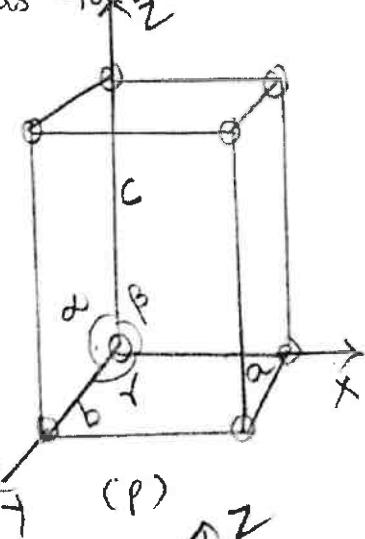


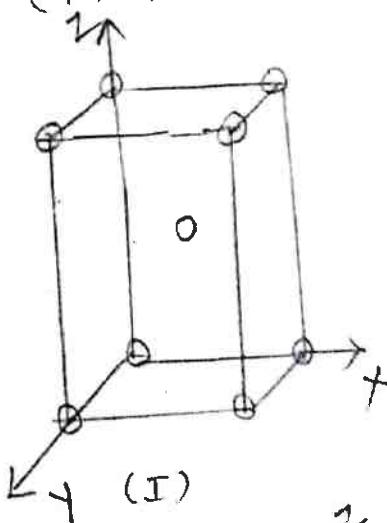
fig: Body centred lattice

(iii) Orthorhombic Crystal System:-

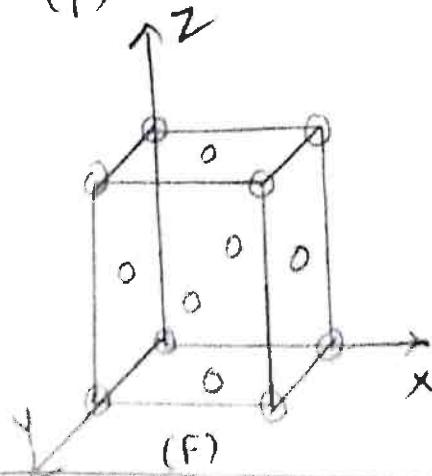
In this Crystal $a \neq b \neq c$, $\alpha = \beta = \gamma = 90^\circ$:
It has four Bravais lattices (P, I, F, C) as shown in figures



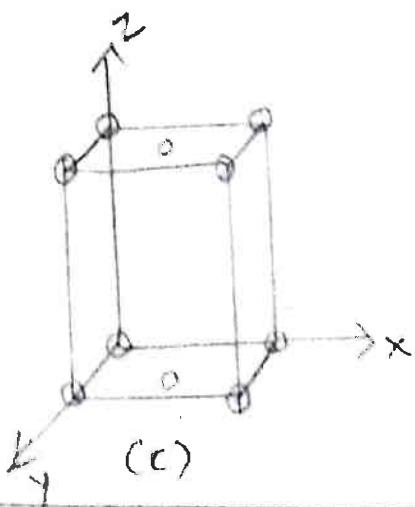
(P)



(I)



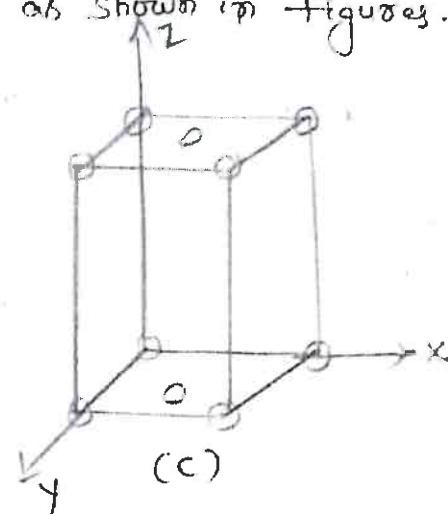
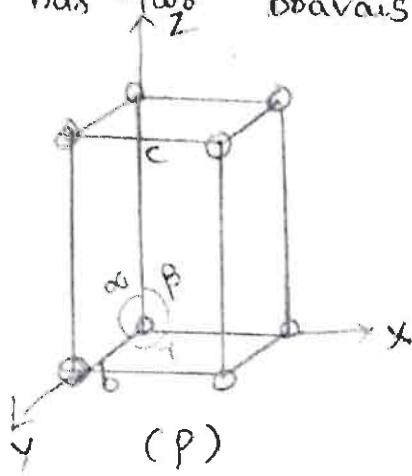
(F)



(C)

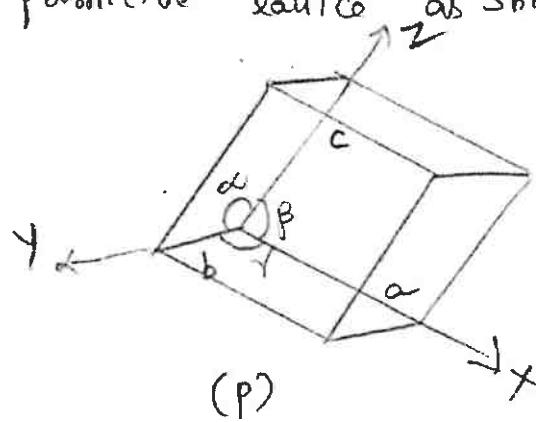
(iv) Monoclinic Crystal System :-

In this crystal system $a \neq b \neq c$, $\alpha = \beta = 90^\circ \neq \gamma$
It has two bravais lattice (P, C) as shown in figures.



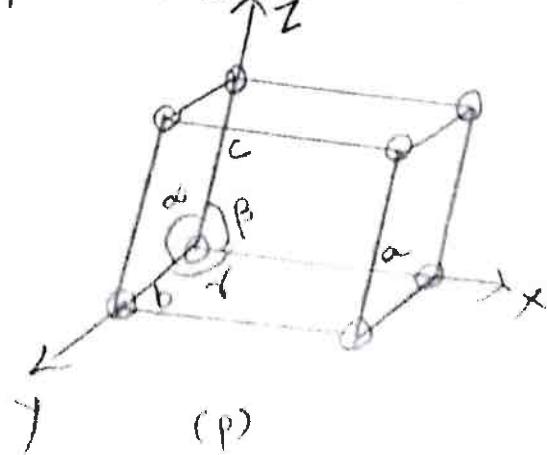
(v) Triclinic Crystal System :-

In this crystal system, $a \neq b \neq c$. $\alpha \neq \beta \neq \gamma \neq 90^\circ$
It has only primitive lattice as shown figure.



(vi) Rhombohedral Crystal System :-

In this crystal system $a = b = c$, $\alpha = \beta = \gamma \neq 90^\circ$
It has only primitive lattice as shown in figure.

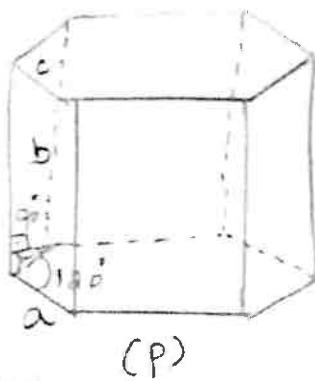


(Vii) Hexagonal crystal system:-

In this crystal system, $a = b \neq c$

$$\alpha = \beta = 90^\circ, \gamma = 120^\circ$$

It has only primitive lattice.



Co-ordination Number:-

The number nearest neighbours atom to an atom is called Co-ordination number.

Nearest Neighbour distance (a₀):-

The distance b/w the centres of two neighbouring atoms is called Nearest neighbour distance.

Packing factor:-

It is defined as the ratio of Volume occupied by the atoms in a unit cell to the volume of the unit cell.

$$P.F = \frac{\text{Volume occupied by atoms}}{\text{volume of Unit cell}}$$

(i) Simple Cubic Structure [SC] :-

In Simple cubic crystal, $a = b = c, \alpha = \beta = \gamma = 90^\circ$.

Atoms are present only at the corners of the unit cell. The corner atom is shared by adjacent 8 unit cells. So, the contribution of each corner atom is $\frac{1}{8}$. The cube has eight corners.

So, the number of atoms present in Simple cubic crystal $18 = 8 \times \frac{1}{8} = 1$.

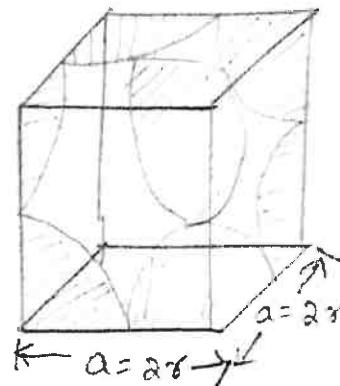
→ In SC, distance b/w the centres of two neighbouring atoms i.e., nearest neighbour distance ($2r$) = a .

→ Co-ordination number = 6

→ Atomic packing fraction =

$$\frac{\text{Volume of atoms in Unitcell}}{\text{Volume of Unitcell}}$$

$$\begin{aligned} \text{APF} &= \frac{1 \times \frac{4}{3} \pi r^3}{a^3} \\ &= \frac{4}{3} \frac{\pi r^3}{(2r)^3} \end{aligned}$$



$$\text{APF} = \frac{\pi}{6} = 0.52 = 52\%$$

→ Void space :- Empty space present in crystal is 48%.

→ Body-Centred Cubic Structure (BCC) :-

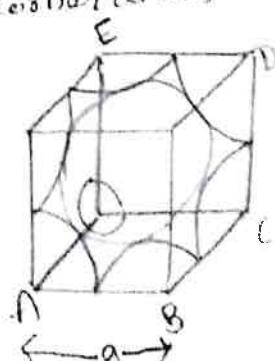
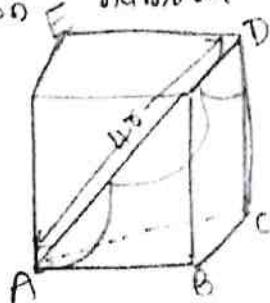
(a) Body - Centred Cubic Structure (BCC) :-
→ For this unit cell, atoms are present at the corners of the cube and one atom is completely present at the centre.

→ Contribution of each corner atom is $\frac{1}{8}$

$$\frac{1}{8} \times 8 + 1 = 2$$

→ The total number of atoms = 2.

→ Centre atom is surrounded by 8 corner atoms. So, the coordination number is 8.



(5)

From fig $AD = 4\alpha$

$$\begin{aligned} \rightarrow AD^2 &= AC^2 + CD^2 = AB^2 + BC^2 + CD^2 \\ &= \alpha^2 + \alpha^2 + \alpha^2 = 3\alpha^2 \end{aligned}$$

$$(4\alpha)^2 = 3\alpha^2$$

$$4\alpha = \sqrt{3}\alpha$$

$$\alpha = \frac{4}{\sqrt{3}} \alpha$$

Atomic packing factor (APF) :-

$$\text{APF} = \frac{\text{Volume of atoms in Unitcell}}{\text{Volume of Unitcell}}$$

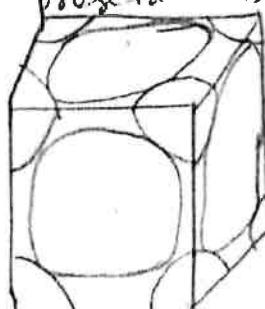
$$= \frac{2 \times \frac{4}{3} \pi r^3}{\alpha^3}$$

$$= \frac{2 \times \frac{4}{3} \pi r^3}{\left(\frac{4}{\sqrt{3}} \alpha\right)^3} = \frac{8 \pi r^3 3 \sqrt{3}}{3 (4r)^3}$$

$$= \frac{\sqrt{3} \pi}{8} = 0.68 = 68\%$$

Void space = 32 %

- (3) Face Centred Cubic Structure (FCC) :-
- In this structure atoms are present at the corners and at the face centres of this cubic structure.
 - Corner atom is shared by 8 unit-cells and a face centred atom shared by two unit-cell.
 - No. of atoms present $r_s = \frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$



Face centred cubic cell

→ In FCC coordination number is 12.

→ From fig: ΔABC

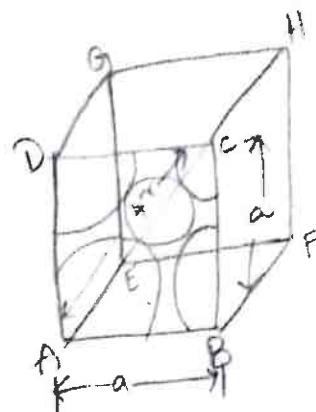
$$AC^2 = AB^2 + BC^2$$

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

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

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

→ Nearest neighbour distance ($2r$) = $\frac{a}{\sqrt{2}}$



→ Atomic packing factor is

$$\text{Volume of one atom} = \frac{4}{3}\pi r^3$$

$$\text{Volume of unit cell} = a^3$$

$$\begin{aligned} \text{APF} &= \frac{4 \times \frac{4}{3}\pi r^3}{a^3} \\ &= \frac{4 \times \frac{4}{3}\pi \left(\frac{a}{2\sqrt{2}}\right)^3}{a^3} = \frac{\pi}{3\sqrt{2}} \end{aligned}$$

$$\text{APF} = 0.74 = 74\%$$

∴ void space is = 26%

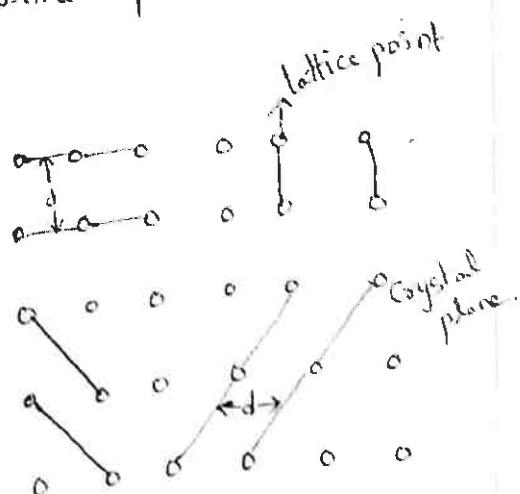
Miller Indices :-

The plane passing through the lattice points is known as crystal planes.

→ the perpendicular distance b/w two adjacent crystal

planes is called "Interplanar Spacing (d)".

→ Miller devised a method of representing the orientation of



a crystal plane.

→ "the crystal plane is represented by three smallest integers known as miller indices".

→ "miller indices are three smallest integers which have the same ratio as the reciprocals of the intercepts of the crystal plane with the coordinate axes".

procedure to find miller indices :-

→ the intercepts made by the crystal plane along x, y and z axis in terms of lattice parameters a, b, c are noted.

→ Express the reciprocal intercepts as multiples of a, b, c .

→ Take the reciprocals of intercepts.

→ Convert the reciprocals in to integers by multiplying each of them with their LCM.

