Annamacharya Institute of Technology and Sciences, Tirupati (Autonomous)

Engineering Physics Course Material
Common to all branches of 1st B. Tech

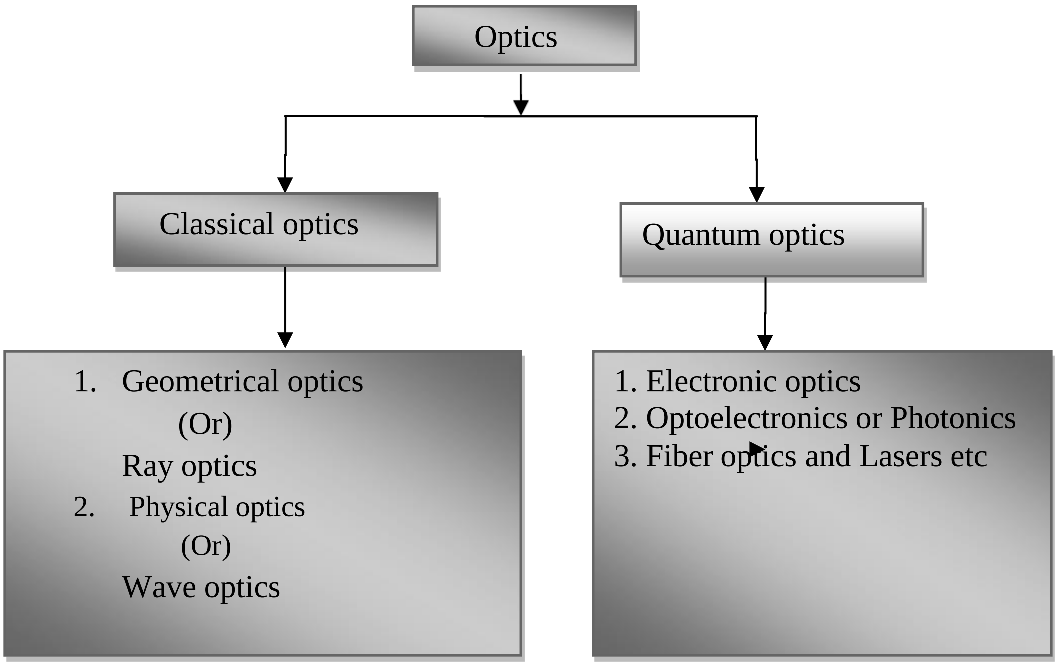
Subject Code: 23ABS9903 (AK23 Regulation)

Unit-1
Wave Optics

Introduction:

The English word optics comes from the Greek word ***"Opticks (Οπτικη)"*** which means look (or) appearance.

Optics is the branch of the physics, which deals with nature, properties, generation, and propagation of light and its interaction with matter.



It is classified into three sections.

Geometrical optics or Ray optics:

In this section, it is assumed that light travels in straight lines and we explain the images are formed by mirrors, prism, lenses etc., by geometrical constructions, without considering the nature of light.

Physical optics or wave optics:

In this section, the nature of light considered and we explain various phenomena like reflection, refraction, interference, diffraction and polarization of light etc., by assuming light as a wave form.

Quantum optics:

In this section, the interaction of light with atomic particles is studied and we explain various phenomena like photo electric effect, Compton Effect and atomic excitation, etc.

Electronic optics is applied to study the stream of particles in electronic microscope, cathode ray tubes etc.

Fiber optics deals with the transmission of light through transparent fibers, using the principle of total internal reflection.

1. INTERFERENCE

Introduction:

Is it possible that light added to light produces darkness? Yes, when the two light waves are out of phase.

Light + Light = Brighter light, if two light waves are in phase .This phenomenon is called interference, which is based on the principle of superposition.

Definition of Interference:

The formation of bright and dark fringes on superimposing two coherent light waves is called interference.

Principle of superposition:

When two or more waves meet, they interfere and produce a resultant wave whose properties can be calculated by using the principle of superposition

The principle of superposition states that whenever two or more waves travelling in the same region superpose, the total displacement(y) at any point is equal to the vector sum of their individual displacements(y_1, y_2, y_3…..) at that point .i.e,

$$\mathbf{y = y_1 \pm y_2 \pm y_3 + \ldots..}$$

If there only two waves, then the resultant displacement is given by;

$$\mathbf{y = y_1 \pm y_2}$$

Case1:

- If the two waves are in phase with each other, they undergo constructive interference producing maximum intensity of light called bright band or fringe.

$$y = y_1 + y_2$$

$$A_{max} = a_1 + a_2 \qquad \text{(since } I \alpha A^2\text{)}$$

$$I_{max} = (a_1^2 + a_2^2)$$

- The condition for constructive interference to occur is

Path difference = $n\lambda$ (or) phase difference $=2n\pi$

Case: 2

- If the two waves are out of phase, then they undergo destructive interference producing zero intensity of light called dark band or fringe.

$$y = y_1 - y_2$$

$$A_{min} = a_1 - a_2$$

$$I_{min} = (a_1^2 - a_2^2)$$

- The condition for destructive interference to occur is

$$\text{Path difference} = (2n-1)\frac{\lambda}{2} \quad \text{(or)} \quad \text{phase difference} = (2n-1)\pi$$

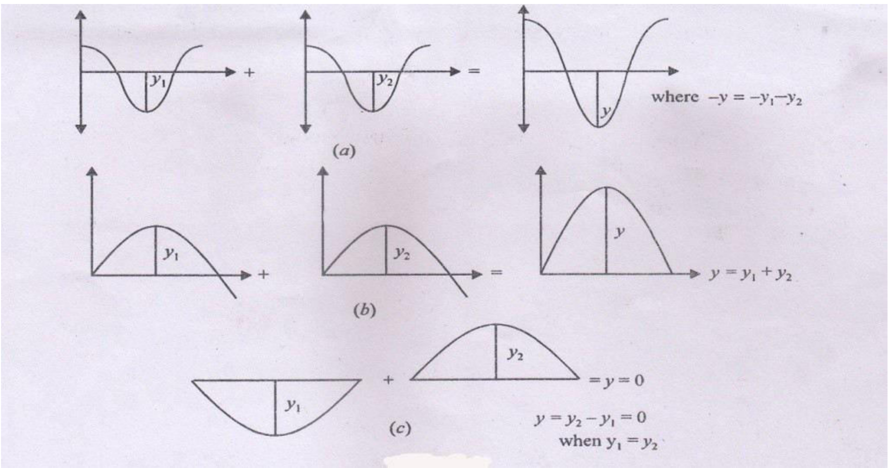


Fig: Superposition of two waves

Case3:

- If the two waves are in phase with each other, they undergo constructive interference producing maximum intensity of light called bright band or fringe.
- The condition for constructive interference to occur is

Path difference $\Delta = n\lambda$ (or)
Phase difference $\emptyset = 2n\pi$

Case 4:

- If the two waves are out of phase, then they undergo destructive interference producing zero intensity of light called dark band or fringe.
- The condition for destructive interference to occur is

Path difference $\Delta = (2n-1)\frac{\lambda}{2}$ (or)
Phase difference $\emptyset = (2n-1)\pi$

Coherence:

The two light waves are said to be coherent if they have same frequency (wavelength) and maintaining same (or) constant phase relationship.
Coherence is two types. (1)Temporal coherence (2) Spatial coherence.

Conditions for interference:

1. To produce interference, we require two coherent light sources.
2. The two sources must be monochromatic.
3. The two sources must be narrow and parallel.
4. The two sources must emit light in same direction.
5. The distance between the two sources must be small.
6. The distance between the two coherent sources and the screen must be large.
7. Background should be dark to view interference fringes.
8. The amplitudes of the light should be equal or nearly equal.
9. The two sourcs of light must emit contineous light waves of same wavelength and frequency.

Interference in uniform thin films by reflection of light:

Plane parallel thin film:

A transparent thin film of uniform thickness which is bounded by two plane parallel surfaces is known as plane parallel thin film.

Principle:

When light is incident on plane parallel thin film, some portion of light gets reflected from the top surface and the reaming portion is transmitted into the film. Again, some portion of the transmitted light is reflected back into the film by the bottom surface and emerges through the top surface. These reflected light waves superimpose with each other, producing interference and forming interference patterns. This is the principle of interference in thin films by reflection.

Theory:

- Let us consider a transparent film of uniform thickness't' bounded by two parallel surfaces, as shown in fig.
- Let the refractive index of the material be μ.The film is surrounded by a common medium say, air on both sides.
- Let a monochromatic light ray AB is incident on the top surface at an angle ***'i'***.
- The ray AB is partly reflected along BC and is partly transmitted into the film along BF makes an angle ***r*** with the normal FG and meets the lower surface.
- At F, it is again partly reflected back into the film along FD, while major portion refracts into the outer medium along FK.
- The reflected ray FD refracts at the outer surface and emerges out along DE which is parallel to the ray BC.
- The waves travelling along directions BC and BFDE are obtained from the incident wave AB.

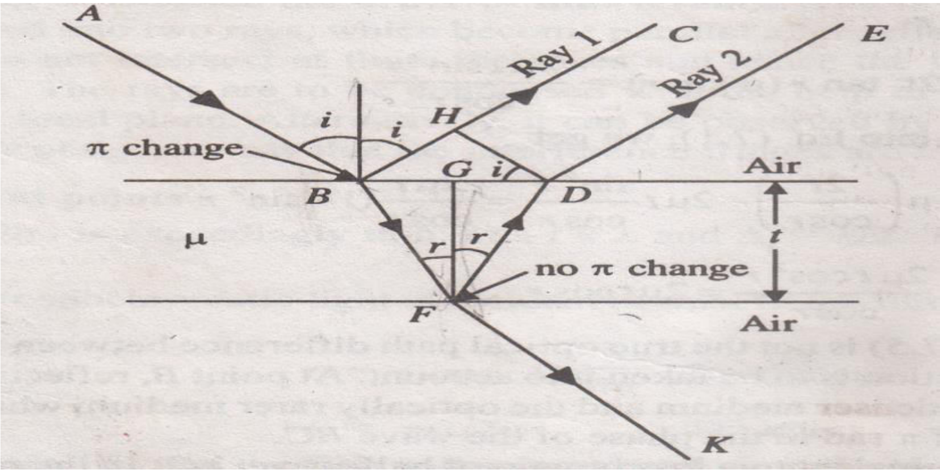


Fig: Interference in thin films by reflection of light

- Therefore, these two light rays superimpose and produce interference patterns. Condition of interference depends on the optical path difference between the rays 1 and 2.
- Let us now calculate the optical path difference between the reflected ray BC (ray1) and the refracted ray BFDE (ray 2).

- A normal DH is drawn on line BC. From points H and D onwards the rays HC and DE equal distances.
- The reflected ray BC travels in air while the refracted ray (BF+FD) travels in the film of refractive index***μ.***
- The Optical path difference (OPD**)** between the rays (1) and (2) is

Total path difference(T.P.D) = (μX geometrical path BFD in film) - (μ X geometrical path BH in air)

$$= \mu\,(BF+FD) - \mu_{air}\,(BH) \qquad [\text{Since } \mu_{air} = 1]$$

$$= \mu\,(BF+FD) - BH \quad ---\longrightarrow(1)$$

Step 1: Calculation of geometrical path BFD in film

Let us calculate path BF+ FD in film,

From fig; ΔBFG, $\text{Cos r} = \frac{GF}{BF}$

$$BF = \frac{t}{\text{Cos r}} \quad --------\longrightarrow(2)$$

Similarly;

From ΔDFG, $\text{Cos r} = \frac{GF}{FD}$

$$FD = \frac{t}{\text{Cos r}} \quad ------\longrightarrow(3)$$

$$\therefore BF+FD = \frac{t}{\text{Cos r}} + \frac{t}{\text{Cos r}}$$

$$\therefore \; BFD = BF+FD = \frac{2t}{\text{Cos r}} \quad ------\longrightarrow(4)$$

Step 2: Calculation of geometrical path BH in air

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

From ΔBGF; $\tan r = \frac{BG}{FG} = \frac{BG}{t}$

$$BG = t.\tan r \quad ------\longrightarrow(5)$$

Similarly;

From ΔDGF; $\tan r = \frac{GD}{FG} = \frac{GD}{t}$

$$GD = t.\tan r \quad ------\longrightarrow(6)$$

$$\therefore BD = BG+GD = t.\tan r + t.\tan r$$

$$= 2t \tan r \quad ------\longrightarrow(7)$$

From ΔBHD; $\text{Sin i} = \frac{BH}{BD}$

$$BH = BD \text{ Sin i}$$

$$= 2t \tan r \text{ Sini} \; ----\longrightarrow(8)$$

From Snell's law $\mu = \frac{\text{Sini}}{\text{Sinr}}$

$$\text{Sin i} = \mu \text{ Sin r}$$

From equation (8)

$$BH = 2t \tan r \; \mu \text{ Sin r}$$

$$= 2\mu t \tan r. \text{ Sin r}$$

$$= 2\mu t \; \frac{\text{Sin r}}{\text{Cos r}} . \text{ Sin r}$$

$$T.P.D = 2\mu t \frac{\text{Sin}^2 r}{\text{Cos r}} \; -------\longrightarrow(9)$$

Substituting equation (4) and equation (9) in equation (1); we have,

$$= \frac{2\mu t}{\text{Cos r}} - 2\mu t\,\frac{\text{Sin}^2\text{r}}{\text{Cos r}} ------\rightarrow(10)$$

$$= \frac{2\mu t}{\text{Cos r}}\,(1 - \text{Sin}^2\text{r})$$

$$= \frac{2\mu t}{\text{Cos r}}\,\text{Cos}^2\text{r}$$

$$\text{T.P.D} = 2\mu t\,\text{Cos r} ----\rightarrow(11)$$

This is called Cosine law.

According to stoke principle, if a light wave traveling from rarer medium to denser medium under goes a phase of π or path change $\frac{\lambda}{2}$ (i.e., the wave loses half of wavelength) when it gets reflected at the boundary of a rarer to denser medium.

$$\boxed{\text{T.P.D} = 2\mu t\,\text{Cos r} - \frac{\lambda}{2}} \quad \text{---------------- (12)}$$

Case 1: Condition for bright band (or) maximum (or) constructive interference:

Bright band occurs when the total path difference (T.P.D) = $n\lambda$ $----\rightarrow(13)$

From equations (12) and (13); we have

$$2\mu t\,\text{Cos r} - \frac{\lambda}{2} = n\lambda$$

$$2\mu t\,\text{Cos r} = n\lambda + \frac{\lambda}{2}$$

$$2\mu t\,\text{Cos r} = (2n+1)\,\frac{\lambda}{2} \quad ---\rightarrow(14)$$, where n= 0, 1, 2, 3…

This is the condition for maxima. The film appears bright under this condition.

Case2: Condition for dark band (or) minimum (or) Destructive interference:

Dark band occurs when the path difference = $(2n-1)\,\frac{\lambda}{2} ------\rightarrow(15)$

From equations (12) and (15); we have

$$2\mu t\,\text{Cos r} - \frac{\lambda}{2} = (2n-1)\,\frac{\lambda}{2}$$

$$2\mu t\,\text{Cos r} = (2n-1)\left(\frac{\lambda}{2} + \frac{\lambda}{2}\right)$$

$$2\mu t\,\text{Cos r} = n\lambda \quad -------\rightarrow(7)$$, where n=0, 1, 2, 3…

This is the condition for minima. The film appears dark under this condition.

Newton’s rings:

Newton’s rings are one of the best examples for the interference in a no uniform thin film.

Definition:

If a Plano-convex lens with its convex surface is placed on a plane glass plate, then air film is formed between the lower surface of the Plano-convex lens and the upper surface of the glass plate. The thickness of the air film is zero at point of contact and gradually increases from the point of contact outer wards.

If a monochromatic light is allowed to fall normally on this air film, a system of alternate bright and dark circular rings is formed in the air film. These rings were discovered by Newton and are called Newton’s rings.

Principle:

Newton's rings are formed due to interference between the light rays reflected from the top and bottom surfaces of air film between the glass plate and the Plano-convex lens.

Experimental Arrangement:

1. The experimental arrangement for producing Newton rings is as shown in fig (1).
2. Keep the convex surface of the Plano-convex lens over the plane glass plate and arrange glass plate G at an angle of 45^0 over the base set.
3. Switch on the monochromatic light source 'S' (Sodium vapor lamp) and it is focus on the Double convex lens (L). This sends parallel beam of light. This beam of light falls on the glass plate B at 45^0.
4. The glass plate 'G' reflects a part of light towards the air film enclosed by the Plano-convex lens and the plane glass plate.
5. A part of the light is reflected by the curved surface of the Plano-convex lens and a part is transmitted which is reflected back from the plane surface of the plane glass plate.
6. These reflected light rays superimpose with each other producing interference and forming interference and forming interference patterns in the form of bright dark circular rings.
7. These rings are seen with a microscope (M) focused on the air film.

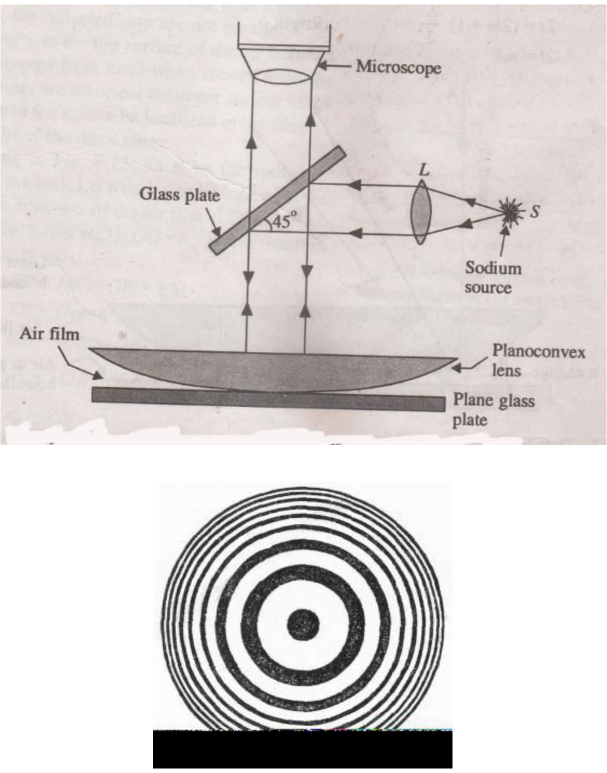


Fig: The experimental arrangement for producing Newton rings.

Explanation of Newton's rings:

- Newton's rings are formed due to interference between the light rays reflected from the top and bottom surfaces of air film between the glass plate and the Plano-convex lens.
- The formation of Newton's rings can be explained with help of fig.

- When a light ray (AB) is incident on the systems, a part of the light is reflected by the curved surface of the lens and a part is transmitted which is reflected back from the plane surface of the glass plate. Ray 1 undergoes no phase change but ray 2 under goes a phase of **π** or path change $\frac{\lambda}{2}$ (i.e., the wave loses half of wavelength) when it gets reflected at the boundary of a rare to denser medium.
- These reflected light rays superimpose with each other producing interference and forming interference and forming interference patterns in the form of bright dark circular rings as shown in fig.
- We know that; the path difference between two reflected rays in uniform thin film is ,

$$\text{Path difference } \Delta=2\mu t \cos r - \frac{\lambda}{2} \quad \longrightarrow (1)$$

For non-uniform thin film :

For air film $\mu = 1$ and

For normal incidence r =0.

$$\text{Path difference } \boxed{\Delta=2t - \frac{\lambda}{2}}$$

$$\text{Thus the path difference } \Delta=2t - \frac{\lambda}{2} \quad - - - - - \longrightarrow (2)$$

This is the path difference between two reflected rays in non-uniform thin film.

Special Case : Dark central spot

At the point of contact 'O' of the lens and glass plate, the thickness of air film is approximately is zero.

i.e., $t \approx 0$

$$\therefore \text{The path difference } \Delta = 2t - \frac{\lambda}{2}$$

$$= 2(0) - \frac{\lambda}{2}$$

$$\Delta = - \frac{\lambda}{2} \quad - - - - - \longrightarrow (3)$$

Thus the two waves are at the centre, out of phase and interference destructively. Hence the central spot is dark.

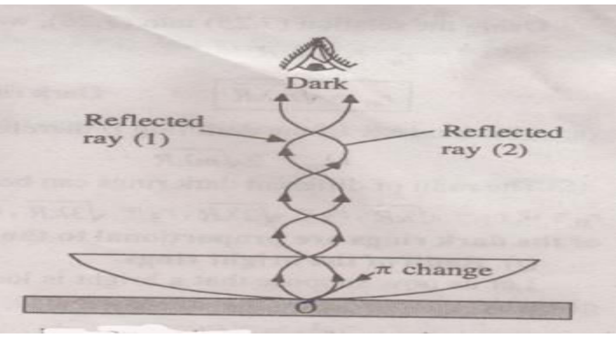


Fig: Two waves are at the centre are opposite in phase

Theory of Newton's rings:

To find the diameters (radii) of dark and bight rings, let 'L' be a Plano convex lens placed on

a glass plate P.

The convex surface of the lens is the part of spherical surface with centre at C as shown in fig.

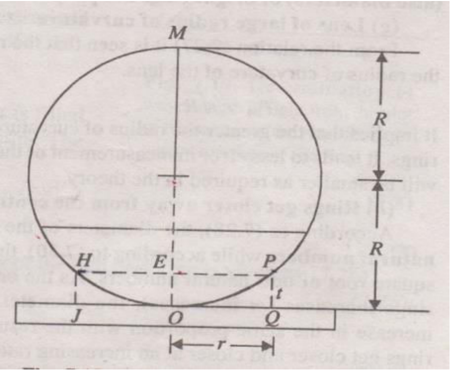


Fig: Theory of Newton's rings

Case1: Diameters (Radii) of the dark rings:

Let 'R' be the radius of curvature of the lens.
Let a dark be located at the point Q is PQ= t.
The radius of the ring at Q is OQ= r.
When the additional path difference due to reflection at Q is taken into account, path difference between the two reflected beams becomes $2t + \frac{\lambda}{2}$.