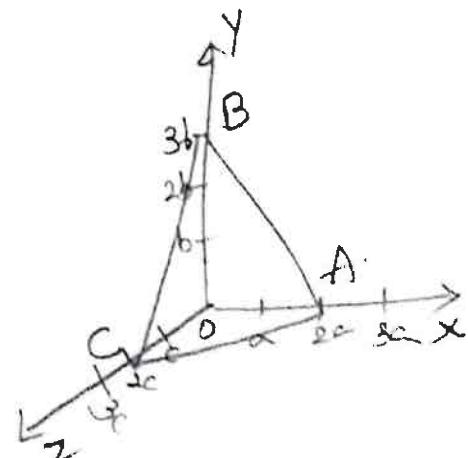
→ Enclose these integers in smallest parentheses. This represents the miller indices of the crystal plane.

For example :

→ ABC is crystal plane with intercepts $ab, 3b$ and ac along x, y and z axes.

a, b, c are lattice parameters.

→ The intercepts as multiples of a, b, c are $2, 3, 2$.



→ Reciprocals of intercepts are $\frac{1}{2}, \frac{1}{3}, \frac{1}{2}$. Their LCM is 6.

→ Multiply reciprocals by 6. So that they become $3, 2, 3$.

→ The integers are written within the parenthesis as $(3, 2, 3)$.

→ $(3, 2, 3)$ represents miller indices of the crystal plane ABC.

Separation b/w Successive Chord planes :-

Consider a plane ABC intercepting all three axes at distances OA, OB and OC as shown in fig.

- let the normal to the plane from the origin intercept the plane at N with a distance d.
- let the normal to the plane from the origin intercept the plane at N₁ at distance d₁.
- α, β, γ are the angles b/w ON and x, y, z axes respectively.

$$\text{From fig, } \Delta ONA, \cos \alpha = \frac{ON}{OA} = \frac{d}{h} = d(\frac{h}{a})$$

$$\Delta ONB, \cos \beta = \frac{ON}{OB} = \frac{d}{k} = d(\frac{k}{b})$$

$$\Delta ONC, \cos \gamma = \frac{ON}{OC} = \frac{d}{l} = d(\frac{l}{c})$$

According to Cosines Law $\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = 1$

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

$$d^2 = \frac{a^2}{h^2+k^2+l^2} \quad (\text{for cubic axis } a=b=c)$$

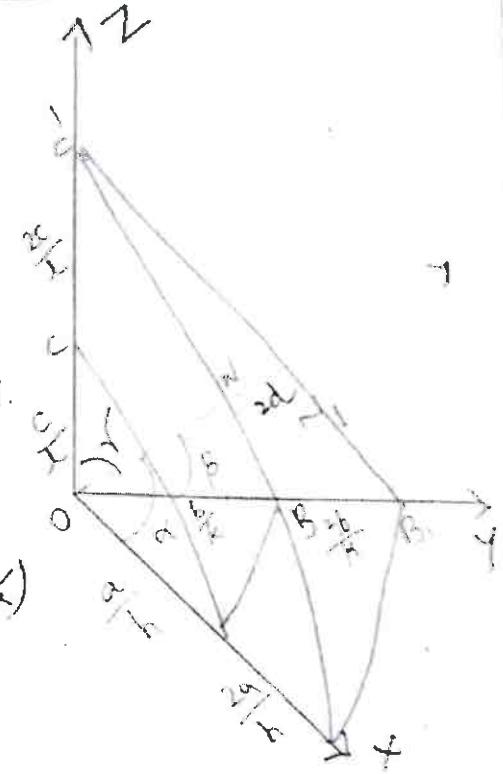
$$d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

Consider a parallel plane intercepting the three axes at A, B, and C at a distance of $2ah$ ($\propto a$), $\frac{2k}{l}$ ($\propto b$) and $\frac{2l}{c}$ ($\propto c$). From origin O. It makes the angles α, β, γ with x, y and z axes respectively. Its planar distance from the origin O is ON_1 ($= d_1$) and is given by

$$d_1 = \frac{2a}{\sqrt{h^2+k^2+l^2}}$$

Hence the interplanar distance b/w the two planes is given by $(ON, -ON)$. i.e., $(2d - d_1)$. $2d - d_1 = \frac{2a}{\sqrt{h^2+k^2+l^2}} = \frac{a}{\sqrt{h^2+k^2+l^2}}$

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



X-Ray Diffraction

X-Ray diffraction :-

- For diffraction to occur, the size of obstacle must be comparable with wavelength of incident light.
- Due to small wavelength of x-rays (0.1 nm) grating cannot be used for x-ray diffraction studies as the spacing cannot be comparable to wavelength of x-rays.
- Laue suggested that a crystal which consists of a three dimensional array of regularly spaced atoms will produce diffraction effects for x-rays.
- Crystal will acts as diffraction grating.

Bragg's law :-

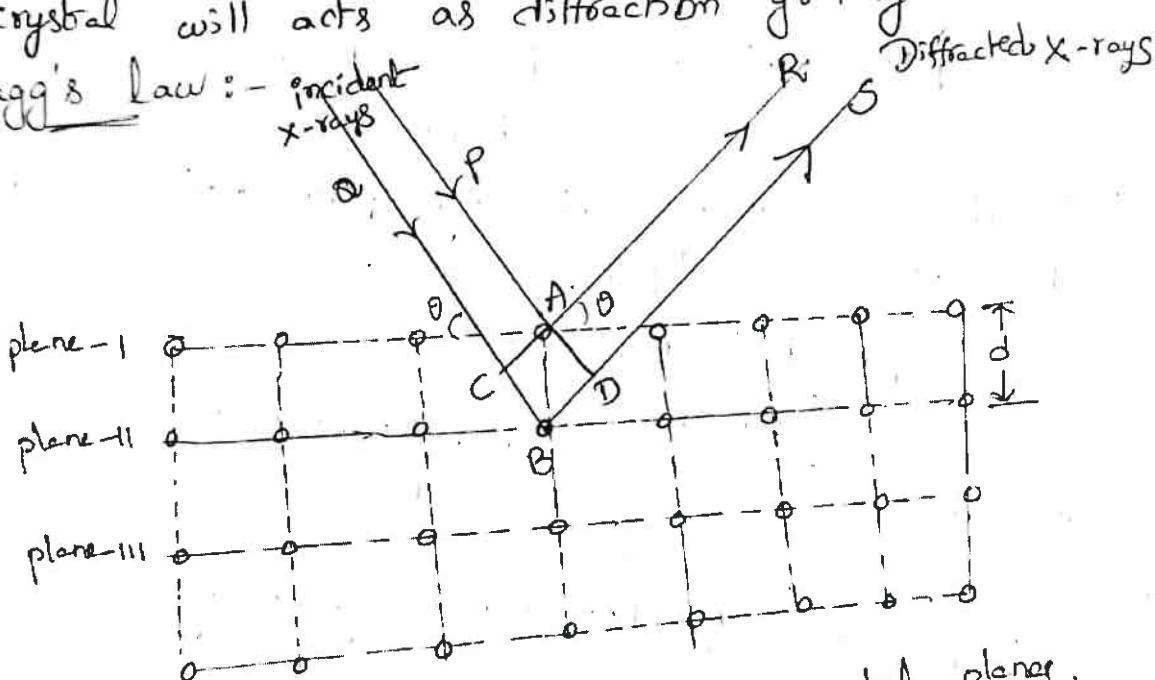


fig: Diffraction of x-rays by crystal planes.

Consider a crystal which consists of equidistant parallel planes with the interplanar spacing 'd' as shown in figure. When x-rays of wavelength (λ) fall on these crystal planes, the atoms in the planes diffract the x-rays in all directions.

Let the x-ray PA incident at angle ' θ ' with the plane I be reflected at atom A in the direction AP and another x-ray QB reflected at an atom 'B' in the direction BS. These diffracted rays will interfere constructively or destructively depending on the path difference b/w the x-rays. To calculate the path difference, two normal AC and AD are drawn from A to QB and BS.

$$\text{path difference} = CB + BD$$

$$\text{From } \triangle ACB; \sin\theta = \frac{CB}{AB}$$

$$CB = AB \sin\theta = d \sin\theta$$

$$\text{From } \triangle ADB, BD = d \sin\theta$$

$$\therefore \text{path difference} = d \sin\theta + d \sin\theta \\ = 2d \sin\theta$$

To get maximum Intensity, path difference should be equal to integral multiple of λ .

$$\text{path difference} = n\lambda$$

$$2d \sin\theta = n\lambda, \text{ where } n=1, 2, 3 \dots$$

The above expression represents Bragg's Law.

Importance of Bragg's Law:

- 1) From Bragg's law by knowing ' λ ', glancing angle ' θ ' can be calculated.
- 2) knowing 'd' the lattice constant 'a' can be known.
- 3) knowing 'a'; ρ (density) and M (molecular weight) the number of atoms in unit cell can be calculated.

4) For cubic crystal, $d = \frac{a}{\sqrt{h^2+k^2+l^2}}$

Knowing 'd', and 'a' the value $\sqrt{h^2+k^2+l^2}$ can be calculated.

- 5) Depending on the values of $h^2+k^2+l^2$, we can classify the crystals as BCC, FCC, simple cubic etc.

X-ray diffractometer :-

- X-ray diffractometers consists of - three basic elements an X-ray tube, a sample holder, and an X-ray detector.
- X-ray diffractometry or XRD machine is a device for analyzing and measuring the structure of materials.
- X-ray diffractometers are used to measure residual stress.
- These are used to measure various sample sizes and geometries.
- X-rays are generated in cathode ray tube by heating a filament to produce electrons, accelerating the electrons toward a target and bombarding the target material with electrons.
- We have two methods, XRD methods used for crystal structure studies.

(i) Laue method (ii) powder method.

Crystal Structure determination by Laue method :-

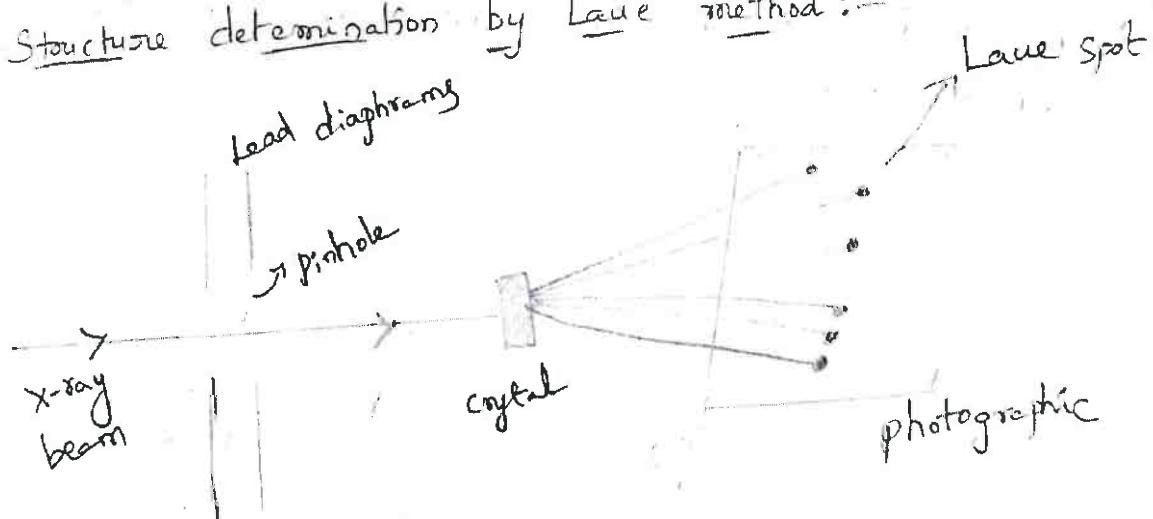


fig: Laue method.

- The Laue method is one of the X-ray diffraction techniques used for crystal structure studies as shown in figure.
- The crystal whose structure has to be studied is held stationary in a continuous X-ray beam.
- After passing through the pin holes of lead diaphragms.

we obtain a fine beam of x-rays.

→ These x-rays are allowed to fall on the crystal.

→ the crystal planes in the crystal diffract the x-rays satisfying Bragg's law.

→ the diffracted x-rays are fall on a photographic plate.

→ the diffraction pattern consists of a series of bright spots corresponding to interference maximum for a set of planes.

→ The distribution of spots depends on the symmetry of the crystal and its orientation with respect to x-ray beam.

→ For simple cubic crystal the true photograph is shown in figure.

merits:-

1) This method is used for determination

of crystal orientation Symmetry

2) It is also used to study Crystalline imperfections.

Demerits:-

This method is not convenient for actual crystal structure determination.