Case1: Condition for bright Ring :

$$2t + \frac{\lambda}{2} = n\lambda \qquad \text{where } n=1,2,3,\text{-------}$$

$$2t= (2n-1))\frac{\lambda}{2} \quad \text{– – – –}\longrightarrow (4\ )$$

Case2: Condition for Dark Ring :

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

$$2t \ = n\ \lambda \quad \text{-------– – – –}\longrightarrow (\ 5)$$

By the theorem of intersecting chords,

$$EP \times HE=OE \times EM$$

$$\text{But} \quad EP=OQ=HE= r;\ OE=PQ= t$$

$$\text{And} \quad EM= OM-OE =2R-t$$

From equation (1),

$$r \times r = t \times (2R-t)$$

$$\text{(Or)} \quad r^2 = 2Rt-t^2$$

As $2Rt \gg t^2$; t^2 can be neglected.

$$r^2 = 2Rt \quad \text{-------– – – –}\longrightarrow (\ 6)$$

(1) Calculation of Diameters (Radii) of the bright rings:

Let us now suppose that a bright ring be located at the point Q.

Therefore, the radius of the nth bright ring will be given by

$$r_n^2 = 2Rt$$

We know that, the condition of the bright band is $2t= (2n-1)\ \frac{\lambda}{2}$

From above equations we have,

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

$$r_n= \sqrt{(n - \frac{1}{2}\ )\ \lambda R} \qquad \longrightarrow (7)$$

This is the condition for radii of the bright rings.
The diameter of the bright ring is therefore given by

$$\frac{D_n^2}{4} = \left(n - \frac{1}{2}\right) \lambda R \qquad \left[\text{Since, } r_n = \frac{D_n}{2}\right]$$

$$\frac{D_n^2}{4} = \left(\frac{2n-1}{2}\right) \lambda R$$

$$D_n = \sqrt{(2n-1)2\,\lambda R} \quad \longrightarrow (8)$$

∴ The radii (diameters) of the bright rings is directly proportional to (i) $\sqrt{2n-1}$
(ii) $\sqrt{\lambda}$

(iii) $\sqrt{R}$

(2)Calculation of diameter (Radii) of the dark rings :

Thus, the radius of the nth dark ring will be given by,

$$r_n^2 = 2Rt$$

We know that, the condition of the dark ring is $2t = n\lambda$

From the above equations we have,

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

$$r_n = \sqrt{n\lambda R}$$

This is the condition for radii of the dark rings.

The diameter of the dark ring is therefore given by

$$\frac{D_n^2}{4} = n\lambda R \qquad \left[\text{Since, } r_n = \frac{D_n}{2}\right]$$

$$D_n = \sqrt{4n\lambda R}$$

$$D_n = 2\sqrt{n\lambda R} \quad \longrightarrow (9)$$

∴ The radii (diameters) of the dark rings is directly proportional to (i) $\sqrt{n(\text{ natural nuber})}$
(ii) $\sqrt{\lambda}$
(iii) $\sqrt{R}$

Applications:
The theory of Newton's rings can be used
(i) To determine the wavelength of monochromatic light and
(ii) To determine the refractive index of a given liquid.

Application (i): Determination of wavelength of monochromatic light source.

Let 'R' be the radius of curvature of a Plano-convex lens, λ be the wavelength of monochromatic light source.

Let D_m and D_n are the diameters of mth and nth dark rings respectively.

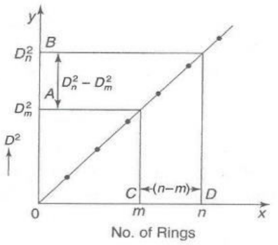


Fig: A graph between (D^2) and number of rings.

Then,

$$D^2_m = 4m\lambda R,$$

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

$$\text{and } D^2_n - D^2_m = 4n\lambda R - 4m\lambda R$$

$$= 4(n-m)\lambda R$$

$$\boxed{\lambda = \frac{D_n^2 - D_m^2}{4(n-m)R}} \longrightarrow (9)$$

Graph:

A graph is drawn with the number of rings on the x- axis and the square of the diameter of the ring (D^2) on the y-axis. The graph is straight line passing through the origin. Form the graph the values of D_m^2 and D_n^2 corresponding to nth and mth rings are found. From the graph, the slope is calculated.

From graph,

$$\frac{D_n^2 - D_m^2}{(n-m)} = \frac{AB}{CD}$$

The radius of curvature 'R' of the Plano-convex lens is found by Boy's method or spherometer.

Substituting the values of R and the values of $D_n^2 - D_m^2$ in the above formula (9), λ can be calculated.

Application 2: Determination of refractive index of a given liquid:

To find the refractive index of a given liquid, the Plano convex lens and glass plate set up is placed in a small container 'C'. The transparent liquid of refractive index 'μ'is introduced between the lens L and the glass Plate 'G' as shown as fig. Then a film of liquid formed between the lens and glass plate. The diameters of mth and nth dark rings are determined with help of travelling microscope.

We know that;

The diameters of mth and nth dark rings in the air film are given by

$$D^2_m = 4m\lambda R,$$

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

$$\text{and } D^2_n - D^2_m = 4n\lambda R - 4m\lambda R$$

$$= 4(n-m)\lambda R \quad -------\!\!\longrightarrow (9)$$

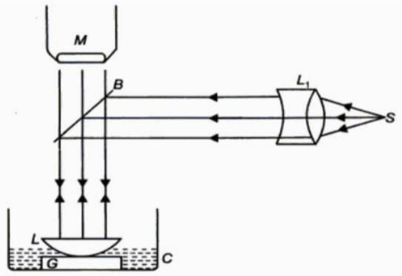


Fig: Determination of refractive index of a given liquid.

With liquid film, the diameters of mth and nth dark rings are determined;

$$D^2{}_m{}^I = \frac{4m\lambda R}{\mu}$$

$$D^2{}_n{}^I = \frac{4n\lambda R}{\mu}$$

$$\text{And } D^2{}_n{}^I - D^2{}_m{}^I = \frac{4n\lambda R}{\mu} - \frac{4m\lambda R}{\mu}$$

$$= \frac{4\lambda R(n-m)}{\mu} \; -------\longrightarrow (10)$$

From equations (9) and (10); $D^2{}_n{}^I - D^2{}_m{}^I = \frac{D_n^2 - D_m^2}{\mu}$

$\mu = \frac{D_n^2 - D_m^2}{D_n^2 I - D_m^2 I}$. Using the above formula μ can be calculated.

2. 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 ‘dirrfactus’ which means to break pieces. It is common experience that waves bends around the obstacles placed in their path. When light waves encounter an obstacle, they bend round the edges of the obstacle. This bending is predominant when size of the obstacle is comparable to the wavelength of light. The bending of light waves around the edge or corner of an obstacle is diffraction .It was first observed by Gremaldy.

As shown in figure 2.1, when light falls on an obstacle then the corresponding geometrical shadow on the screen should be completely dark. In practice, the geometrical shadow consists of bright dark fringes. These fringes are due to the superposition of bended light waves around the edges or corners of an obstacle. The amount of bending depends upon the size of an obstacle and wavelength of light.

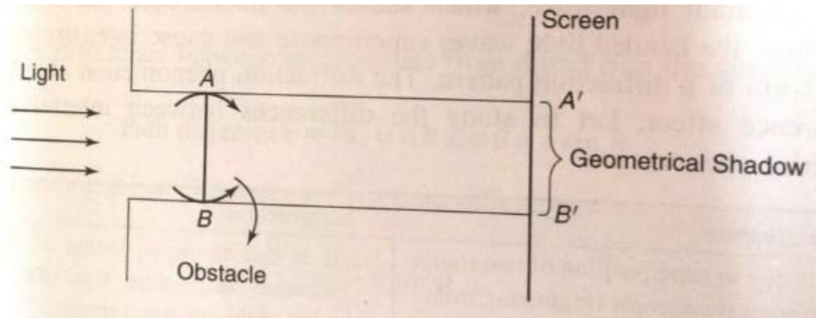


Figure 2.1 Diffraction

Diffraction definition:

When a light falls on an obstacle whose size is comparable with wavelength of light,then light bends around the edges or corners of an obstacle.This bending nature of light tacle is called diffraction.

The diffraction phenomenon is brodly devided into two types.They are

1. Fresnel's diffraction
2. Fraunhoffer's diffraction.

Difference between Interference and diffraction :

Interference	Diffraction
1.Superposition is due to two separate wavefronts originating from two cohenent sources. 2.The fringenormally have equal widths. 3.All the bright fringes have same intensity. 4.All the dark fringes have zero intensity.	1.Superposition is due to secondary wavelets originating from different parts of the same wavefront. 2.The width between frines is never equal. 3.The intensity of bright fringes usually decreases with increase of order. 4.The intensity of dark fringes is not zero.

Difference between Fresnel's diffraction and Fraunhoffer diffraction:

Fresnel's Diffraction	Fraunhoffer diffraction
1.For diffraction to occur,the light source and screen are at finite distance from the obstacle. 2.No lenses are necessary to study the diffraction. 3.Study of diffraction is complicated. 4.Either a point source or an illuminated narrow slit is used. 5.Diffraction can be studied only in the direction of propagation of light. 6.In this case the incident wavefronts are either cylindrical (or) spherical.	1.For diffraction to occur,the light source and screen are at infinite distance from the obstacle. 2. Lenses are necessary to study the diffraction. 3.Study of diffraction is easy. 4.Extended source at infinite distance is used.. 5. Diffraction can be studied in any direction of propagation of light. 6.In this case, incident wavefronts are plane.

Fraunhoffer diffraction at Single Slit:

- Consider a slit AB of width 'e' perpendicular to the plane of the paper. Let a plane wave front of monochromatic light of wavelength 'λ' incident at this slit.
- At slit, each and every point is able to generate secondary wavelets. These wavelets are focused through the lens 'L'.
- The wavelets travelling normal to the lens are brought to focus at at P_0 and the wavelets travel with an angle θ are focused at P_1 .Now the intensity at P_O is central maximum with bright fringe ,and intensity at P_1 is either maxima or minima depends upon the angle 'θ'.

- To find the intensity at P_1, first we should calculate the phase difference at point P_1.For this AC is perpendicular to BC.