Powder Method :-

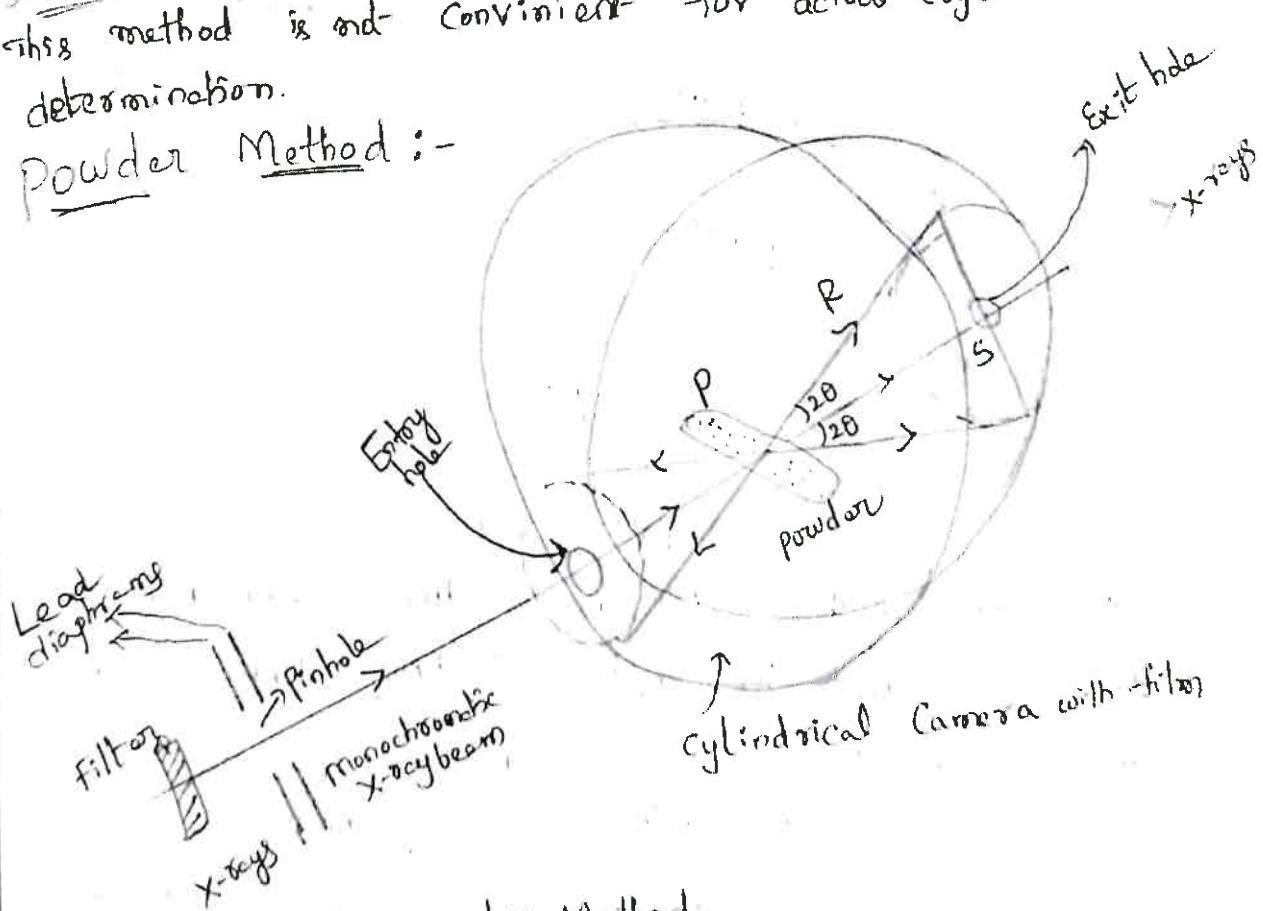
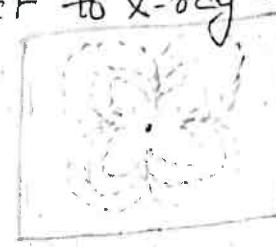
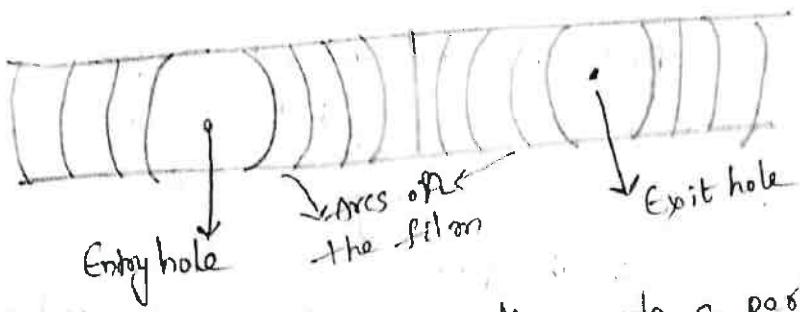


Fig: powder Method.



- The powder method is an XRD technique used to study the structure of microcrystals in the form of powder.
- This method gives information regarding the size and orientation of the crystallites in the powder.
- It is also known as Debye-Scherrer method as shown in fig.
- The experimental arrangement consists of a cylindrical camera, called the Debye-Scherrer Camera consisting of a film in the inner position.
- The powder sample is filled in the capillary tube.
- The incident X-rays after passing through the filter and pin holes of lead diaphragms, produce a fine beam of X-rays.
- The fine beam of monochromatic X-ray after passing through the entable falls on the capillary tube P containing powder crystals.
- The oriented crystallites in the powder all possible θ and d values are available for diffraction of X-rays.
- They satisfy Bragg's law $2d \sin\theta = n\lambda$.
- For particular value of θ various orientations of a particular set of planes are possible.
- Different cones are observed for different sets of d and θ for a particular order of n . The diffraction pattern is shown in figure.
- The diffraction pattern is in the form of arcs on either side of the exit and entry holes with their positions coinciding with hole.



The angle θ corresponding to a particular pair of arcs is related to the distance 'S' b/w the arcs as

$$4\theta = \frac{S}{R} \quad [\because \text{angle} = \frac{\text{arc}}{\text{radius}}]$$

R is the radius of the corner.

$$4\theta = \frac{S}{R} \left[\frac{180}{\pi} \right]$$

$$= \frac{57.296}{R} S$$

From above Expression ' θ ' can be calculated. Then the interplanar spacing for first-order diffraction is

$$d = \frac{\lambda}{2 \sin \theta}$$

knowing all parameters the crystal structure can be studied.

Merits:

- 1) Using filter, we get monochromatic x-rays
- 2) All crystallites are exposed to x-rays and diffraction takes place with all available planes.
- 3) Knowing all parameters, crystal structure can be studied completely.

UNIT-III

DIELECTRIC

&

MAGNETIC MATERIALS

Dielectrics and Magnetic Materials

Dielectric Materials :-

Introduction :-

- "Dielectrics are materials which contain no free electrons such that no current can flow through them. As a result, the electrical conductivity of a dielectric is poor and for an ideal dielectric it is zero".
- the ratio of the capacitance immersed in dielectric to that of same capacitor in Vacuum is called dielectric constant or permittivity it is denoted by κ or ϵ_0 .

$$\kappa = \frac{C}{C_0}$$

- The ratio of permittivity of medium to that of Vacuum is called dielectric constant.

$$\kappa = \frac{E}{E_0}$$

Dielectric polarization :-

"The process of dipole alignment in a dielectric in the presence of external electric field is called Dielectric polarization." The dielectric dipole moment induced per unit volume of the dielectric material is called dielectric polarization. It is represented by \vec{P} .

$$\text{polarization } P = \sigma P$$

Polarization may also be defined as the surface density of charge appearing at faces perpendicular to the direction of applied field. Unit of polarization is C/m^2 .

Dielectric polarizability :-

When an external electric field is applied to a dielectric material this material becomes polarized, which

means that acquires a dipole moment. This property of dielectrics is known as polarizability.

induced dipole momentum $P \propto E$

$$P = \alpha E$$

where ' α ' is called as dielectric polarizability.

Dielectric Susceptibility:-

"when a dielectric material is placed in an electric field, it becomes electrically polarized. For most materials, the polarization is proportional to electric field E such that

$$P \propto E$$

$$P = \epsilon_0 \chi E$$

where χ is called Dielectric Susceptibility

ϵ_0 is permittivity of free space.

Dielectric displacement vector (D):-

"the dielectric displacement vector D is generated by free charges". It is proportional to electric field 'E'.

$$D \propto E$$

$$D = \epsilon E$$

$$\therefore \epsilon = \kappa \epsilon_0$$

absolute permittivity of medium.

Relationship between the dielectric vectors:

The three electric vectors are D , E and P .

' q ' be the charge. According to Gauss's law the total electric flux due to this charge will be

$$\int \epsilon_0 E_0 \cdot dA = q$$

$$\epsilon_0 E_0 A = q$$

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

where E_0 - Electric field due to free charge 'q'.

when dielectrics is present, the induced charge on surface is ' q' ' then

$$\int \epsilon_0 E \cdot dA = q - q'$$

$$\epsilon_0 E A = q - q'$$

$$E = \frac{q - q'}{\epsilon_0 A} = \frac{q}{\epsilon_0 A} - \frac{q'}{\epsilon_0 A}$$

$$\frac{q}{\epsilon_0 A} = E + \frac{q'}{\epsilon_0 A}$$

$$\frac{q}{A} = \epsilon_0 E + \frac{q'}{A}$$

$$D = \epsilon_0 E + \sigma P$$

$$\begin{cases} \frac{q}{A} = \frac{q \epsilon_0}{A \epsilon_0} = \epsilon_0 \epsilon_r \\ = \epsilon_0 \epsilon_r E \\ = D \end{cases}$$

Types of polarization:-

there are four types of polarization.

- 1) Electronic polarization (or) Induced polarization
- 2) Ionic (or) atomic polarization
- 3) Orientation (or) dipolar polarization
- 4) Space-charge (or) interfacial polarization.

1) Electronic polarization:-

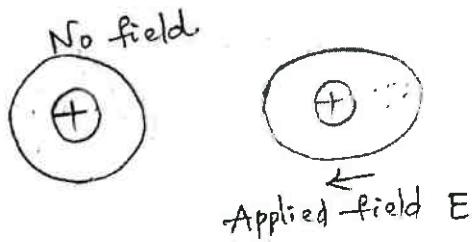
Electronic polarization occurs due to the displacement of positively charged nucleus and electron clouds of atoms in opposite direction by an external electric field. It creates a dipole moment in the dielectric. This is called electronic polarization. This polarization is independent of temperature.

The polarization is $P_e = N \alpha_e E$

where N - no. of molecules per unit volume

α_e - Electronic polarizability

$$[\epsilon_r = 1 + \chi \\ = 1 + \frac{\rho_e}{\epsilon_0 E} \\ = 1 + \frac{N \kappa_e E}{\epsilon_0 E}]$$



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No

From the figure, when the atom of the dielectric is placed in an electric field (E). Two types of forces are arise.

1) Lorentz force: force which separates electrons and positive nucleus due to applied field.

2) Coulomb force: An attractive force which is produced after separation.

$$\text{Lorentz force} = (\text{charge of electron}) \times (\text{Intensity of applied field})^2 \\ = (ze)E$$

$$\text{Coulomb force} = \frac{-ze^2 d}{4\pi\epsilon_0 R^3}$$

At equilibrium, Coulomb force and Lorentz force must be equal.

$$(ze)E = \frac{-ze^2 d}{4\pi\epsilon_0 R^3}$$

$$E = \frac{zed}{4\pi\epsilon_0 R^3} \Rightarrow d = \frac{4\pi\epsilon_0 R^3 E}{ze}$$

Now the electric charges $+ze$ and $-ze$ are displaced by a distance ' d ' under the influence of the field and form induced dipole moment which is

induced dipole moment (μ_e) = charge of electron \times displacement

$$\mu_e = ze \frac{4\pi\epsilon_0 R^3 E}{ze}$$

$$\boxed{\mu_e = 4\pi\epsilon_0 R^3 E}$$

$$\frac{\mu_e \propto E}{(\mu_e = \alpha E)}$$

\rightarrow Limit case when $\alpha = 1$ in polarization.

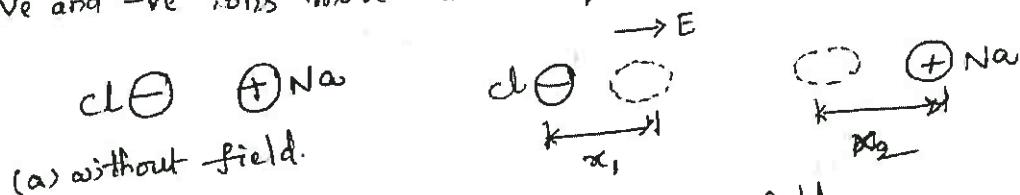
(3)

(2) Ionic polarization :-

"Ionic polarization occurs in ionic crystals. It is brought about by the elastic displacement of positive and negative ions from their equilibrium positions".

Ex: NaCl, it consists of Na^+ ions bound to Cl^- ions through ionic bond.

Let us assume that there is one cation and one anion representing each unit of the ionic crystal. When an electric field is applied, let x_1 and x_2 be the distance to which +ve and -ve ions move their equilibrium position.



The resultant displacement per unit volume due to ionic displacement is

$$\mu_i = \text{charge} \times \text{displacement}$$

$$\mu_i = e [x_1 + x_2] \rightarrow (1)$$

When field is applied restoring force produced is proportional to the displacement

$$\text{For +ve ion restoring force } F \propto x_1, F = \beta_1 x_1 \rightarrow (2)$$

$$\text{For -ve ion restoring force } F \propto x_2, F = \beta_2 x_2 \rightarrow (3)$$

β_1 and β_2 are restoring constants.

$$\beta_1 = m \omega_0^2 \rightarrow (4)$$

$$\beta_2 = M \omega_0^2 \rightarrow (5)$$

where m and M are mass of +ve and -ve ion.

$$\text{eq (2) & (5) can be written as } \frac{F}{x_1} = m \omega_0^2$$

$$F = m \omega_0^2 x_1 \rightarrow (6)$$

My form ③ q ⑦

$$F = M \omega_0^2 x_2 \rightarrow ⑦, F = eE \rightarrow ⑧$$

From equations ⑥, ⑦ and ⑧

$$m\omega_0^2 x_1 = eE$$

$$x_1 = \frac{eE}{m\omega_0^2} \rightarrow ⑨$$

$$x_2 = \frac{eE}{M\omega_0^2} \rightarrow ⑩$$

$$x_1 + x_2 = \frac{eE}{\omega_0^2} \left[\frac{1}{m} + \frac{1}{M} \right] \rightarrow ⑪$$

Substitute eq ⑪ in eq ⑫

$$\mu_i = \frac{e^2 E}{\omega_0^2} \left[\frac{1}{m} + \frac{1}{M} \right] \rightarrow ⑫$$

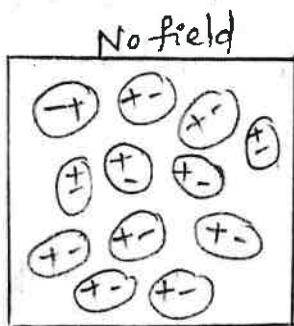
$$\mu_i = \alpha_i E$$

α_i is ionic polarizability

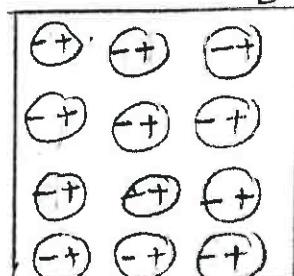
$$\boxed{\alpha_i = \frac{e^2}{\omega_0^2} \left[\frac{1}{m} + \frac{1}{M} \right]}$$

3) orientational polarization :-

The orientational polarization is due to existence of a permanent dipole moment in the dielectric medium. Polar molecules have permanent dipole even the absence of an electric field.



→ Applied electric field E



The orientational polarizability α_o is calculated to be

$$\boxed{\alpha_o = \frac{\mu^2}{3KT}}$$

(4)

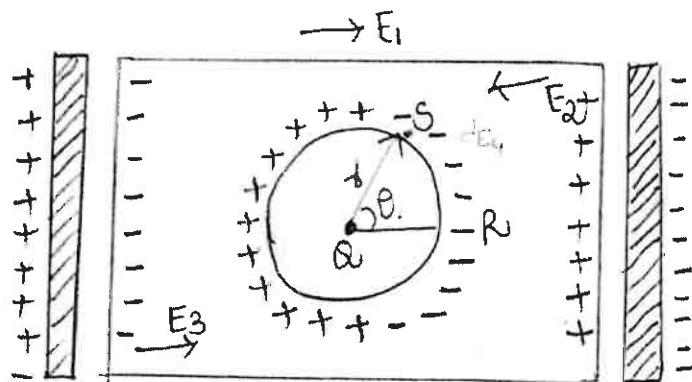
4) Space charge polarization :-

The space charge polarization occurs due to the diffraction of ions along the field direction giving rise to redistribution of charge in the dielectric. Without external field, the ions are orderly arranged. When the field is applied, the ions diffuse w.r.t. the directions of applied field, thus the polarization occurs, known as space charge polarization.