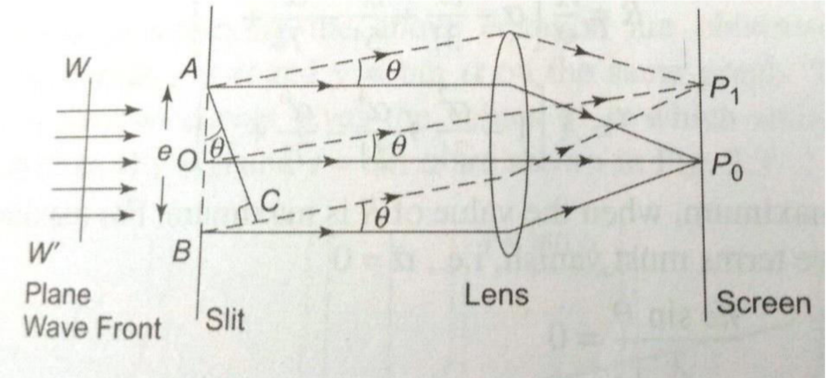


Figure 2.2 Fraunhofer diffraction—single slit

Path difference between the wavelets along P_o & P_1 is given by,

$$\delta = BC$$

From ΔACB, $\text{Sin}\theta = \frac{BC}{AB}$

$$BC = AB \sin\theta$$

$$BC = e \sin\theta$$

$$\therefore\ \delta = BC = e \sin\theta$$

But the phase difference $\phi = \frac{2\pi}{\lambda}$ (Path difference δ)

$$\therefore\ \phi = \frac{2\pi}{\lambda}(e \sin\theta) \text{ --------------->(1)}$$

Let the slit ‘s’ is decided into ‘n’ number of small slits of each with amplitude ‘a’, then,

Phase difference at each slit (d) = $\frac{Total\ phase\ difference}{number\ of\ slits}$

$$d = \frac{\phi}{n} = \frac{2\pi}{n\lambda}(e \sin\theta) \text{ -------------> (2)}$$

After diffraction, the resulting amplitude R can be obtained by using vector addition method with each of amplitude ‘a’.

$$R = \frac{a\ Sin\left(\frac{nd}{2}\right)}{Sin\ d/2} \text{ ----------------}\rightarrow\text{(3)}$$

Substitute eq(2) in eq(3) we get,

$$R = \frac{a\ Sin\ (n\{\frac{2\pi e Sin\theta}{n\lambda}\})/2}{Sin\ \{\frac{2\pi e Sin\theta}{n\lambda}/2\}}$$

$$R = \frac{a\ Sin\ \left(\frac{\pi e Sin\theta}{\lambda}\right)}{Sin\ \left(\frac{\pi e Sin\theta}{\lambda}\right)/n}$$

Put $\frac{\pi}{\lambda}e\sin\theta = \alpha$,then

$$R = \frac{aSin\alpha}{Sin\left(\frac{\alpha}{n}\right)}$$

Since $\frac{\alpha}{n}$ is small, $Sin(\alpha/n) \approx \alpha/n$

$$R = a\frac{Sin\alpha}{\alpha/n}$$

$$R = n\, a\frac{Sin\alpha}{\alpha}$$

$$R = A\frac{Sin\alpha}{\alpha} \text{ ------------------}\rightarrow\text{ (4)}$$

Intensity at P_1 is given by,

$$I = R^2 = \left(A\frac{Sin\alpha}{\alpha}\right)^2 = A^2\frac{Sin^2\alpha}{\alpha^2} \text{ -------------------}\rightarrow\text{ (5)}$$

(1) Principal maximum :

From eq(4) if write the Sinα expansion we have,

$R = \frac{A}{\alpha}[\alpha - \frac{\alpha3}{3!} + \frac{\alpha5}{5!} - \frac{\alpha7}{7!}----------]$

$= \frac{A\alpha}{\alpha}[\alpha - \frac{\alpha2}{3!} + \frac{\alpha4}{5!} - \frac{\alpha6}{7!}----------]$

In above equation for 'R' maximum negative terms and higher order terms vanishes i.e, α=0.

But $\frac{\pi}{\lambda}$ esinθ =α =0

$\therefore$ Sinθ =0 ⇒θ=0°

Then R = A ⇒ $I^2 = A^2 = R^2$

At θ =0°, the maximum intensity is formed at P_o known as principal maximum.

2.Minimum intensity position :

From eq(5) for '$I_{minimum}$, Sinα=0

$\therefore \alpha = \pm m\pi$, m= 0,1,2,3,---------

For m=0, α =0 which gives principal maxima and for α = ±π,±2π,±3π ,------------ minimum intensity is observed at P_1,

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

$\frac{\pi}{\lambda}$ esinθ = ±mπ

esinθ = ±mλ

The above condition is for minimum intensity position.

3. Secondary Maxima:

Between two secondary minima, the secondary maxima can be obtained by differentiating eq(4) w.r.to α and equating to zero , we get

$\frac{dI}{d\alpha} = 0 \Rightarrow \frac{dI}{d\alpha} = \frac{d}{d\alpha}[A^2 (\frac{Sin\alpha}{\alpha})^2] = 0$

$A^2(\frac{2Sin\alpha}{\alpha})[\frac{\alpha Cos\alpha - Sin\alpha}{\alpha^2}] = 0$

$A^2 (\frac{2Sin\alpha}{\alpha}) \neq 0$, then $\frac{\alpha Cos\alpha - Sin\alpha}{\alpha^2} = 0$

α Cosα – Sinα = 0

α Cosα = Sinα

α = Tanα

which is interms y=α and y=Tanα

Now draw graphs y=α and y=Tanα

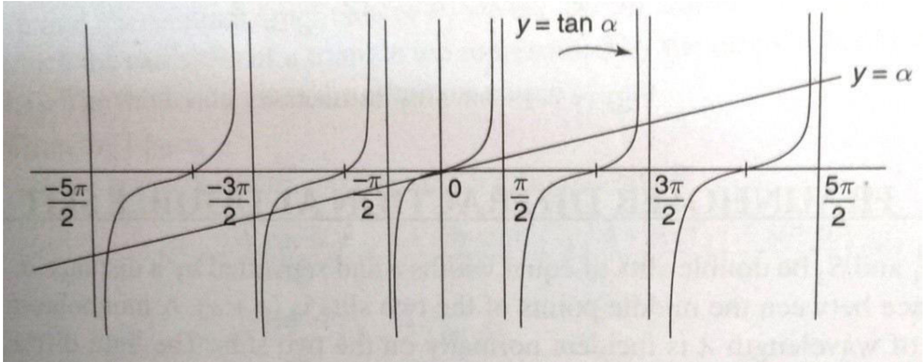


Figure 2.3 Plots of $y = \alpha$ and $y = \tan \alpha$

From graph, it is clear that y=α line touches the y=Tanα curves at

$\alpha = 0, \pm\frac{3\pi}{2}, \pm\frac{5\pi}{2}, \pm\frac{7\pi}{2}$ -------.

So, at these α values, secondary maxima can be obtained.We already know that α = 0 is principal maxima. So,

1. $\alpha = \pm\frac{3\pi}{2}$, $I = A^2\left[\frac{Sin(\frac{3\pi}{2})}{(\frac{3\pi}{2})}\right]^2 = \frac{A^2}{\frac{9\pi^2}{4}} = \frac{4A^2}{9\pi^2}$ ---→ first secondary maxima

2 .$\alpha = \pm\frac{5\pi}{2}$, $I = A^2\left[\frac{Sin(\frac{5\pi}{2})}{(\frac{5\pi}{2})}\right]^2 = \frac{A^2}{\frac{25\pi^2}{4}} = \frac{4A^2}{25}$ ---→ second secondary maxima

4. Intensity distribution :

The intensity distribution of diffraction intensity depends on α values, i.e, α = 0 , principal maxima.

$\alpha = 0, \pm\frac{3\pi}{2}, \pm\frac{5\pi}{2}, \pm\frac{7\pi}{2}$-------. Secondary maxima.

for $\alpha = \pm\pi, \pm2\pi, \pm3\pi$,------------Minimum distribution of intensity.

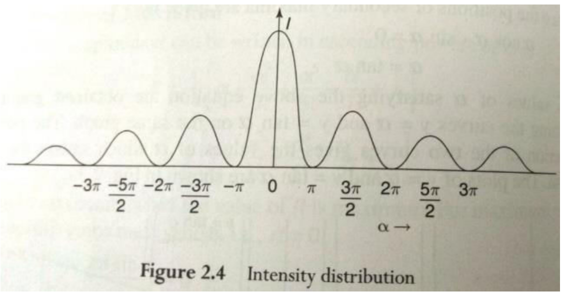


Figure 2.4 Intensity distribution

Fraunhoffer diffraction at double slit:

- Let S1 and S2 be double slits of equal widths ‘e’ and separated by a distance‘d’. The distance between the middle points of the two slits is (e+d).
- A monochromatic light of wavelength of λ is incident normally on the two slits .The light diffracted from these slits is focused 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 wave front is incident normally on two slits, the secondary wavelets from the slits travels uniformly in all directions. The wavelets travelling in the direction of incident light comes to a focus at P_o while the wavelets travelling in a direction making an angle θ, come to focus at P_1 (see figure 2.5).

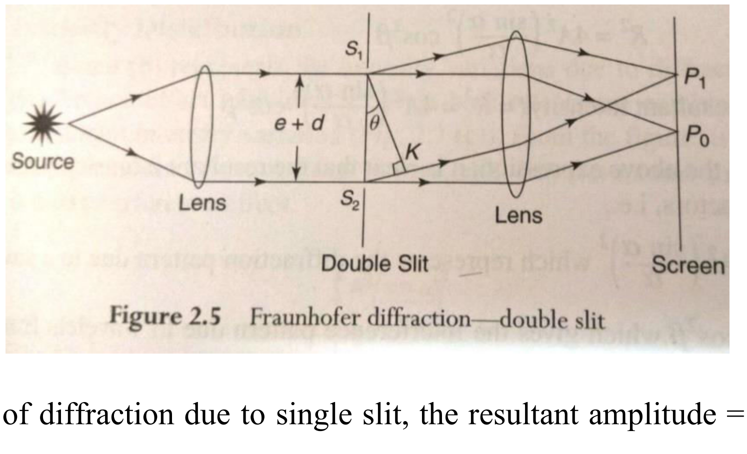


Figure 2.5 Fraunhofer diffraction—double slit

From the study of diffraction due to single slit, the resultant amplitude = $\frac{ASin\alpha}{\alpha}$ where $\alpha = \frac{\pi eSin\theta}{\lambda}$.

Since we use double slit,from each slit we get a wavelet of amplitude $\frac{ASin\alpha}{\alpha}$ in a direction θ.These two wavelets interfere and meet at a point P_1 on the screen .To calculate the path difference between the wavelets,let us draw a normal S_1K to the wavelet through S_2 .

Path difference = S_2K = (e+d)Sinθ

$$\text{Phase difference } \delta = \frac{2\pi}{\lambda}(e+d)Sin\theta$$

To find the resultant amplitude at P_1 we use vector addition method (see fig.2.6) in which the two sides of a triangle are represented by the amplitudes through S_1 and S_2.The third side gives the resultant amplitude.