Lorentz Internal field :-

Consider a dielectric material and is subjected to external field of intensity E_1 . The charges are induced on the dielectric plates and the induced electric field intensity is taken as E_2 . Let E_3 be the field at the center of the material. E_4 be the induced field due to the charges on the spherical cavity. The total internal field of material

$$E_i = E_1 + E_2 + E_3 + E_4$$



$$E_1 = \frac{D}{\epsilon_0}$$

$$D = \epsilon_0 E + P$$

Substitute electric flux density D in E_1 .

$$E_1 = \frac{E\epsilon_0 + P}{\epsilon_0}$$

$$E_1 = E + \frac{P}{\epsilon_0} \rightarrow (1)$$

E_2 is the electric field intensity due to induced or polarized charges.

$$E_2 = \frac{-D}{\epsilon_0}$$

Here the charge is induced due to induced field. So, the electric flux density D changes to the electric polarization P

$$E_2 = -\frac{P}{\epsilon_0} \rightarrow (2)$$

For non polar dielectric material dipole moment is zero and hence the electric field intensity at the centre is zero due to symmetric structure.

$$E_3 = 0 \rightarrow (3)$$

In order to calculate E_4 on the surface of spherical cavity, the polarization should be calculated by resolving it into two components.

$$\text{polarization } p = \frac{q'}{A}$$

$$p \cos \theta = \frac{dq}{ds} \Rightarrow dq = p \cos \theta ds$$

$$\text{Electric field Intensity } E = \frac{1}{4\pi\epsilon_0} \frac{q}{r^2}$$

$$E_4 \cos \theta = \frac{1}{4\pi\epsilon_0} \times \frac{q \cos \theta}{r^2}$$

$$E_4 = \frac{1}{4\pi\epsilon_0} \propto \frac{dq \cos \theta}{r^2 \cos \theta}$$

$$E_4 = \frac{1}{4\pi\epsilon_0} \times \frac{p \cos \theta ds \times \cos \theta}{r^2} \rightarrow (4)$$

from figure $ds = 2\pi \times (RG) \times (\theta s)$

$$d\theta = \frac{RQ}{r}$$

$$RQ = r d\theta$$

The angle of the Sector $\theta = \frac{\text{length of the arc } (l)}{\text{radius of the circle } (r)}$

$$\sin\theta = \frac{QS}{OQ}$$

$$QS = r \sin\theta$$

$$ds = 2\pi (r d\theta) (r \sin\theta)$$

$$ds = 2\pi r^2 \sin\theta d\theta$$

equation (4) becomes

$$\begin{aligned} E_4 &= \frac{1}{4\pi\epsilon_0} \times \frac{p \cos\theta ds \times \cos\theta}{r^2} \\ &= \frac{1}{4\pi\epsilon_0} \times \frac{p \cos\theta}{r^2} \times 2\pi r^2 \sin\theta d\theta \cos\theta \end{aligned}$$

$$E_4 = \frac{p}{2\epsilon_0} \sin\theta \cos^2\theta d\theta$$

Integrate above equation with the limits 0 to π

$$\begin{aligned} E_4 &= \int_0^\pi \frac{p}{2\epsilon_0} \sin\theta \cos^2\theta d\theta \\ &= \frac{p}{2\epsilon_0} \int_0^\pi \sin\theta \cos^2\theta d\theta \end{aligned}$$

$$E_4 = \frac{p}{2\epsilon_0} \times \frac{2}{3}$$

$$E_4 = \boxed{\frac{p}{3\epsilon_0}}$$

Hence the local or Lorentz field is

$$E_i = E_1 + E_2 + E_3 + E_4$$

$$E_i = E + \frac{p}{\epsilon_0} - \frac{p}{\epsilon_0} + 0 + \frac{p}{3\epsilon_0}$$

$$E_i = E + \boxed{\frac{p}{3\epsilon_0}}$$

Columbus - Mossotti Equation :-

It gives the relation between the dielectric constant and the ionic polarizability of atoms in dielectric material. If there are N number of atoms, the dipole moment per unit volume which is called polarization is given by

$$P = N \alpha_e E_i$$

we know that Internal field

$$E_i = \left(E + \frac{P}{3\epsilon_0} \right)$$

from above equations

$$P = N \alpha_e \left[E + \frac{P}{3\epsilon_0} \right]$$

$$P = \frac{N \alpha_e}{3\epsilon_0} (3\epsilon_0 E + P)$$

$$\frac{N \alpha_e}{3\epsilon_0} = \frac{P}{3\epsilon_0 E + P} \rightarrow ①$$

we know polarization from the relation b/w polarization and dielectric constant.

$$P = E\epsilon_0 (\epsilon_r - 1) \rightarrow ②$$

From equations ① & ②

$$\frac{N \alpha_e}{3\epsilon_0} = \frac{E\epsilon_0 (\epsilon_r - 1)}{3E\epsilon_0 + E\epsilon_0 (\epsilon_r - 1)}$$

$$\frac{N \alpha_e}{3\epsilon_0} = \frac{E\epsilon_0 (\epsilon_r - 1)}{E\epsilon_0 (3 + \epsilon_r - 1)}$$

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

Complex dielectric constant :-

(6)

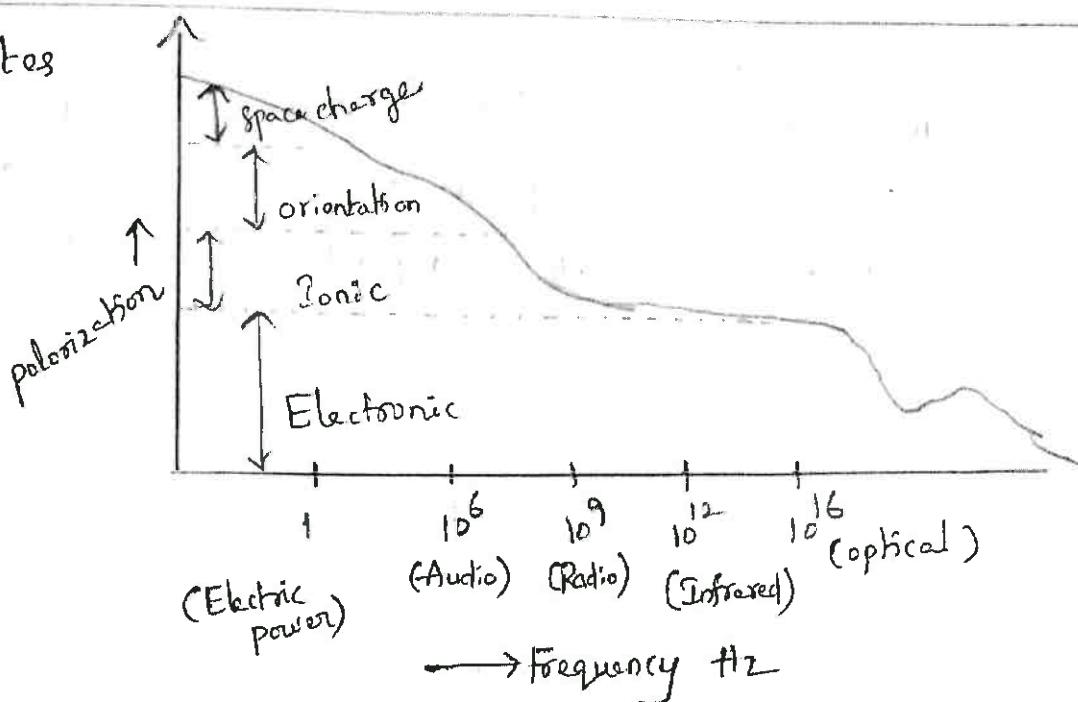
The Complex dielectric constant is a physical quantity that express the capability of materials to withstand external fields that have a strong dependence from the frequency.

Frequency dependence of polarization :-

when a dielectric is placed in an alternating electric field the dipoles attempt to maintain alignment with the field. This process a finite time that is different for each polarization mechanism. At relaxation frequency the dipoles will only just be able to reorient themselves in time with the applied field. At this frequency the dielectric loss and energy lost in the form of heat.

The dielectric loss at a maximum frequency of a given polarization mechanism. At frequency above relaxation frequency the dipoles will no longer be able to keep up with changes in the applied field and the contributes polarization mechanism becomes effectively frozen and longer

Contributes

Dielectric loss :-

The loss of energy involved in heating a dielectric material in an electric domain is called dielectric loss. These are generally based on the frequency and the dielectric material. These losses is considerately used in industries for drying lumber and various other fibrous materials.

Dielectric loss is measured using the loss of tangent which is also commonly referred to as $\tan \delta$. The higher the value of $\tan \delta$ is the more dielectric loss is likely to be.

Magnetic Materials

Introduction:

- Magnetic materials play an important role in industrial and scientific research fields.
- The magnetism of materials is mainly due to the interactions of uncompensated magnetic moments of the constituent atoms or molecules.
- Depending on the alignment of magnetic moments within the materials, they are classified as dia, para, ferro, antiferro and ferrimagnetic materials.
- The attracting properties exhibited by the magnet is known as magnetism.
- A magnet consists of north and south poles. Any two opposite poles separated by a finite distance constitute a magnetic dipole.

Magnetic dipole moment :- If 'm' is the magnetic pole strength and '2l' is the length of the magnet then its magnetic dipole moment or magnetic moment is given by the product of $m \times 2l$. It is denoted by μ_m

$$\mu_m = IA, A-m^2$$

Magnetic field :- the space surrounding the magnet up to which its attracting influence is felt is known as magnetic field.

Magnetic field strength (H) :- the magnetic field strength H is the force experienced by a unit north pole placed at a given point in a magnetic field. expressed in A/m

Magnetisation or Intensity of Magnetisation (M) :-

The magnetisation M is defined as the magnetic moment per unit volume. It is expressed in A/m.

Magnetic Susceptibility (χ) :- The magnetic susceptibility 'χ' is defined as the ratio of magnetisation produced in a sample to the magnetic field strength.

$$\chi = \frac{M}{H} \quad \chi \text{ has no units.}$$

Magnetic lines of forces :- The magnetic field is characterised by magnetic lines of forces.

Magnetic flux density (B) :- The number of magnetic lines of forces passing through a unit area of Cross Section of magnetic material.

$$B = \frac{\Phi}{A} \quad \text{wb/m}^2 \text{ or Tesla}$$

Magnetic permeability (μ) :-

It is a measure of the amount of magnetic lines of forces penetrating through a materials. It is defined as the ratio of the magnetic flux density in a material to the applied magnetic field intensity H. i.e.

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

Magnetic permeability of free Space (μ_0) :-

It is defined as the ratio of magnetic induction field strength B_0 of a free space to the applied magnetic field strength H. $\mu_0 = \frac{B_0}{H} \Rightarrow B_0 = \mu_0 H$

$$\mu_0 = 4\pi \times 10^{-7} \text{ H/Am}$$

Atomic origin of Magnetism :-

- Materials made up of atoms, these atoms consist of a nucleus surrounding which electrons are revolving in their orbits.
- These orbital motions of electron establish a magnetic field and hence we get orbital magnetic moment of the electrons.
- while revolving around the nucleus, the electrons spin about their own axes which results in a magnetic field and we get Spin magnetic momentum of the electrons.
- the nucleons in the nucleus also spin, resulting in magnetic field and we get Spin magnetic moment of the electrons.

Orbital magnetic moment of electron :-

- Consider an electron of mass 'm' charge 'e' revolving around the nucleus in a circular orbit of radius 'r' in anticlockwise direction. v be the linear velocity and ' ω ' is angular velocity.

$$\text{The linear frequency of revolving electron} = \frac{\omega}{2\pi}$$

$$\text{Time period of revolutions} = \frac{2\pi}{\omega}$$

Revolving electron establishing a current

$$I = \frac{\text{charge}}{\text{Time period}} = e \frac{\omega}{2\pi}$$

The current I establishes a magnetic field so that the upper surface of the orbit is act as South pole lower surface is north pole. The area of orbit

$$A = \pi r^2$$

Corresponding magnetic moment

$$\mu_{\text{orbital}} = IA$$

$$\mu_{\text{orbital}} = e \frac{\omega}{2\pi} \pi r^2$$

$$\mu_{\text{orbital}} = \frac{e\omega r^2}{2} \rightarrow ①$$

The angular momentum of the revolving electron is

Angular momentum = Linear momentum \times Radius.

$$= mv\tau \quad (\because v = \omega r)$$

$$= m\omega r^2$$

$$\mu_{\text{orbital}} = \frac{e\omega r^2}{2} = \left[\frac{e}{2m} \right] (mr\omega^2)$$

$= -\left(\frac{e}{m} \right)$ (orbital angular momentum)

The -ve sign indicates the orbital angular momentum and magnetic moment are in opposite directions then

$$\text{orbital gyromagnetic ratio } (\gamma) = \frac{\text{Magnetic moment}}{\text{orbital angular momentum}}$$

$$\boxed{\gamma = \frac{e}{2m}}$$

According to modern atomic theory

$$\text{Angular momentum} = l \left(\frac{h}{2\pi} \right)$$

$$\mu_{\text{orbital}} = -\frac{e}{2m} \left(\text{orbital angular momentum} \right)$$

$$= -\frac{e}{2m} \left(\frac{lh}{2\pi} \right)$$

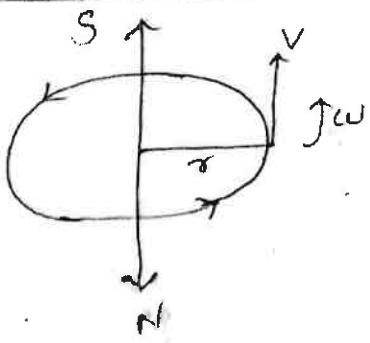
$$= -\left(\frac{elh}{4\pi m} \right)$$

$$\mu_{\text{orbital}} = -\mu_B l \quad \text{where } l = 1, 2, 3, \dots$$

$$\mu_{\text{orb}} = -\mu_B, -2\mu_B, -3\mu_B, \dots$$

where $\mu_B = \frac{eb}{4\pi m}$ is a fundamental unit of magnetic moment

Known as "Bohr magneton". Its value is $9.27 \times 10^{-24} \text{ Am}^2$



a) Spin magnetic moment of electron:-

→ the surrounding electron about its own axis establishes the magnetic field and we get magnetic moment known as spin magnetic moment which is

$$\beta_{\text{spin}} = \gamma \left(\frac{e}{2m}\right) S$$

where ' γ ' is the spin gyromagnetic ratio.