From figure,

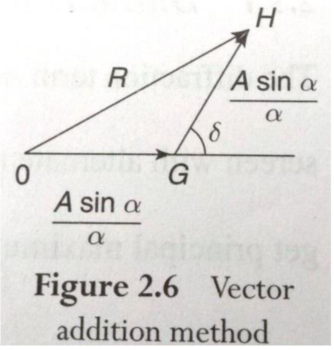


Figure 2.6 Vector addition method

$$(OH)^2 = (OG)^2+(GH)^2+2(OG)(GH)\,Cos\delta$$

$$R^2 = \left(\frac{ASin\alpha}{\alpha}\right)^2 + \left(\frac{ASin\alpha}{\alpha}\right)^2 + 2\left(\frac{ASin\alpha}{\alpha}\right)\left(\frac{ASin\alpha}{\alpha}\right)Cos\delta$$

$$= A^2\,\frac{Sin^2\alpha}{\alpha^2}[2+2\cos\delta]$$

$$=2\left(\frac{ASin\alpha}{\alpha}\right)^2(1+Cos\delta\,)$$

$$= 2\left(\frac{ASin\alpha}{\alpha}\right)^2\,(1+2\,Cos^2(\delta/2)\,-1)$$

$$R^2 = 4A^2\left(\frac{Sin\alpha}{\alpha}\right)^2 Cos^2\left[\frac{\pi(e+d)Sin\theta}{\lambda}\right]$$

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

$$R^2 = 4A^2\left(\frac{Sin\alpha}{\alpha}\right)^2 Cos^2\beta$$

The resultant intensity I = $R^2 = 4A^2\left(\frac{Sin\alpha}{\alpha}\right)^2 Cos^2\beta$

From the above expression it is clear that the resultant intensity is the product of two factors i.e,

1. $4A^2\left(\frac{Sin\alpha}{\alpha}\right)^2$ which represents the diffraction pattern due to a single slit.
2. $Cos^2\beta$ which gives the interference pattern due to wavelets from double slits.

The resultant intensity is due to both diffraction and interference effects.

<u>1.Diifraction effect :</u>

The diffraction term $4A^2\left(\frac{Sin\alpha}{\alpha}\right)^2$ gives the principal maximum at the centre of the screen with alternate minima and secondary maxima of decreasing intensity.

We get principal maximum for θ=0.We get minima for Sinα=0.

$\alpha = \pm m\pi$, where m=1,2,3,4---

$$\frac{\pi eSin\theta}{\lambda} = \pm m\pi$$

$$eSin\theta = \pm m\lambda$$

The positions of secondary maxima occur for $\alpha = \frac{\pm 3\pi}{2}, \frac{5\pi}{2}, \frac{\pm 7\pi}{2}, ------$

2. Interference effect :

The interference term $Cos^2\beta$ gives the equidistant bright and dark fringes.

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

$\beta = \pm n\lambda$ where n=0, 1,2,3-------

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

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

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

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

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

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

Intensity Distribution:

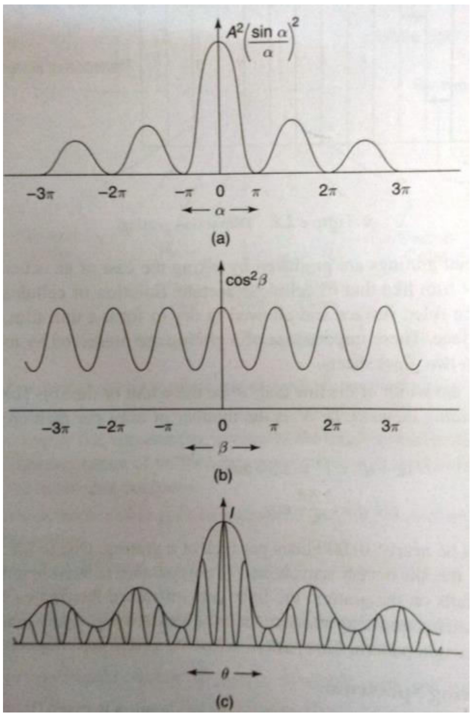


Figure: (a) Diffraction effect, (b) Interference effect, and (c) Resultant Intensity.

The figures shown here represents the intensity variations due to diffractions as well as interference effect individually (fig.(2.7 a) and fig.(2.7 b)) . When both effects are combined, then we get the resultant intensity variations (fig.2.7(c). From the figure, it is clear that the resultant minima are not equal to zero still they have some minimum intensity due to interference effect.

Diffraction Grating:

Definition of diffraction grating:

An arrangement which consists of a large number of parallel slits of the same width and separated by equal opaque spaces is known as Diffraction grating.

Explanation :

✓ Fraunhoffer used the first grating consisting of a large parallel wires placed side by side very closely at regular intervals.

✓ Now gratings are constructed by ruling equidistant parallel lines on a transparent material such as glass with a fine diamond point.

✓ The ruled lines are opaque to light while the space between any two lines is transparent to light and acts as a slit (Fig 2.8).

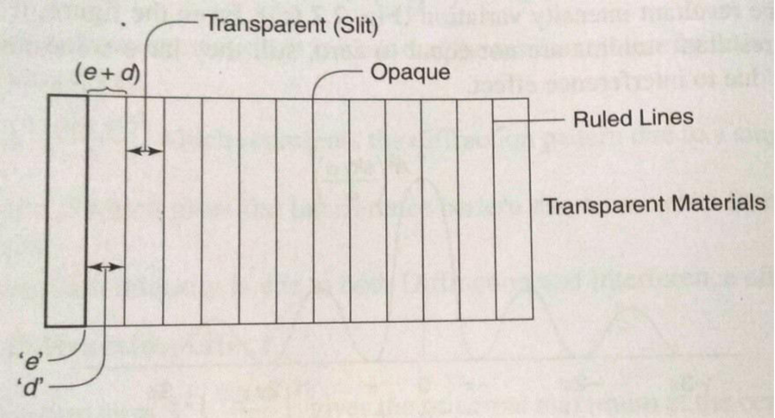


Figure 2.8 Diffraction grating

✓ Commercial gratings are produced by taking the cast of an actual grating on a transparent film like that of cellulose acetate.

✓ Solution of cellulose acetate is poured on the ruled surface and allowed to form a thin film, detachable from the surface. These impressions of a grating are preserved by mounting the film between two glass sheets.

Let 'e' be the width of the line'd' be the width of the slit. Then (e+d) is called grating element. If 'N' be the number of lines per inch on the grating, then

$$N(e+d) = 1 \text{ inch} = 2.54 \text{ cm}$$

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

✓ There will be nearly 30000 lines per inch of a grating. Due to above fact, the width of the slit is very narrow and is comparable with the wavelength of light. When light falls on the grating, the light gets diffracted through each slit.

✓ As a result, both diffraction and interference of diffracted light gets enhanced and forms a diffraction pattern. This pattern is known as diffraction spectrum.

Grating spectrum:

- The condition to form the principal maxima in a grating is given by,

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

Where (e+d) is the grating element and the above equation is known as grating equation. From the grating equation, the following points are clear.

- For a particular wavelength ' λ' the angle of diffraction θ is different for principal maxima of different for principal maxima of different orders.
- As the number of lines in the grating are large , maxima appears as sharp , bright parallel lines and are termed as spectral lines.

- For white light and for a particular order of 'n 'the light of different wavelengths will be diffracted in different directions.
- At the centre, $\theta = 0$ which gives the maxima of all wavelengths which coincides to form the central image of the same colour as that of the light source. This forms zero order (Fig 2..9).

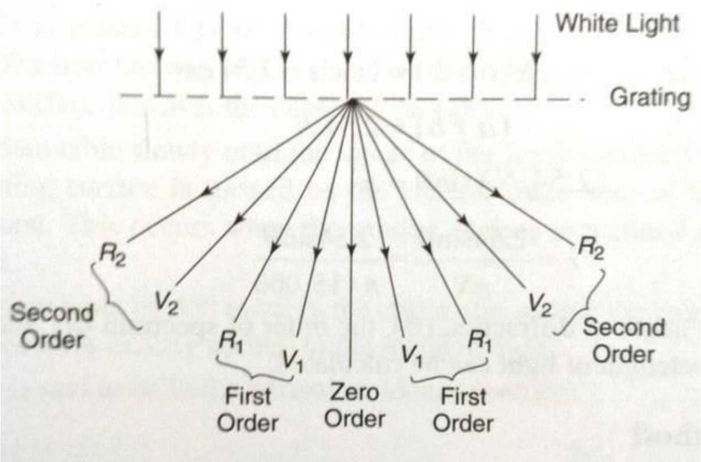
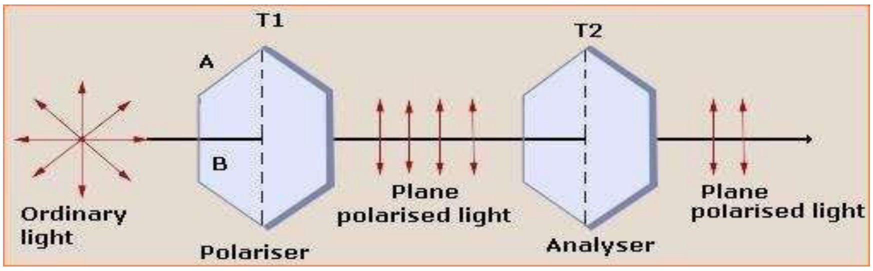


Figure 2.9 Grating spectrum

- The principal maxima of all wavelengths form the first, second-------order spectra for n=1,2,------
- The longer the wavelength, greater is the angle of diffraction .Thus ,the spectrum consists of violet being in the innermost position and red being in the outermost positions.
- Most of the intensity goes to zero order and the rest is distributed among other orders. Spectra of different orders are situated symmetrically on both sides of zero order.
- The spectral lines are more and more dispersed as we go to higher orders ($\sin\theta=\sin 90^0=1$)
- The maximum number of orders available with the grating is $n_{max} = \frac{(e+d)}{\lambda}$.

3. POLARIZATION

The phenomena of interference and diffraction shows that the light has wave nature,but they do not confirm that the light is a transverse wave or longitudinal wave. The phenomena of polarization proved that the nature of light is transverse wave nature.



Light is nothing but an Electromagnetic (EM) wave because of it has both electric and magnetic fields. Both electric field (E) vector and magnetic field (B) vectors are perpendicular to each other and also perpendicular to the direction of propagation.

Polarization

The process of converting unpolarized light into polarized light is called polarization. (or) The process of converting Ordinary light into extraordinary light is called polarization.

The light which vibrates in a single plane is called polarized light. The light which vibrates in more than one plane is called unpolarized.

Polarizer: The material which is used for polarization is called polarizer.

Analyzer: The material which is used to analyze the polarized light is called analyzer. Calcites, Quartz, Tourmaline, Nichol's prism are examples of polarizer and analyzer.

Plane of Vibration:

The plane in which the electric vector (E) vibrates, is called plane of vibration

Plane of Polarization:

The plane which is perpendicular to the plane of vibration is called plane of polarization.

Types of polarization

1) Linearly plane polarized light: When the amplitudes of electric (E) vectors of light changes, but orientation remains constant, then the path traced by electric vectors is a straight line. Hence, that polarized light is said to be linearly plane polarized light.