S is the spin angular momentum.

For an electron, $S = \frac{\hbar}{4\pi}$

$$\mu_{\text{spin}} = \gamma \left(\frac{e}{2m}\right) \left(\frac{\hbar}{4\pi}\right) = -9.4 \times 10^{-24} \text{ Am}^2$$

The value of μ_{spin} is nearly equal to the orbital magnetic moment.

b) Magnetic moment due to nuclear spin:-

In addition to electronic contribution, nuclear spin also contributes to magnetic moment of atoms.

The nuclear spin magnetic moment is

$$\mu_{\text{nuclear spin}} = \frac{e\hbar}{4\pi M_p}$$

where M_p represents the mass of proton.

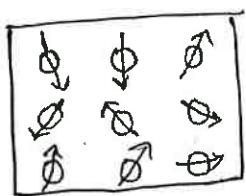
$$\mu_{\text{nuclear spin}} = 5.05 \times 10^{-27} \text{ Am}^2$$

Classification of magnetic materials:-

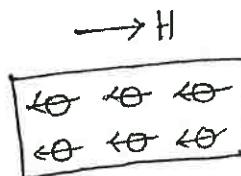
The magnetic materials have been classified into five types based on the influence of external field on them

1) Diamagnetic materials :-

- the atoms in the diamagnetic material will have random orientations of magnetic moments in the absence of a magnetic field.
- once the magnetic field is applied all the magnetic moments of its atoms will align in the opposite direction of the applied field.



fig(a): $H = 0$
Absence of magnetic field



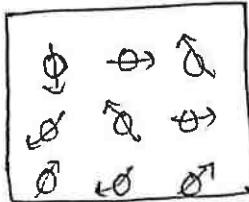
fig(b): presence of magnetic field

- there is an induced magnetism opposite to applied field.
- Diamagnetic materials repels the magnetic lines of force due to the external magnetic fields.
- Relative permeability $\mu_r < 1$
- The intensity of magnetisation ' μ ' is negative
- Susceptibility ' χ ' is negative
- ' χ ' is independent of temperature.
- Examples: organic materials

2) paramagnetic materials :-

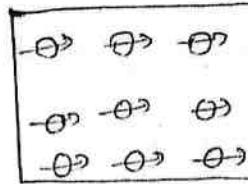
- In the absence of magnetic field all atoms in the paramagnetic material will have random magnetic moments. Net magnetic moment is zero.
- In the presence of magnetic field, all magnetic moments align into the direction of applied field and exhibit net magnetic moment along the field.

$$H = 0$$



fig(a) Absence of field

$$\rightarrow H$$



fig(b) presence of field.

→ There is an induced magnetism in the direction of field

→ It allows the magnetic lines of forces pass through it

$$\mu_s > 1$$

→ Intensity of magnetisation m is positive and moderate.

→ χ is low and +ve

$$\rightarrow \chi = \frac{C}{T}, \text{ where } C = \text{Curie Constant}$$

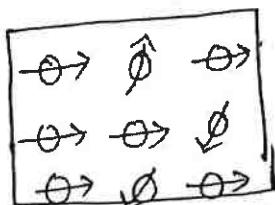
→ Examples : Alkali metals and transition metals.

3) Ferro magnetic materials:

→ In this the magnetic moments will be aligned parallel to each other to a maximum extent in absence of field due to spin magnetic moment of electron

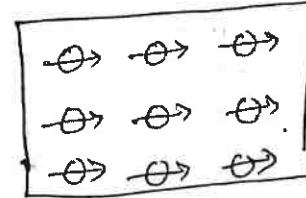
→ when a magnetic field (H) is applied, magnetic moments align in its field direction exhibiting large net magnetic moment along H .

$$H = 0$$



fig(a) Absence of field

$$\rightarrow H$$



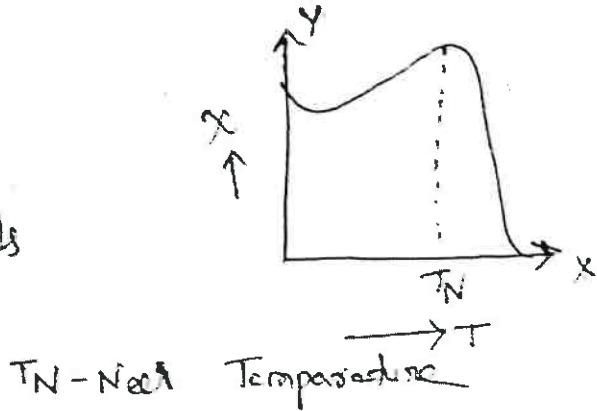
fig(b) presence of field

→ There is strong induced magnetism in the direction of the field

→ It allows a large number of magnetic lines of forces to pass through it.

- $\mu_b \gg 1$
- Intensity of magnetisation m is +ve and high
- α is high and positive
- $\alpha = \frac{C}{T \pm T_c}$, T_c = Curie Temperature
- Examples - Transition and rare earth metals.
- 4) Ferrimagnetic material :-
- The materials with anti parallel magnetic moments are known as antiferromagnetic materials.

- Net magnetic moments exist in the direction of applied magnetic field
- It allows magnetic lines of forces to pass through it.
- $\mu_b > 1$
- Intensity of magnetisation m is positive and modest.
- α is low and +ve
- $\alpha = \frac{C}{T \pm T_c}$
- Ex: Salts & transition metals

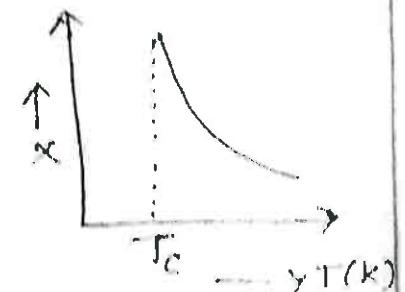


5) Ferri magnetic material :-

- The substances which consists of anti parallel magnetic moments of different magnitudes are known as ferri magnetic materials.



- Net large magnetic moment exists in the direction of applied magnetic field
- There is a large induced magnetism in the direction of field.
- It allows large number of lines of forces to pass through it
- $\mu_s \gg 1$.
- M is +ve and high
- χ is high and +ve, $\chi = \frac{C}{T - T_c}$
- Ex: ferrites.



Domain concept of ferromagnetism:

- The ferromagnetic materials have permanent magnetic properties which can be explained on the basis of domain theory.
- The domain theory was proposed by Weiss in 1907.
- According to this theory, ferromagnetic material consists of a large numbers of tiny regions, and each region gets spontaneously magnetised to saturation.
- The domains are free to move among these tiny regions.
- The spin magnetic moments of all the atoms in a domain are oriented in a particular direction.
- These domains are prone to the influence of external magnetic fields.
- Initially, the direction of those domains is such that they are randomly oriented and the magnetization due to these cancel out each other. So the resultant magnetism

of the material is zero in the absence of an external magnetic field. Thus, we get weak magnetization.

- In the presence of strong magnetic field, these domains get aligned in one particular direction and as a result strong magnetisation gets produced.
- In case of ferromagnetic materials, after all the domain gets aligned in one particular direction and the external field is removed, the domain boundaries do not change their orientation.
- thus ferromagnetic materials do not get demagnetized that's why they are used widely to make permanent magnets.

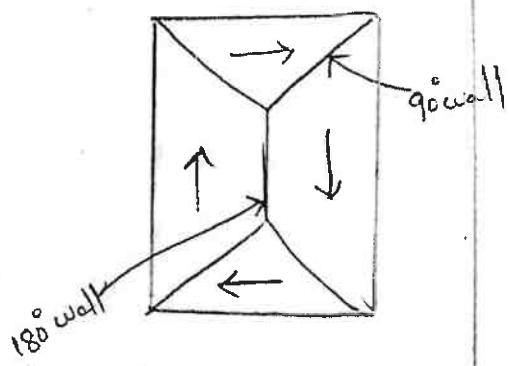
Domain walls:

Domain walls are the regions between domains where the direction of magnetization must change usually by either 180° or 90° .

- The width of domain walls is controlled by the balance of two energy contributions.

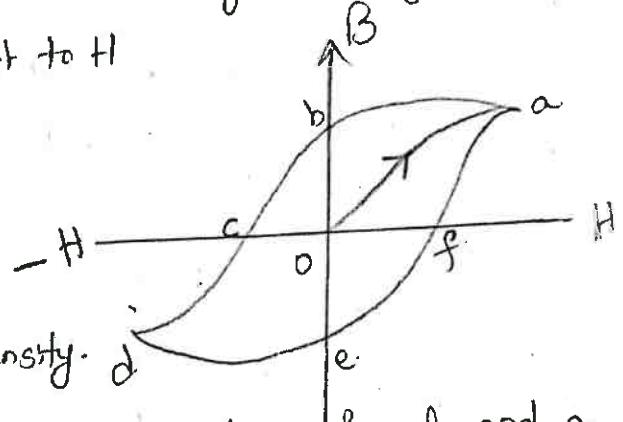
- * Exchange energy
- * Magneto-crystalline energy

- The most favourable domain walls are those which do not require an external demagnetising field.



Hysteresis :-

- when a specimen of ferromagnetic material is placed in a magnetic field, the specimen is magnetized by induction.
- the magnetic Intensity H is varied, the flux density B in ferromagnetic material does not vary linearly with H .
- the variation in B with respect to H is shown in figure.
- the point O represents initially unmagnetized Specimen with zero magnetic intensity. d
- H increases B also increases but not uniformly and a point such as 'a' is reached.
- H decreases, B also decreases but following a path ab.
- thus B lags behind H . when H becomes zero B still has a value equal to ob.
- this magnetic flux density remaining in the Specimen in the absence of any external field is called the "residual magnetization."
- the power of retaining this magnetism is called "retentivity" or "remanence".
- "the retentivity of a specimen is measure of magnetic flux remaining in the Specimen when the magnetizing force is removed.
- If H increased in the reverse direction, the value of B further decreases, still lagging behind H , and becomes zero



when H has a value equal to Oc .

→ This value of magnetic intensity is called as Coercive force or coercivity.

→ Thus Coercivity Hc is a measure of the magnetic intensity required to destroy the residual magnetization of the Specimen.

→ As H increases beyond Oc , the Specimen is increasingly magnetized in the opposite direction and a point 'd' is reached.

→ By taking H back from its negative max value through zero, to its original +ve max value, a similar curve defa is obtained

→ At points e and b where the Specimen is magnetized in the absence of any External magnetic intensities. It is said to be a 'permanent magnet'.

→ It is found that B always lags behind H . The lagging of B behind H is called hysteresis. The closed curve abcdefa which represents a cycle of magnetization is known as the 'hysteresis curve' of the Specimen.

Based on the area of hysteresis loop ferro magnetic materials they are classified in to Soft and hard magnetic materials.

Soft magnetic materials :-

→ the ferromagnetic materials which are easily magnetized and demagnetized are known as soft magnetic materials.

Properties :-

- 1) These shows a very steep hysteresis loop
- 2) The area of the loop is very small hence H
- 3) the hysteresis loss is also small
- 4) These materials show high values of Susceptibility and permeability.
- 5) Due to steep nature of loop it is clear that it has low value of Coercivity
- 6) It exhibits low and value of retentivity
- 7) They exhibit high resistivity
- 8) They require low magnetic field for magnetisation, Sensors, also used in microwave isolators.
- 9) These are used in transformers, motors, relays and sensors also used in microwave isolators.
- 10) Ex: Iron - Silicon alloys
Nickel - Iron alloys
Iron - Cobalt alloys

Hard magnetic materials :-

→ The ferromagnetic materials which are hard to magnetize and demagnetize are known as hard magnetic materials.

Properties :

- 1) They are very hard to magnetize and demagnetize
- 2) They require high magnetic field
- 3) their corresponding hysteresis loop is broad. H
- 4) Hysteresis loss is large due to large area of loop $-B$

-
- 5) They exhibit low values of Susceptibility and permeability
 - 6) They have high coercivity and retentivity
 - 7) They are used to make permanent magnets used in dc motors and measuring devices also used in Sensors in automobiles, motors etc
 - 8) Ex: Carbon Steels, tungsten steels, chromium sheets.

UNIT-IV

QUANTUM MECHANICS

QUANTUM MECHANICS AND FREE ELECTRON THEORY

Quantum Mechanics:-

- Classical mechanics successfully explained the motion of macroscopic particles but it fails to explain the motion of microscopic particles.
- But quantum mechanics successfully explained the motion of microscopic particles as well as some topics like photo electric effect, Compton effect and black body radiation.

Dual Nature of matter :-

- In 1924, DeBroglie extended dual nature of matter according to these hypothesis when particles are accelerated those will be spread like a wave particles with certain wavelength.
- The particles like electrons, protons, neutrons possess dual nature in every moving particle is associated with a wave.
- These particles are controlled by the waves, these waves are called matter waves (or) DeBroglie waves (or) pilot waves.
- According to Planck's quantum theory, the energy of photon

$$E = h\nu \rightarrow (1)$$

According to Einstein Energy mass relation is

$$E = mc^2 \rightarrow (2)$$

From eq (1) & (2) we get

$$h\nu = mc^2$$

$$h\left(\frac{c}{\lambda}\right) = mc^2 \quad (\because \gamma = \frac{c}{\lambda})$$

$$\lambda = \frac{h}{mc}$$

The wavelength of the electron associated with a particle of mass 'm' moving with velocity γ is

$$\lambda = \frac{h}{mv} \rightarrow (3)$$

When a charge of electron 'e' is accelerated by potential difference 'V' Volts then

$$\text{workdone} = ev$$

wavelength inversely of K.E :-

The Kinetic Energy of a moving particle

$$K.E = \frac{1}{2}(mv^2)$$

$$ev = \frac{1}{2}mv^2$$

$$mv^2 = 2ev$$

$$mv^2 = 2mv \Rightarrow mv = \sqrt{2mev}$$

Substitute in eq (3)

$$\lambda = \frac{h}{\sqrt{2mev}} \quad (\because E = ev) \quad [\because E = ev]$$

where $h = \text{Planck's constant} = 6.626 \times 10^{-34} \text{ Js}$

$m = \text{mass of } e = 9.1 \times 10^{-31} \text{ kg}$

$e = \text{charge of } e = 1.6 \times 10^{-19} \text{ C}$

$$\lambda = \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19}}} = \frac{12.27 \times 10^{-10}}{\sqrt{V}}$$

$$\boxed{\lambda = \frac{12.27}{\sqrt{V}} \text{ A}}$$

Matter wave properties :-

From the equation $\lambda = \frac{h}{mv}$, the following properties of matter waves are deduced.

- Light $v \rightarrow 0$, $\lambda \rightarrow \infty$ this implies matter wave can be associated only with moving particles.
- These waves can travel faster than the velocity of light.
- The wave number of an electron is given by
- The wave number of an electron is given by
- $$\frac{1}{\lambda} = \frac{\sqrt{2mev}}{n} m^{-1}$$

$$\text{The matter wave velocity } v = \frac{h}{2m\lambda}$$

Heisenberg's Uncertainty principle :-

- In 1927, Heisenberg proposed Uncertainty principle which is a direct consequence of dual nature of matter.
- It states that the product of Uncertainties of two variables is equal or greater than $\frac{h}{4\pi}$.
- Consider a pair of variables as a position and momentum we have

$$\Delta p \cdot \Delta x \geq \frac{h}{4\pi}$$

where Δp = Uncertainty in determining the momentum of the particle

Δx = Uncertainty in determining the position of the particle.

- Uncertainty in determining the energy and time are
- $$\Delta E \cdot \Delta t \geq \frac{h}{4\pi}$$

- If one measures the position accurately then the measurement of momentum becomes zero and momentum

accurately than the measurement of position becomes incorrect.

Significance of wave function :-

- 1) The wave function ψ has no direct physical meaning it is a complex quantity and represents the variation of matter wave if connects the particle nature and if associates wave nature satisfactorily.
- 2) $\psi^* \psi$ (or) $|\psi|^2$ is the probability density function.
 $\psi^* \psi dx dy dz$ gives the probability of finding the electron in the region of space b/w x and $x+dx$, y and $y+dy$ and z and dz
- 3) If the particle is present- $\int_{-\infty}^{\infty} |\psi|^2 dx dy dz = 1$

- 4) If there is no particle then $\int_{-\infty}^{\infty} |\psi|^2 dx dy dz = 0$
- 5) It can be considered as probability amplitude, since it is used to find the location of particle.

Schrodinger Time Independent wave equation:-
→ Schrodinger develops a wave equation for a moving particle by using de Broglie Concept of matter waves.

→ Let us consider a particle has mass 'm' moving velocity v is associated with a wave

→ Let ψ is a wave function of particles, then it can be represented as follows.

$$\psi = \psi_0 \sin(\omega t - kx) \rightarrow 0$$

where, ψ_0 : Amplitude ω : angular frequency

t = time, k = wave vector, x = displacement

(3)

Differentiating the equation (1) with respect to x in two times we get

$$\frac{d\psi}{dx} = \psi_0 \cos(\omega t - kx) (-k)$$

$$\frac{d^2\psi}{dx^2} = \psi_0 (-\sin(\omega t - kx)) (-k)(-k)$$

$$\frac{d^2\psi}{dx^2} = -k^2 \psi$$

$$\frac{d^2\psi}{dx^2} + k^2 \psi = 0 \quad [\because \text{Eq } 0]$$

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

$$\frac{d^2\psi}{dx^2} + \frac{4\pi^2}{\lambda^2} \psi = 0$$

Acc to deBroglie w.r.t $\lambda = \frac{h}{mv}$

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

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

Total Energy of the particle can be written as

Sum of PE and KE

$$E = PE + KE$$

$$E = V + \frac{1}{2} mv^2 \Rightarrow mv^2 = 2(E-V)$$

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

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

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

The above eq is Schrodinger's time dependent
above equation

Schrodinger Time dependent wave equation:-

For deriving time & dependent Schrodinger's one dimensional wave equation let us eliminate the total energy E from time-dependent wave equation.

The wave function given by

$$\psi(x,t) = A e^{i(kx - \omega t)}$$

Differentiating w.r.t 't' we get

$$\begin{aligned}\frac{\partial \psi}{\partial t} &= -i\omega A e^{i(kx - \omega t)} \\ &= -i(2\pi)^2 A e^{i(kx - \omega t)}\end{aligned}$$

$$\frac{\partial \psi}{\partial t} = -2\pi i \delta \psi$$

$$E = \hbar \delta, \quad \delta = \frac{E}{\hbar}$$

$$\frac{\partial \psi}{\partial t} = \frac{-2\pi i E}{\hbar} \psi, \quad \frac{1}{\hbar} = \frac{b}{2\pi}, \quad b = 2\pi \hbar$$

$$\frac{\partial \psi}{\partial t} = \frac{-2\pi i E}{2\pi \hbar} \psi$$

$$\frac{\partial \psi}{\partial t} = \frac{-iE}{\hbar} \psi = \frac{E \psi}{i\hbar}$$

$$E\psi = i\hbar \frac{\partial \psi}{\partial t}$$

$$\frac{\partial \psi}{\partial t} + \frac{2m}{\hbar^2} (E - V)\psi = 0$$

$$\text{we get, } \frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V)\psi = 0$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} \left(i\hbar \frac{\partial \psi}{\partial t} - V\psi \right) = 0$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{2m}{\hbar^2} \left(i\hbar \frac{\partial \psi}{\partial t} - V\psi \right)$$

$$\boxed{-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar \frac{\partial \psi}{\partial t}}$$

The above eq represents Schrodinger Time dependent wave equation

(21)

Particle in a one dimensional potential well:

Let us consider a particle moving inside a box along x-direction its moving between walls $x=0$ and $x=a$. The potential energy of the particle inside the box is constant and it is taken as zero and outside the box the potential energy is infinity.

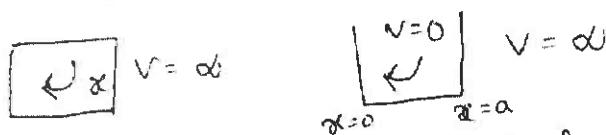


Fig: Square well potential.

The potential energy may be expressed as

$$V=0 ; 0 < x < a \quad [x \text{ is greater than zero } (x>0, x<a)]$$

$$V=\infty ; 0 \geq x \geq a \quad (x \leq 0, x \geq a)$$

The wave function ψ within the box b/w $x=0$ and $x=a$

The Schrödinger wave equation

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m(E-V)}{\hbar^2} \psi = 0$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2} \psi = 0 \quad [\because V=0]$$

$$\frac{\partial^2 \psi}{\partial x^2} + K^2 \psi = 0, \text{ where } K = \frac{\sqrt{2mE}}{\hbar} \rightarrow ①$$

The general solution of the above equation is

$$\psi(x) = A \sin Kx + B \cos Kx \rightarrow ②$$

By applying boundary conditions on equation ①

If $\psi=0$, at $x=0$

$$\Rightarrow B=0$$

If $\psi=0$ at $x=a$, $\Rightarrow A \sin k a = 0$ [$\because B=0$]

But $A \neq 0$, $\sin k a = 0$

$$\sin k a = \sin n\pi$$

$$ka = n\pi \Rightarrow k = \frac{n\pi}{a} \rightarrow (3)$$

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

Here 'n' can not be taken as zero

If $n=0$, then $k=0$, E_0 and $\psi=0$

The energy of the particle is not equal to zero at anywhere

Sub eq(3) in eq(2)

$$\psi_0(x) = A \sin\left(\frac{n\pi}{a}x\right) \rightarrow (4) (\because B=0)$$

From eq(1) & (3) we get

$$k^2 = \frac{n^2\pi^2}{a^2} \Rightarrow \frac{4\pi^2 2mE}{h^2} = \frac{n^2\pi^2}{a^2}$$

$$4\pi^2 \frac{2mE}{h^2} = \frac{n^2\pi^2}{a^2} \Rightarrow E_n = \frac{n^2 h^2}{8ma^2} \rightarrow (5)$$

$$E_1 = \frac{h^2}{8ma^2} \text{ where } n=1$$

$$E_2 = \frac{4h^2}{8ma^2}, \text{ when } n=2$$

$$E_3 = \frac{9h^2}{8ma^2} \neq 9E_1 \text{ when } n=3$$

For each value of 'n' there is an energy level and corresponding wave function is given by equation(4). The particle in the box have discrete energy level specified by eqn(5) each value of E_n is called Eigen Value and corresponding wave function is called Eigenfunction.

Free electron Theory:-

- the electron theory of metals aims to explain the structure and properties of metals through their electronic structure.
- the electron theory of metals explain the bonding in metals, ferromagnetism, electrical and thermal conductivity of metals, elasticity, cohesive and repulsive forces in metals.

Classical free electron theory :-

- the classical free electron theory of metals proposed by Drude and Lorentz in 1900 is based on following assumptions
- A solid metal composed of atoms and atoms have nucleus around which there are revolving electrons.
- The electrons in metals behaved as gas molecules in gas container.
- In the absence of electric field electrons in metals move in random directions makes collisions with +ve nucleus. Here all the collisions are elastic.
- the electrons in metals obeys the Maxwell Boltzmann distribution law.
- Due to random motion of electrons in metals velocity of electrons continuously changes but they are move with average velocity & Rms value which is given by

$$v_{\text{rms}} = \sqrt{\frac{3k_B T}{m}}, \quad k_B - \text{Boltzmann constant} \\ = 1.38 \times 10^{-23} \text{ J/K}$$

- Drift velocity :- Under the influence of electric field, the electrons in metals freely move opposite to the field direction and gain same velocity. Velocity is called drift velocity.
- Relaxation time (τ) :- The time taken by free electrons to reach their original position from disturbed position in the presence of electric field.
- Mean free path (λ) :- The mean distance travelled by electrons b/w any two successive collisions is known as mean free path. $\lambda = T_c v_{avg}$

→ Mean Collision time (T_c) :- The mean time taken by an electron to make any two successive collisions is known as mean collision time.

$$\tau = \frac{T_c}{(1 - \cos\theta)}$$

Drawbacks :-

- 1) This theory fails to explain electrical conductivity of Semiconductors and insulators.
- 2) CFT fails to explain contribution of electron to specific heat and magnetic Susceptibility.
- 3) This theory fails to explain optical properties of metals.
- 4) Fails to explain paramagnetic behaviour of electron.

Success :-

- 1) It is used to verify ohm's law.
- 2) It is used to explain electrical and thermal conductivities of metals.
- 3) It is used to derive Wiedemann-Franz law ($\frac{K}{\sigma} \propto T$).

Quantum free electron theory :-

- To overcome the drawbacks of classical free electron theory Sommerfeld proposed quantum free electron theory.
- based on electrostatic hypothesis of matter waves and Schrödinger wave equation.
- He treated electron as a quantum particle.
- The electrons obey's the principles of quantum theory.
- According to Sommerfeld only Fermi level electrons are responsible for all types of physical properties in metals.

Electrical Conductivity :-

The relation between momentum 'p' and wave velocity 'k' is

$$p = \hbar k$$

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

$$mv = \hbar k$$

$$p = mv$$

$$v = \frac{\hbar}{m} k \rightarrow ①$$

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

Differentiating the above equation w.r.t 't'

$$\frac{dv}{dt} = \frac{\hbar}{m} \frac{dk}{dt}$$

$$a = \frac{\hbar}{m} \cdot \frac{dk}{dt} \rightarrow ②$$

According to Lorentz force $F = eE$

According to Newton's Second Law $F = ma$

$$ma = eE$$

from eqns ② & ③

$$a = \frac{eE}{m} \rightarrow ③$$

$$\frac{\hbar}{m} \frac{dk}{dt} = \frac{eE}{m}$$

$$-\frac{h}{k} \frac{dK}{dt} = eE$$

$$dK = -\frac{eE}{h} dt \rightarrow (4)$$

By Integrating the above eq we get

$$\Rightarrow K(t) - K(0) = -\frac{eE}{h} t$$

$$\Rightarrow \Delta K = -\frac{eE}{h} T_F \rightarrow (5)$$

- the Current density $J = neV_d$

$$J = ne \Delta V \rightarrow (6)$$

$$\text{from eq(1), } V = \frac{h}{m} K$$

$$\Rightarrow \Delta V = \frac{h}{m^*} \Delta K \rightarrow (7)$$

equations (7) in (6)

$$\Rightarrow J = ne \frac{h}{m^*} \Delta K \rightarrow (8)$$

From equations (8) & (5)

$$J = ne \frac{h}{m^*} \cdot \frac{eE}{h} T_F$$

$$J = \frac{ne^2 T}{m^*} E \rightarrow (9)$$

$$\text{But } J = \sigma E \rightarrow (10)$$

$$\text{From eqns (9) & (10)} \Rightarrow \sigma E = \frac{ne^2 T}{m^*} E$$

Merits:-

$$\sigma = \frac{ne^2 T_F}{m^*}$$

1) It successfully explains the electrical and thermal conductivities of metals

2) phenomena of thermionic emission can be explained by this theory

3) Temperature dependence of conductivity of metals can be explained by this theory

- ④ It explains the specific heat of metals
 ⑤ It explains the magnetic susceptibility of metals.

Demerits:-

- ① It is unable to explain the metallic properties exhibited by only certain crystals.
- ② It is unable to explain why the atomic arrays in metallic crystals should prefer certain structures only.

Fermi-Dirac distribution:-

→ Fermi-Dirac distribution function can be applied on the system of particles of which obeys Pauli's exclusion principle with spin of $\pm \frac{1}{2}$ such as electrons.

→ The particles which obeys F-D statistics are called Fermions.

→ Electrons and holes are fermions.

→ Fermi-Dirac distribution function represents the probability of occupation of electrons in any given energy state and it is given by

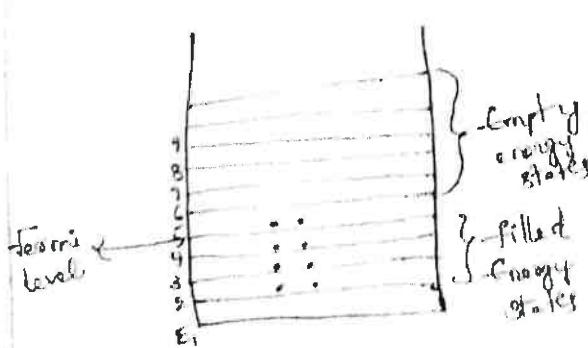
$$F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)}$$

where $F(E)$ = Fermi-Dirac distribution function

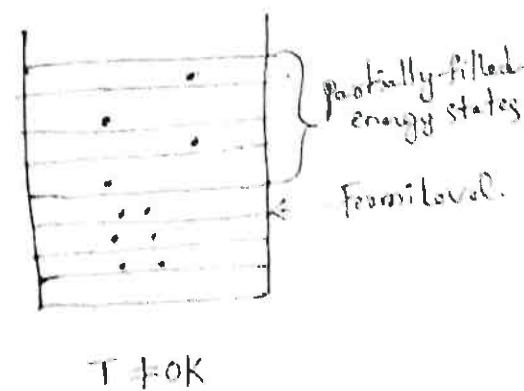
E_F = Fermi energy

k_B = Boltzmann Constant

T = absolute temperature.