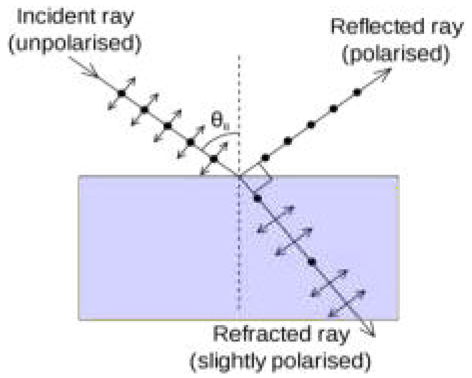
2) Circularly polarized light: When the amplitude of electric (E) vectors of light remains constant but orientation changes, then the path traced by the electric vectors is circular. Hence, that polarized light is said to be circularly polarized light.

3) Elliptically polarized light: When the amplitudes of electric vectors and orientation changes, then the path traced by electric (E) vectors is an ellipse and that polarized light is said to be elliptically polarized light.

Methods of production of plane polarized light

Polarization by reflection from Di-Electric surfaces

1. Polarization by refraction (Pile of plates)
2. Polarization by double refraction (Birefringence)



1) Polarisation by Reflection (Brewster's law):

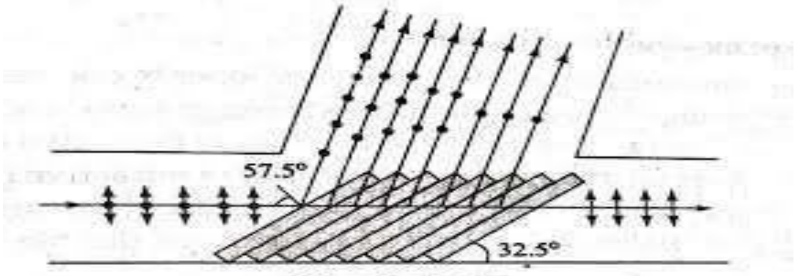
When an ordinary light is incident on the dielectric (glass) surface at a particular angle of incidence (θ_p), thelight which vibrations are perpendicular to the crystal planes is reflected back as polarized light and the light which vibrations are parallel to the crystal planes is refracted into the glass. This refracted light is partially polarized.

Brewster's angle (θ_p): It is the angle of incident light at which the reflected light is completely polarized. It is known as angle of polarization.

Brewster's law: The refractive index (μ) of a material is equal to the tangent of angle of polarization (θ_p). $\mu = \text{Tan}\,(\theta_p)$

2) Polarisation by Refraction (Pile of Plates):

When a beam of ordinary light is incident on the first glass plate of a pile of platesat Brewster's angle, some part of light is reflected up and some part of light is refracted.The light which vibrates perpendicular to the glass planes is reflected up as polarized light and the light which vibrates parallel to the glass planes is refracted as partially polarized light as shown in the figure.



Pile of plates

Partially polarized light is incident again on the second glass plate, some part of light gets reflected up as polarized light and some part of light gets transmitted as partially polarized light as said above.

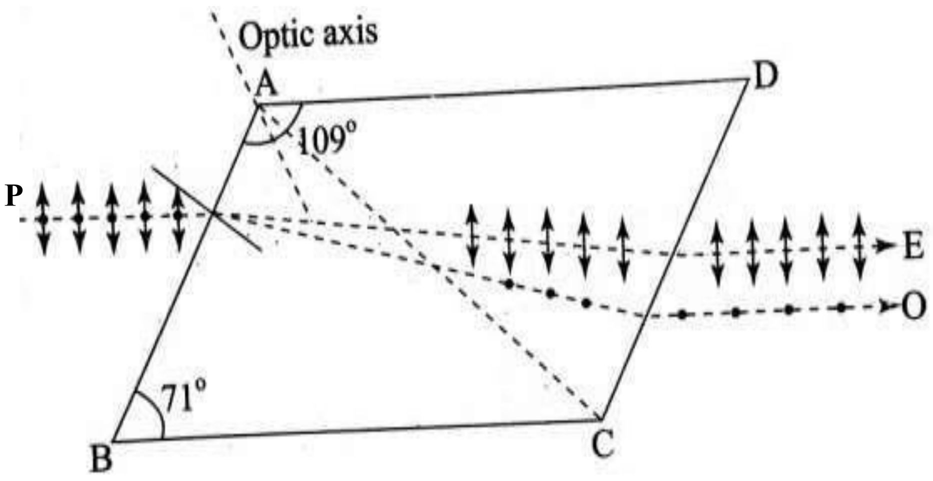
Finally, the refracted light is also completely polarized after passing through the 15(or) 20 glass plates. In this way, we get both reflected and refracted lights as polarizedlights.

3. Polarization by Double Refraction (Birefringence):

When a beam of ordinary light is incident on a calcite or quartz crystal, the refractedlight splits up into two refracted rays, one is ordinary ray (O-ray) and another is extraordinary ray (e-ray). This is called double refraction of light (or) birefringence.

Let grounded angles of principal section of calcite is 71^0 and 109^0. O-ray travels along PO making an angle of refraction r_1 and e-ray travels along PE making an angle r_2 is shown in the figure.

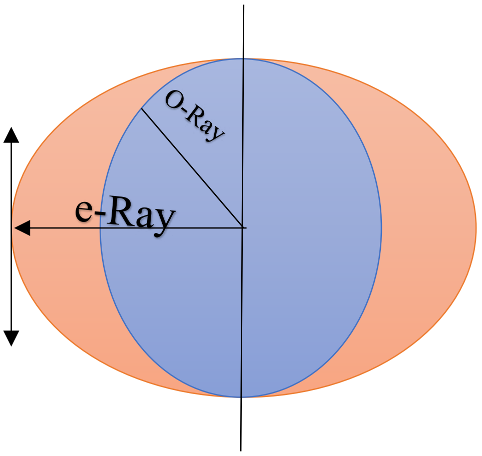
Let the refractive indices of o - ray and e - ray are μ_0 and μ_e, then



$$\mu_o = \frac{sini}{sinr1} \qquad \text{and } \mu_e = \frac{sini}{sinr1}$$

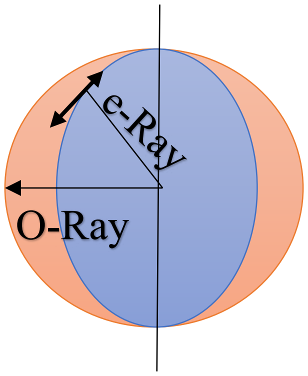
here $r_1 < r_2$ and $\mu_0 > \mu_e$ for calcite crystal, $\mu_0 = 1.6504$, $\mu_e = 1.4864$,

1. O-ray obey Snell's law and e-ray does not obey Snell's law.
2. Velocity of o-ray is same in all directions and velocity of e-ray is different indifferent directions.
3. The velocities of o-ray and e-ray are same along the optic axis inside the crystals.
4. The velocity of o-ray is more in quartz (positive) crystal and velocity of e-ray ismore in calcite (negative) crystal.
5. For positive crystals ellipsoid is within the sphere and for negative crystals sphereis within the ellipsoid is shown in the figure.
6. When the crystal is rotating about the beam of axis, e-ray rotates about the beam of axis around the fixed o-ray is shown in the below figure.



$\mu_e < \mu_o$

Negative Crystal



$\mu_e > \mu_o$

Positive Crystal

Difference between unpolarized light and polarized light

Unpolarized Light (O-ray)	Polarized Light (e-ray)
1. O-ray obey Snell's law and other laws of refractions.	1. E-ray doesn't obey Snell's law and other laws of refractions.
2. Refracted angle of O-ray is less than the refracted angle of e -ray.	2. Refracted angle of e-ray is more thanthe refracted angle of O-ray.
3. Vibrations of electric vectors are perpendicular to the optic axis.	3. Vibrations of electric vectors areparallel to the optic axis.
4. O-ray travels with same speed in all directions in the crystals.	4. E-ray travels with different speeds in different directions in the crystals.
5. Velocity of O-ray is more in Quartz /positive crystals.	5. Velocity of e-ray is more in calcite / negative crystals.
6. Speed of o-ray and e-ray is same along the optic axis.	6. Speed of o-ray and e-ray is samealong the optic axis.
7. For positive crystals, ellipsoid iswithin the sphere.	7. For negative crystals, sphere is within the ellipsoid.

Construction and working of Nicol's prism

Nicol's Prism is a good polarizer as well as good analyzer. Nicol's prism is working on the basic principle of Total Internal Reflection.

Working Principle: Total Internal Reflection

When the light travels from a denser medium to rarer medium, if the angle of incidenceis greater than the critical angle,the light totally reflected in the denser medium, this phenomenon is called Total Internal Reflection.

Description of Nicol's Prism:

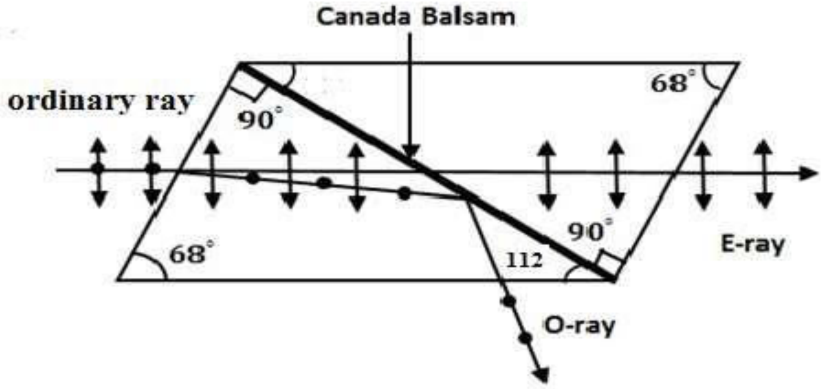
1. Nicol's prism is an important optical instrument, used to produce plane polarized light.
2. It was invented by William Nicol in 1828, hence it was called Nicol's prism.
3. It was made from calcite crystal by cemented two pieces of calcite with Canada balsam(μ=1.55).
4. Nicol's Prism eliminates O-ray by total internal reflection and produce only thepolarized light.
5. Nicol's Prism is a good polarizer as well as good analyzer.

Construction of Nicol's Prism:

1. Length of the calcite crystal is taken 3 times of its width.
2. Grounded angles of principal section of calcite is 68^0 and 112^0 instead of 71^0 & 109^0.
3. The calcite crystal cuts along its diagonal. After polished two faces cemented togetherin its original positions with Canada balsam is called Nicol's Prism.
4. Canada balsam is a transparent cement with refractive index μ = 1.55.
5. Canada balsam layer and optic axis makes an angles 90^0 and 48^0 with the end face ofprincipal section is as shown in the figure.

Working of Nicol's Prism:

When a beam of ordinary light is incident on a Nicol's prism, the refracted light splits up into two refracted rays, one is ordinary ray and another is extraordinary ray. This is called double refraction of light.