$T = 0K$



- Acc to quantum theory electrons occupies in any energy level through governance by pauli exclusion principle. i.e., not more than two electrons can occupy the same energy level.
- At absolute zero Temp ($T=0K$) first two electrons occupy in ground state and two in each state of next higher energy levels.
- So the highest energy level occupied by electrons at $T=0K$ is known as Fermi Energy Level.
- The reference energy level which represents both filled states and empty energy states is also called fermi energy level.
- The energy of fermi level is called fermi energy.

$$E_F = 3.65 \times 10^{-19} \times n^{2/3} \text{ eV}$$

- If the external energy supplies to the metal then electrons are excited from lower energy level to highest energy level.
- Below Fermi Energy level all are filled and above the level are partially filled.

Effect of temperature on Fermi - Dirac distribution :-

Fermi - Dirac distribution function is given by

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)}$$

Case (1)
At $T = 0K$, $E < E_F$ then,

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{0}\right)}$$

$$f(E) = \frac{1}{1 + e^{-\infty}}$$

$$f(E) = \frac{1}{1+0} = 1 = 100\%$$

i.e., Below the Fermi Level there is a 100% chance to be filled with electrons at $T = 0K$.

Case (2): At $T = 0K$; $E > E_F$ then

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

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

at $T = 0K$ above the Fermi level all the energy states are empty. There is 0% chance to be filled with electrons above Fermi level.

Case (3): At $T > 0K$, if $E = E_F$ then

$$F(E) = \frac{1}{1 + e^0} = \frac{1}{1+1} = \frac{1}{2} = F(E)$$

At this case there is 50% chance to be filled with electrons above or below the Fermi level.

Density of Energy States:-

"Density of states defined as the number of quantum states that we have between certain interval of energy level E and $E + dE$. i.e., $\frac{dN}{dE}$ ".

→ Electrons can occupy in certain Energy level corresponding that energy level it has two quantum states one is $+\frac{1}{2}$ and $-\frac{1}{2}$.

→ The number of states that can be occupied by electron up to a certain energy is given by

$$N(E) = \frac{V}{3\pi^2} \left(\frac{2mE}{\hbar^2} \right)^{3/2} \quad \text{--- (i)}$$

where $V = \text{Volume}$

$m = \text{mass of electron}$.

Density of States

$$\frac{dN}{dE} = \frac{V}{3\pi^2} \left(\frac{8m}{\hbar^2} \right)^{3/2} \frac{d}{dE} (E)^{3/2}$$

$$= \frac{3}{2} \frac{V}{3\pi^2} \left(\frac{8m}{\hbar^2} \right)^{3/2} E^{1/2}$$

$$\boxed{\frac{dN}{dE} = \frac{V}{3\pi^2} \left(\frac{8m}{\hbar^2} \right)^{3/2} E^{1/2}}$$

Fermi Energy :-

It is defined as the energy difference between the highest and lowest occupied single-particle states in a quantum system of non-interacting fermions at absolute zero temperature.

- The value of the Fermi level at absolute zero temperature is known as the Fermi energy.
- It is also the maximum kinetic energy an electron can attain at 0K. Fermi energy is constant for each solid.
- Fermi level and Fermi energy both are equal at absolute zero temperature. There are different at other temperature.

Applications :-

- (1) It is used in Semiconductors and insulators.
- (2) It is used to describe insulators, metals and Semiconductors.
- (3) It is applied in determining the electrical and thermal characteristics of the solids.
- (4) It is also important in nuclear physics to understand the stability of nuclei (stars).

UNIT-V

SEMICONDUCTORS

SEMICONDUCTORS

- The properties of materials lies between conductors and insulators are known as Semiconductors.
- The conductivity and resistivity of Semiconductors varies between conductors and insulators.
- These are widely used in Solid-state electronic devices.

Formation of Energy bands:-

- When two isolated atoms are brought together, the electrons in the outer orbit of one of the atoms experience a force from the atom near to it.
- Because of this process the energies of the electrons change.
- This means that the energy levels will not be the same.
- The value of electrons is changed to a higher or lower energy level than the original energy level of the electron.
- Energy levels of the electrons in the same orbit are different every time.
- When you group these varied energy levels the energy band is formed.
- Energy levels of electrons at inner orbits are not affected by the atoms which are nearer to them.

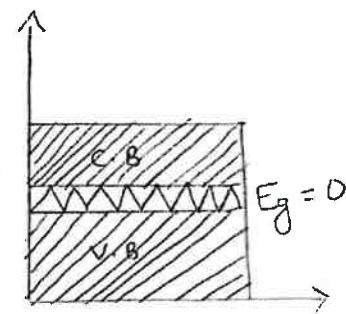
Classification of crystalline Solids :-

Based on the band theory and energy gap between Conduction band and Valence band Solids are classified into 3 types.

- Conductors
- Semiconductors
- Insulators.

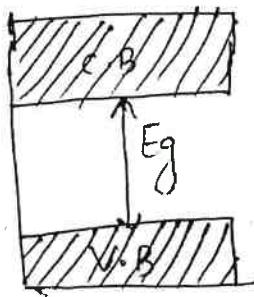
1) Conductors :-

- In conductors Conduction band and valence band both are overlapped to each other.
- Due to overlapping of bands no band gap is exist. i.e., $E_g = 0$
- Due to overlapping of electrons can easily move from conduction band to valence band and valence band to conduction band.
- Due to conduction of more electrons electrical conductivity is more in conductors.
- In conductors as temperature increases conductivity decreases.



2) Semiconductors :-

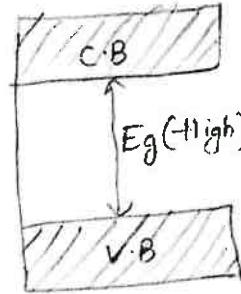
- The Energy gap b/w valence band and conduction band is very small, and it is about 0.5 ev to 3.6 ev.
- Energy band gap is less.
- As the temperature increases the bands in valence band breaks up and electrons move from V.B. to C.B. and creates holes.
- Hence the conduction band is partially filled and valence band is partially empty.
- In Semiconductors electrons and holes are responsible for electrical conductivity.
- In Semiconductors $\rho \propto \frac{1}{T}$
- The Semiconductor behaves as insulators at $T = 0K$
- These are acts as conductors at $T \neq 0K$
- Ex: Ge, Si, Graph, GaAs etc



(2)

(3) Insulators :-

- In insulators conduction band and valence band separated by large gap.
- Band gap is very high is about $E_g = 10 \text{ eV}$
- Even in the presence of electric field electrons cannot move from V.B to C.B since electrons are strongly bounded with nucleus.
- In insulators electrical conductivity is zero.
- No charge carriers are available for conduction in insulators.
- Ex: Glass, plastic, rubber ... etc



Intrinsic Semiconductors:-

- pure form of Semiconductors are known as Intrinsic Semiconductors. Ex: Ge and Si.
- Each Semiconductor has four valence electrons in their outermost orbit. Each of these atoms makes four covalent bonds with the surrounding crystal.
- At all all valence electrons are strongly bound to their atoms and are actively participating in the covalent bond and it acts as insulators.
- The energy band structure consists of conduction and valence bands separated by a forbidden energy gap.

$$E_g = 1.2 \text{ eV} \text{ (for Si)} \quad E_c \rightarrow \text{Conduction band}$$

$$E_g = 0.07 \text{ eV} \text{ (for Ge)} \quad E_v \rightarrow \text{Valence band}$$

$$E_g \rightarrow \text{Energy gap}$$

→ At $T=0K$, all valence electrons are bound to their atoms those electrons occupy all energy levels of the valence band while the conduction band is empty.

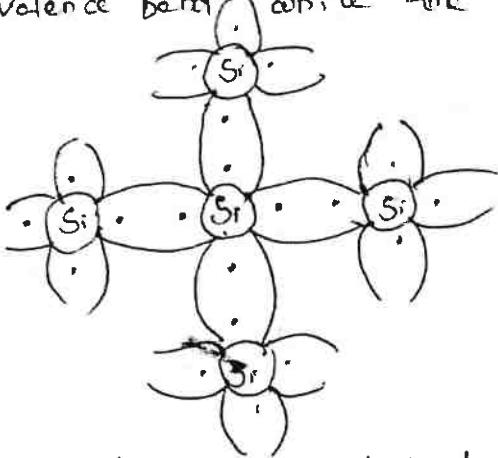


Fig:- At $T=0K$ Bond structure

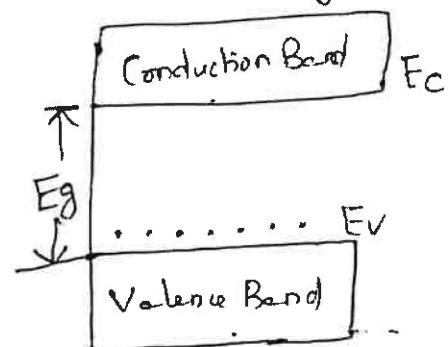
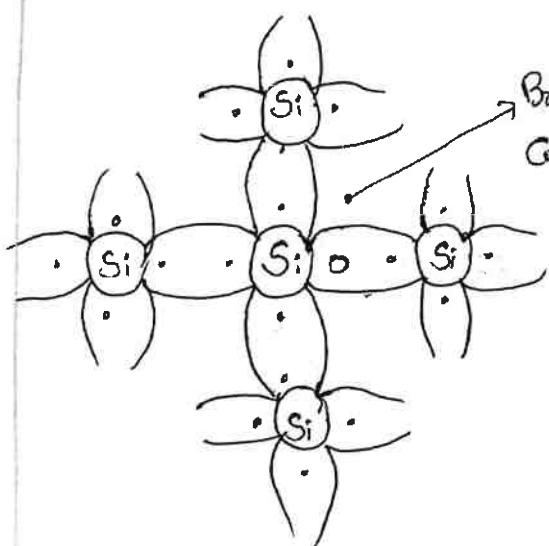
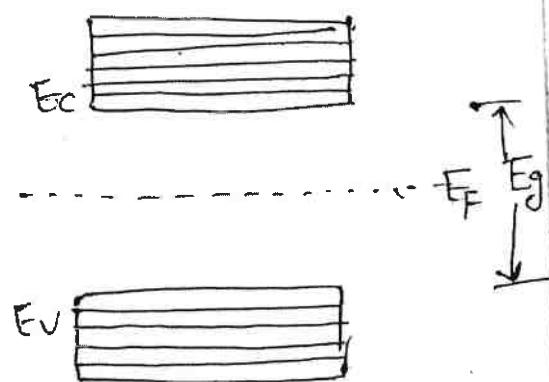


fig: Band structure at $0K$.

- At $T > 0K$, the valence electrons acquire sufficient amount of thermal energy. As a result breakage of covalent bonds takes place releasing free electrons.
- These free electrons create vacancy is known as hole.
- These free electrons excited to the Conduction band. Create holes in Valence bands.



Breakage of
Covalent bond



at $T > 0K$

(3)

Density of charge carriers :-

- In an intrinsic semiconductor there will be - temperature equal to number of holes generated.
- Let 'n' be the number of electrons generated will be - therefore equal to number of holes generated.
- Electron concentration in conductors band and 'p' or electron concentration of holes from unit volume or hole concentration be the number of holes from unit volume or hole concentration in valence band.

$$\text{For Intrinsic S.C. } n = p = n_i$$

$n_i \rightarrow$ Intrinsic Concentration

Electron Concentration is

$$n = N_c e^{-(E_C - E_F)/k_B T}$$

$$\text{Hole Concentration is} \\ p = N_V e^{(-E_F - E_V)/k_B T}$$

$$p = n = n_i$$

where N_c and N_V are known as pseudo constants.

$$n_i^2 = n p \\ = N_c N_V e^{-(E_C - E_F)/k_B T} \times N_V e^{-(E_F - E_V)/k_B T} \\ = N_c N_V e^{-(E_C - E_V)/k_B T}$$

$$E_C - E_V = E_g \\ \therefore n_i^2 = N_c N_V e^{-\frac{E_g}{k_B T}} \\ n_i = (N_c N_V)^{\frac{1}{2}} \cdot e^{-\frac{E_g}{2k_B T}}$$

From the above relation it is clear that

- Intrinsic carrier concentration is independent of the Fermi level.
- It is a function of the band gap E_g .
- It depends on the Temperature.

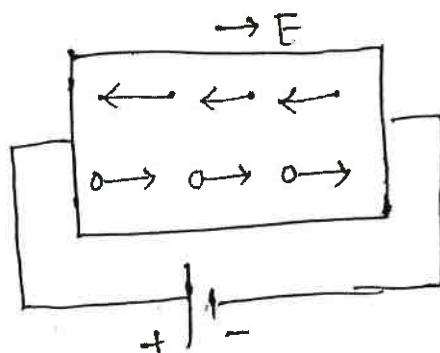
Electrical Conductivity :-

- Consider a semiconductor to which a potential difference 'V' is applied. It establishes an electric field E and the charge carriers are forced to drift in the respective directions to constitute an electric current I .
- The drift velocity acquired by the charge carrier is given by

$$V_d = \mu E$$

' μ ' is mobility of charge carriers

'n' concentration of electrons.



$$\text{Current density } J_n = neV_d$$

$$= ne\mu_0 E$$

μ_0 mobility of the electron.

$$\text{Current density due to holes is } J_p = pe\mu_p E$$

Total current density $J = J_n + J_p$

$$J_n = n e \mu_n e^{-\mu_n k_B T}$$

$$J_p = (n_{un} + n_{sp}) e \mu_p e^{-\mu_p k_B T}$$

Current density $J = \sigma E$

$$\text{Conductivity } \sigma = \frac{J}{E}$$

$$\sigma = (n_{un} + n_{sp}) e$$

For Intrinsic Semiconductors $n = p = n_i$:

$$\sigma = n_i e^{(\mu_n + \mu_p)}$$

$$n_i = (N_c N_v)^{\frac{1}{2}} e^{-\frac{E_g}{2k_B T}}$$

$$\sigma = (N_c N_v)^{\frac{1}{2}} e^{(\mu_n + \mu_p)} \cdot e^{-\frac{E_g}{2k_B T}}$$

$$\boxed{\sigma = A e^{-\frac{E_g}{2k_B T}}}$$

$$A = (N_c N_v)^{\frac{1}{2}} e^{(\mu_n + \mu_p)} = \text{constant.}$$

Fermi level :-

→ The Fermi Energy level indicates the probability of occupation of energy levels in conduction and valence bands.