1. Both o-ray and e-ray travels towards the Canada balsam.
2. When the angle of incidence of o-ray is greater than the critical angle (θ_c= 69^0) at Canada balsam, that o-rays totally reflects into same medium by total internal reflection.

refractive index of Canada balsam is μ = 1.55for calcite crystal, μ_0 = 1.6504, μ_e = 1.4864

Critical angle (θ_c) =$\text{Sin}^{-1}\frac{1.55}{1.6504}$ = 69^0

3. When e-ray is incident on the Canada balsam, it can easily transmit through canadabalsam.
4. Finally, by eliminating O-ray Nicol's prism produce e-ray only is shown in the figure.
5. Nicol's Prism is a good polarizer as well as good analyzer.

Half Wave Plate

Half wave plate is the thickness of the crystal plate at which the path difference between o-ray and e-ray inside the crystal is equal to $\lambda/2$.

Consider a light of wavelength 'λ' falls normally on a crystal surface; the refracted light splits up into o-ray and e-rays.

Let 't' is the thickness of crystal at which path difference of o-ray and e-ray is $\lambda/2$, then

Path difference of o-ray and e-ray = $\lambda/2$ -------------------------------------- (1)
Optical path of o-ray = $\mu_o t$,optical path of e-ray = $\mu_e t$
Optical path difference between o-ray & e-ray = $(\mu_o \sim \mu_e)$ t--------------(2)
from eqns (1) & (2),
$(\mu_0 \sim \mu_e)$ t = $\lambda/2$

$$t = (\lambda/2)/((\mu_o \sim \mu_e)$$

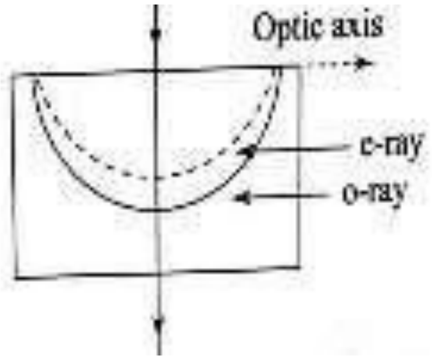


Figure: Half Wave Plate

Quarter Wave Plate

Quarter wave plate is the thickness of the crystal plate at which the path difference between o-ray and e-ray inside the crystal is equal to $\lambda/4$.

Consider a light of wavelength 'λ' falls normally on a crystal surface; the refracted light splits up into o-ray and e-rays.

Let 't' is the thickness of crystal at which path difference of o-ray and e-ray is λ, then

Path difference of o-ray and e-ray = $\lambda/4$ --(1)
optical path of o-ray = $\mu_o t$,optical path of e-ray = $\mu_e t$
optical path difference between o-ray and e-ray = $(\mu_o \sim \mu_e)$ t ------------- (2)
from eqns (1) & (2),
$(\mu_0 \sim \mu_e)$ t = $\lambda/4$

$$t = \lambda/4(\mu o \sim \mu e)$$

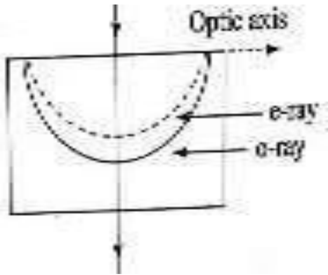


Figure: Quarter Wave Plate

Malus Law: The intensity of polarized light by a polarizer is directly proportional to the square of cosine angle between polarizer and analyzer.

$I \alpha \cos^2\theta$.

Hence $I= I_0 \cos^2\theta$

Optical Activity: The property of rotating the vibrations of plane polarized light by a substance is called as optically activity and the substance is called as optically active substance.

Specific rotation: The angle of rotation of plane polarized light produced by 1decimeterslength in an optically active substance of concentration of 1gr/cc.

Polari meter: The optical instrument which measure the angle of rotation of vibrations of plane polarized light by optically active substance.

Saccharimeter: The optical instrument used to determine the angle of rotation of polarized light by sugar solution is called as saccharimeter.

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Engineering Physics Material
Common to all branches of 1st B. Tech

Subject Code: 23ABS993 (AK23 Regulation)
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Unit-II

Crystal structures and X-ray diffraction

Introduction:

The matter in this beautiful world is found to exist in many states, namely solids, liquids and gases, plasma and Bose-Einstein condensation etc.

All that is limited by form, semblance, sound, color is called object.
Among them all, man alone is more than an object.
Though, like objects, he has form and semblance,
He is not limited to form.
He is more.
He can attain to formlessness. ..Chang Tzu

Solid:

- All that is (The whole) limited by form, semblance (shape), size, sound, color is called solid.
- It is one of the states of matter.
- It consists of a large number of closely packed atoms or molecules. The physical structure of a solid and its properties related to the arrangement of atoms or molecules within it.

Every solid element has its own internal structure.
It may be crystal or amorphous in the nature.

Crystallography is the way to study the crystal structures as they are.

Crystallography:

The word "crystallography" derives from the Greek words ***krystallon*** = clear ice, with its meaning extending to all solids with some degree of transparency, and ***grapho*** = write.
The study of the geometrical form and other physical properties of crystalline solids by using X-Ray, electron beams and neutron beams etc. is termed as the science of crystallography.
It is the

a) Experimental science of determining the arrangement of atoms in solids.

b) The study of crystals.

Note:X-ray are most widely used to study the crystal structure because, the wavelength of X-rays (10^{-12} to 10^{-10} m) is almost equal to that of the interatomic distance and hence diffraction can easily occur, when they are passed through the crystal.

Classification of solids:

Every solid element has its own internal structure. The internal structure of solid depends on the internal arrangement of atoms or molecules or ions.
Solid are classified in two categories based on the internal arrangement of atoms or molecules.

1. Crystalline solid or crystals
2. Amorphous solids or no-crystalline solids

1. Crystalline solids or crystals:

Solids that have a definite shape and size are called crystalline solids.
The word crystal comes from Greek word ***krystallone*** which means "**clear ice** ''

Properties of crystalline solids:

- In Crystal solids, the atoms or molecules are arranged in a regular and periodically in three-dimensional manner.
- If the crystal breaks, the broken pieces also have regular shape.
- They have characteristic geometrical shape.
- Some crystalline solids are anisotropic i.e. the magnitude of physical properties (such as refractive index, electrical conductively, thermal conductively, etc.) are different along different directions of the crystals.
- Melting point of crystalline solids is extremely sharp. Because, when the temperature increases, bonds break at the same time.
- They are most stable.
  Examples**: i. Metallic crystals:** Gold, Silver, Aluminum, etc.

ii. None-metallic crystals: Diamond, Silicon, Germanium, and Sodium chloride etc.

Again crystalline solids are classified into two types; they are single crystalline solids and poly crystalline solids.

Single crystals or mono crystals:

- Single crystal which contains only one crystal.
- There are no grain boundaries in these crystals.
- Single crystal may consist of same atoms or different types of atoms and yet all the atoms or molecules are arranged in a regular and periodically in three-dimensional manner.
- Single crystals naturally form as they are and yet they produce artificially from their vapor or liquid state.

- Most of the single crystals have different refractive index, electrical conductivity as well as mechanical strength different in all directions. This is also known as the anisotropic behavior of the crystals.

Examples of Single crystals:

Quartz, salt, diamond, Graphite and snowflakes, pearls, gem stones (such as Sapphire, Ruby, Fluorite and emeralds et...)

Poly crystals:

- Poly crystals which composed of many microscopic or tiny crystals are called grains.
- Fig (b) shows the diagram of poly crystalline material. Notice that this type of material there exists some mismatch within the region where two grains meet. This area is called grain boundary.
- Due to the mismatch math of grains, defects are formed in the crystals.
- Examples of polycrystalline solids include the common metals, and ceramics, sulfur, etc.

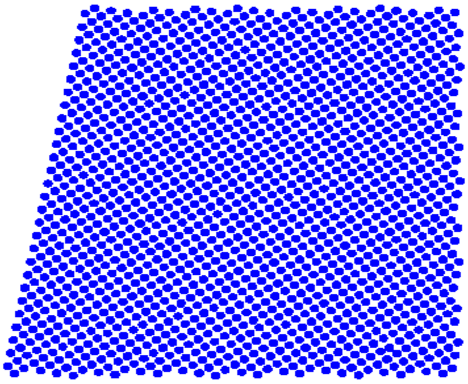


Fig (a) Model of a perfect single crystal

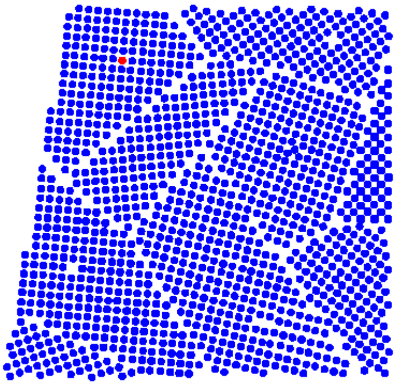
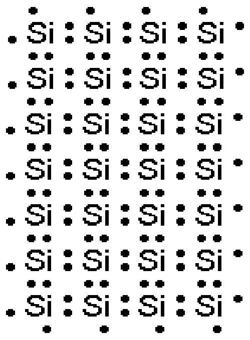
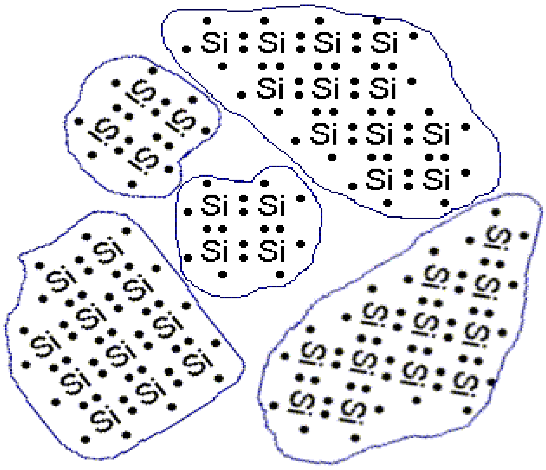


Fig (b) Model of a poly-crystal with many defects

Example:



Monocrystalline

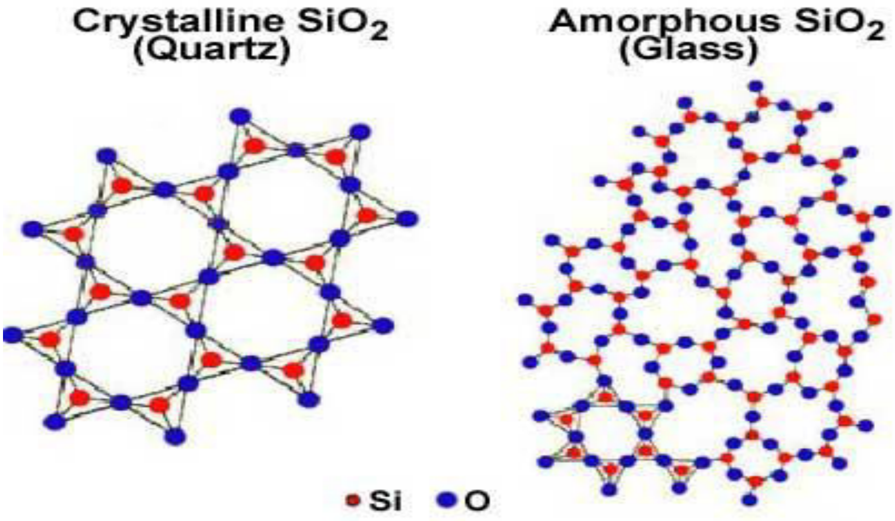


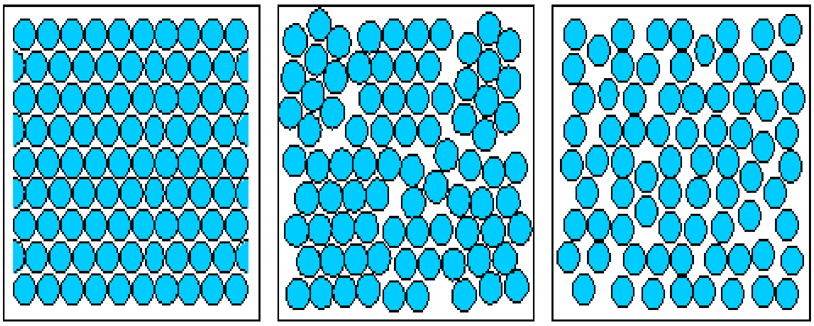
Multicrystalline

Amorphous solids or Non-crystalline solids:

The word **amorphous** comes from the Greek ***a*** means without, and ***morphé***, means shape, form)

- In amorphous solids, the atoms or molecules are arranged in an irregular manner.
- If an amorphous solid breaks, the broken pieces are irregular in shape.
- They do not have sharp melting points.
- They are less stable.
- Example Glasses, plastics, Rubbers etc.