→ In intrinsic Semiconductors the probability of occupation of energy level in conduction and valence bands are equal. Due to hole and electron concentrations are equal, thus, the Fermi level lies in the middle of the energy gap. Eg:-

For intrinsic Semiconductor $n = p$

$$\frac{N_c e^{-C(E_c - E_F)/k_B T}}{N_v e^{-(E_c - E_F)/k_B T}} = N_v e^{-(E_F - E_v)/k_B T}$$

$$\frac{N_v}{N_c} = e^{-\frac{(E_F - E_v)/k_B T}{e^{\left[2(E_F - (E_c + E_v))\right]/k_B T}}}$$

$$\log \left(\frac{N_v}{N_c} \right) = \frac{2(E_F - (E_c + E_v))}{k_B T}$$

$$E_F = \frac{E_c + E_v}{2} + \frac{1}{2} k_B T \log \left(\frac{N_v}{N_c} \right)$$

when $N_v = N_c$, then $E_F = \frac{E_c + E_v}{2}$

thus Fermi level is the intrinsic semiconductor lying in the middle of the energy gap and so is independent of exposure.

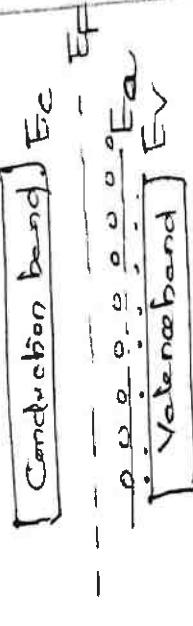
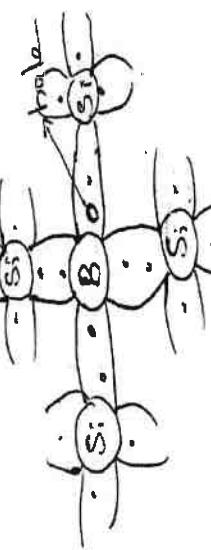
Extrinsic Semiconductors :-
 \rightarrow when impurities are added to an intrinsic Semiconductor

\rightarrow Depending upon the type of impurity added, extrinsic Semiconductors are of two types.

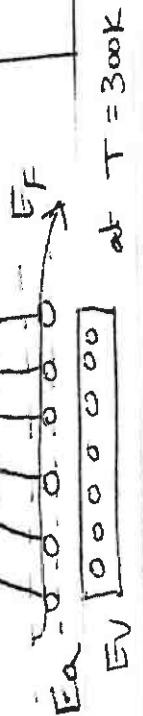
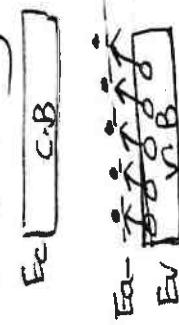
- P-type Semiconductors
- N-type Semiconductors

P-type Semiconductors

- carbon a small amount of silicon at room purity such as boron is added to a pure Si crystal.
- In boron some of Si atoms position in between silicon atoms i.e. between covalent bonds results into neighbouring Si atoms or one bond is left over with the deficiency of an electron i.e. on a hole is created at this position.
- Boron is in a position to accept an electron, it acts as an acceptor. Correspondingly we have an acceptor level (E_A) near the valence band.



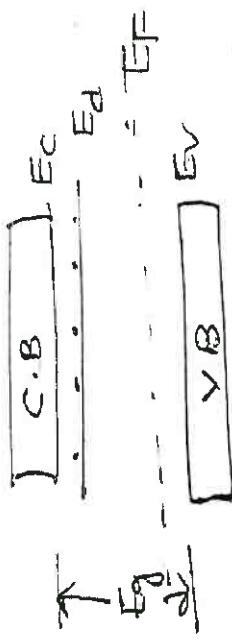
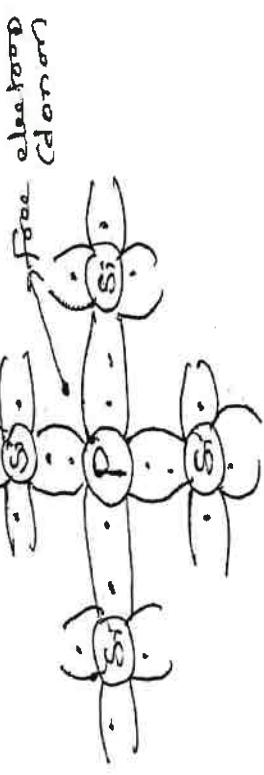
- when the temperature is raised the electrons from the valence band try to occupy the acceptor level and it gets ionized.
- If the temperature is further increased than due to breakage of covalent bonds electrons emanates into the conduction band leaving more holes in the valence band.
- As a result holes becomes majority carriers and electrons becomes minority carriers i.e., $P > n$ is shown in figure.



at $T > 0K$

2) Type Semiconductors

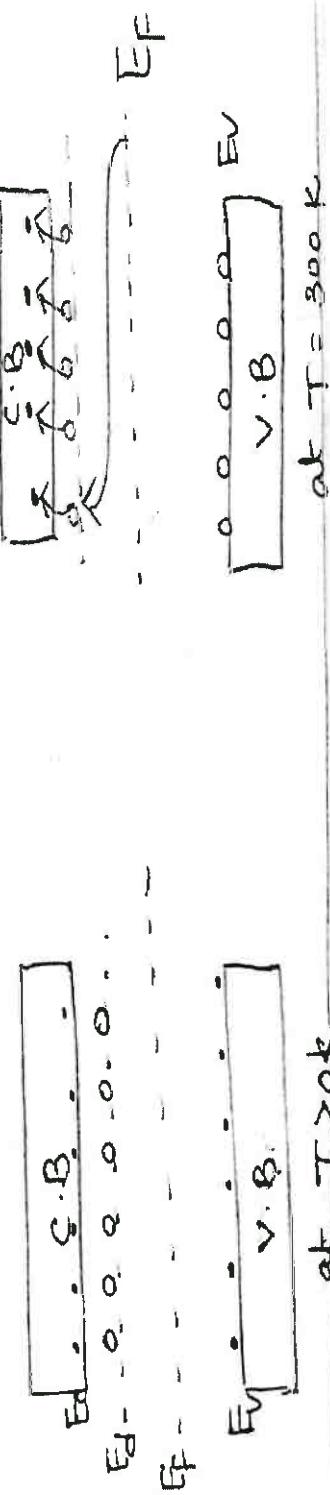
- when a small amount of p-doped impurity such as P^+ is added to the intrinsic semiconductor, then the impurity atoms occupy one of the positions of Si atom.
- Four of the valence electrons of phosphorous form covalent bonds with Si atoms.
- the first electron is left. This free electron is called as donor which is going to donate an electron at high temperature.
- Little that all atoms occupy almost energy levels which are placed near the conduction band.



Band structure at $T = 0K$.

→ when the temperature increased, then the band electrons becomes free electrons and enters into the conduction band.

→ As a result donates levels get ionized. At still higher temperature breakage of covalent bond releases an electron from valence band to conduction band leaving holes in the valence band.



(6)

As a result concentration of electrons increases in the conduction band rather than holes. Hence electrons become majority charge carriers and holes become minority charge carriers.

→ the Fermi level shifted towards conduction band in n-type Semiconductor

Density of charge carriers :-

- In an n-type Semiconductor, the total number of electrons in the conduction band would be equal to the sum of electrons originated from donor atoms and electrons excited from the valence band.
 - Electrons coming from donor levels behind positive donor ions while electrons excited from valence band leave behind holes.
 - These charges have only created any additional charges between positive and negative charges.
- So, that equality is maintained.

→ the charge neutrality condition applied to the n-type Semiconductor simplified that the total negative charge carried in the crystal is equal to the total positive charge carried in the crystal.

$N_D - \text{Donor Concentration}$

$$n_D = N_D + P_N$$

→ the charge neutrality for p-type Semiconductor

$$P_P = N_A + n_N$$

In n-type Semiconductors, $n_D > P_N$; $n_D \approx N_D$ where n_D , P_N are the electron & hole concentrations.

For n-type Semiconductors,

For p-type, $P_P > n_N$; $P_P \approx N_A$ where P_P and n_N are the concentrations of holes in p-type Semiconductor.

Drift Current

- Under the influence of an external electric field, the charge carriers move in a particular direction constituting electric current. Current due to moving electrons is known as Drift.
- Let us consider electrons in a semiconductor under the electric field 'E'. They are drifted with a drift velocity v_d . Then the current density is:

$$\text{J} = nev_d$$

then Conductivity $\sigma = \frac{\text{J}}{E} = \frac{nev_d}{E}$

Drift velocity $v_d = \mu n E$
where mobility of electrons
 $\mu = ne \mu_0 E$

$$\sigma = \frac{1}{\rho} = \frac{1}{ne \mu_0}$$

Drift current density due to electrons
 $J_{n \text{ drift}} = nev_d E$

Drift current density due to holes
 $J_{p \text{ drift}} = pev_d E$

$$\begin{aligned}\text{Total current density } J &= J_{n \text{ drift}} + J_{p \text{ drift}} \\ &= nev_d E + pev_d E \\ &= eE (n + p)\end{aligned}$$

$$\sigma (\text{drift}) = \frac{J}{E}$$

$$\sigma_{\text{drift}} = e n \mu_n + p e \mu_p$$

for intrinsic $n = p = n_i$

$$\sigma_i(\text{drift}) = n_i e (\mu_n + \mu_p)$$

$$\text{Drift current } I_{\text{drift}} = e E_A (n \mu_n + p \mu_p)$$

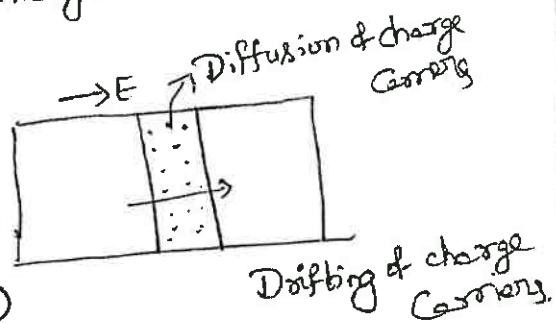
Diffusion Current :-

"Due to non-uniform carriers concentration in a semiconductor, the charge carriers move from a region of higher concentration to a region of lower concentration. This process is known as diffusion of charge carriers".

Let Δn be the excess electron concentration. Then according to Fick's law, the rate of diffusion of electrons

$$\propto -\frac{\partial}{\partial x}(\Delta n)$$

$$= -D_n \frac{d}{dx}(\Delta n)$$



where D_n is the diffusion coefficient of electrons.

The diffusion current density due to electrons is given by

$$J_n(\text{drift}) = -e \left[-D_n \frac{\partial}{\partial x}(\Delta n) \right]$$

$$= e D_n \frac{\partial}{\partial x}(\Delta n)$$

The diffusion current density due to holes

$$J_p(\text{drift}) = +e \left[-D_p \frac{\partial}{\partial x}(\Delta p) \right]$$

$$= -e D_p \frac{\partial}{\partial x}(\Delta p)$$

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

$$J = e D_n \frac{\partial}{\partial x}(\Delta n) - e D_p \frac{\partial}{\partial x}(\Delta p)$$

Diffusion Current

$$I = A e \left[D_n \frac{\partial}{\partial x}(\Delta n) - D_p \frac{\partial}{\partial x}(\Delta p) \right]$$

Einstein's Relation (or) Einstein Equation :-

"The relation between mobility ' μ ' and diffusion Co-efficient 'D' of charge carriers in a Semiconductor is known as Einstein relation".

At equilibrium the drift and diffusion current density due to excess electrons are equal.

$$\therefore \Delta n \neq \mu_n = e D_n \frac{\partial}{\partial x} (\Delta n)$$

-the force on excess electrons restoring equilibrium is equal to the product of excess charge and electric field.

$$F = (\Delta n) e E$$

$$F = e \cdot \frac{D_n}{\mu_n} \frac{\partial}{\partial x} (\Delta n) \rightarrow ①$$

From kinetic theory of gases the force on gas molecules is given by

$$F = k_B T \frac{\partial}{\partial x} (D_n) \rightarrow ②$$

From equations ① & ②

$$\frac{e D_n}{\mu_n} = k_B T$$

$$\frac{D_n}{\mu_n} = \frac{k_B T}{e}$$

By For holes we get

$$\frac{D_p}{\mu_p} = \frac{k_B T}{e}$$

$$\therefore \boxed{\frac{D_n}{\mu_n} = \frac{D_p}{\mu_p} = \frac{k_B T}{e}}$$

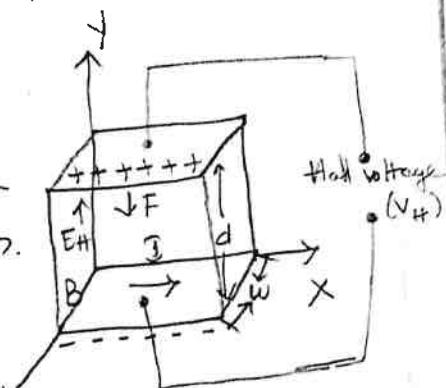
The above relation is known as Einstein's relation.

Hall Effect :-

When a current carrying semiconductor is subjected to a transverse magnetic field, then a potential difference or electric field is developed across the semiconductor or conductor in a direction perpendicular to both current and the applied magnetic field. This phenomenon is known as "Hall Effect".

Working :-

- Consider a semiconductor slab of thickness 'd' and width 'w' in which a current I is flowing along x-direction.
- Magnetic field B along y-direction. The charge carriers inside the semiconductor experiences a force due to the applied magnetic field.
- As a result electrons will be accumulated at the bottom surface of the semiconductor due to the magnetic force on them along y-direction.
- Thus negative charge build up at the bottom surface and the corresponding positive charge on upper surface of the semiconductor.
- Thus a potential difference and electric field is established across the surfaces.
- This developed electric field along z-direction exerts a force on the electrons to prevent further accumulation at the bottom surface.
- At steady state both the forces balances each other and the electrons can move freely to constitute an electric current.



E_H be the Hall electric field on the semiconductor.
 - the force on the electrons due to E_H is eE_H
 - the force on electrons due to magnetic field B is BeV
 at steady state $eE_H = BeV$

$$E_H = BV$$

Hall electric field $E_H = \frac{V_H}{d}$

or get $\frac{V_H}{d} = BV$

$$V_H = BVd$$

current density $J = nev$

$$v = \frac{I}{ne}$$

then $V_H = \frac{BJd}{ne} \Rightarrow J = \frac{I}{A}$

then $V_H = \frac{BdI}{nedw} = \frac{BI}{new} \quad [\because A = dw]$

Hall coefficient R_H is

$$R_H = \frac{1}{ne}$$

$$V_H = \frac{BI R_H}{\omega}$$

$$R_H = \frac{V_H w}{BI}$$

The conductivity in a semiconductor is $\sigma = ne\mu$, $\mu = \frac{\sigma}{ne}$

Applications:-

$$\mu = R_H \sigma$$

- 1) Knowing R_H and σ or the mobility μ can be determined
- 2) By using Hall effect we can easily find out the given semiconductor is either p-type or n-type
- 3) Carrier Concentration can be determined by knowing R_H
- 4) We can measure σ or by knowing μ and R_H
- 5) We can measure the magnetic field strength 'B' by measuring the relative quantities.