Single crystal — Periodic across the whole volume.

Polycrystal — Periodic across each grain.

Amorphous solid — Not periodic.

Language of crystals or crystal geometry:

Crystal geometry is useful to understand the crystal structures. If we want to understand the crystal structures, some basics are needed. Crystal geometry gives us those basics.

Crystal lattice (or) space lattice:

A crystal structure can be studied in terms of an idealized (imaginary) geometrical concept is called a space lattice.

According to this concept,

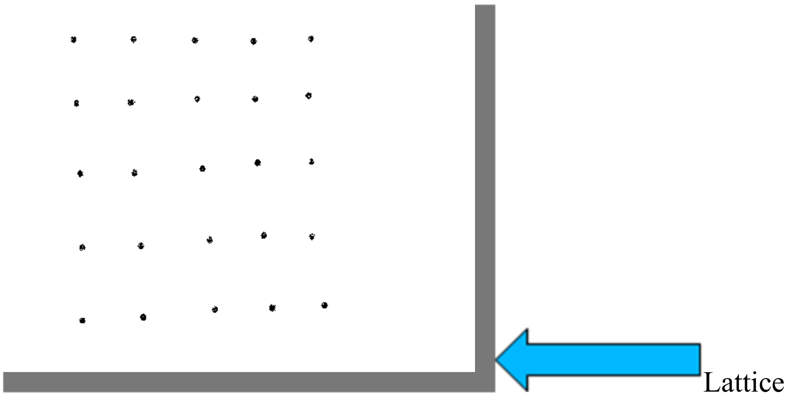
- Each atom in the structure can be replaced by a point in space .These points are known as lattice points.
- A Three dimensional collection of points in space are called space lattice or A Geometrical representation of the crystal structure in terms of lattice points is called "space lattice (or) crystal lattice ".
- Lattice points are an array points in space.
- Lattice points are arranged in regular and periodically in three-dimensional order in space or array of points in space. In which every lattice point has the same environment with respect to all other points.
- Lattice points are geometrical points.
- Lattice points denote the position of atoms (or) molecules or ions in the crystal (fig.1)

It is an imaginary concept.

1D- lattice:

It is defined as an infinite array of points in one-dimensional space in which every lattice point has the same environment with respect to all other points.

- In 1D there is only one kind of lattice
- This lattice can be described by a single lattice parameter (a)
- The unit cell for this lattice is a line segment of length **'a'.**



2D- Lattice:

It is defined as an infinite array of points in two-dimensional space in which every lattice point has the same environment with respect to all other points.
A two dimensional space lattice is shown in fig. Consider an origin “O” a in XY-plane .two translational vectors a and b are taken along X-axis and Y-axis respectively. The resultant vector op = T

$$\vec{T} = n_1 a + n_2 b \text{ -------------------- } (1)$$

Where n_1 and n_2 are the integers and a and b are the fundamental translation vectors along x and y directions.

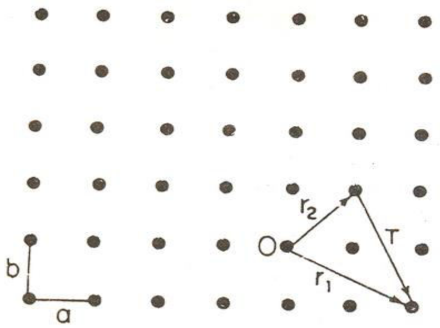


Figure 2: Two-dimensional array of points

(**NOTE:** Consider a lattice point at ‘O’ AS origin. And join the origin to successive lattice points along x and y directions. Let the position vectors of these lattice points be a and b. when a is repeated regularly, then it gives the position of lattice points along the x direction, i.e., 2a, 3a, 4a…similarly, if b is repeated regularly, then it gives the position of lattice points along the y direction,i.e., 2b,3b,4b,…since, a and b when repeated regularly give the array of lattice points in space, they are known as fundamental translational vectors or basic vectors or primitive vectors)..

3D- Lattice:

It is defined as an infinite array of points in three-dimensional space in which every lattice point has the same environment with respect to all other points**.**
In this case, the resultant position vector can be expressed as

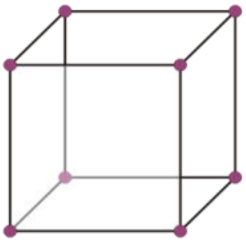
$$\boldsymbol{T = n_1 a + n_2 b + n_3 c} \text{ -------------------- } \mathbf{(2)}$$

Where n_1, n_2 and n_3 are the integers and a, b and c are the fundamental translation vectors along x, y, and z directions.

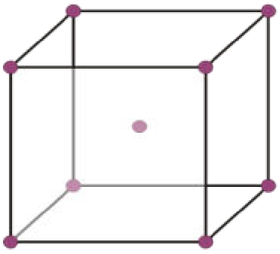
The possible types of Bravias lattices are four and following names and symbols represent them,

Primitive lattice-P, Body centered lattice-I, Face centered lattice-F, and Base centered lattice-C.

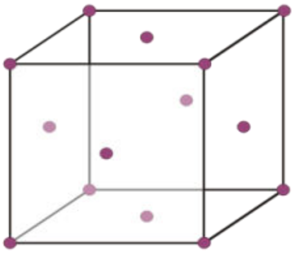
- In the simple primitive lattice (P), the lattice points are situated only at the corners of the unit cell.



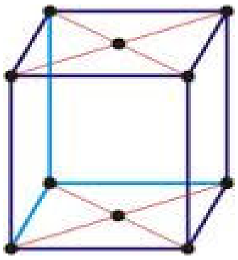
- In the body- centered lattice (I - from the German "Innenzentriert” means inner centered), the lattice points are situated at the corners and also at the intersection of the diagonals (centre) of the unit cell.



- In the face- centered lattice (F- from the German "Flächenzentriert” means face centered), the lattice points are lie at the corners and also at the centers of all the six faces of the unit cell.

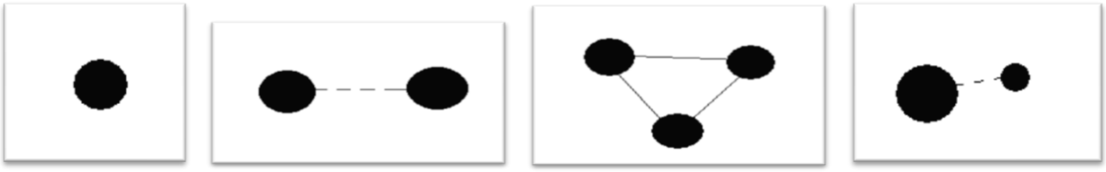


- In the base- centered lattice (C), the lattice points are lie at the corners as well as at the centers of the unit cell, which are opposite to each other.



2. Basis (or) motif: A Group of atoms or molecules or ions is called ‘Basis’

- ❖ Basis may consist of single atom or a group of atoms.



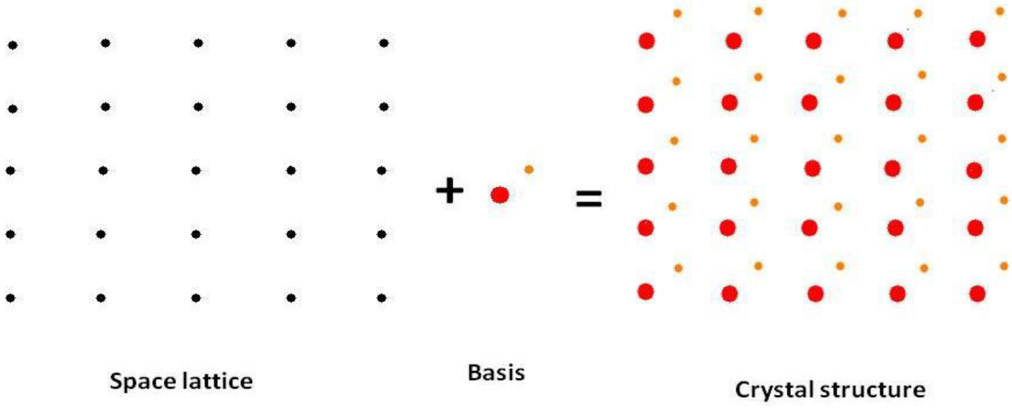
(a) single atom (b) Di atomic molecule (c) Tri atomic molecule (d) Ion

3. Crystal structure:

- ➢ Crystal structure is a combination of lattice and basis.
- ➢ A crystal structure is formed by adding basis (atoms) to every lattice point of the space lattice. The number of atoms in the basis may be one or more than one.
- ➢ Thus the crystal structure is real and the crystal lattice is imaginary

Mathematically

$$\boxed{\textbf{Crystal structure = space lattice + basis}}$$



3. Unit cell:

- ➢ Crystal structure can be defined in terms of unit cell.
- ➢ The unit cell is the smallest block or geometric figure of crystal, from which the entire crystal is built up by repetition in three dimensional manners.
- ➢ It represents the actual structure of crystal.
- ➢ The three dimensional representation of unit cell is as shown in figure.

Definition of Unit cell :

The smallest possible geometrical figure which repeats regularly gives actual crystal structure is called unit cell.

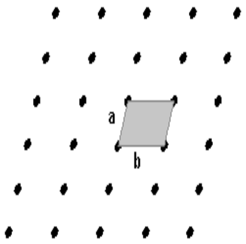


Fig. Unit cell in 2D -space lattice

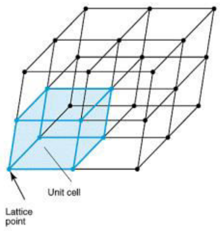


Fig. Unit cell in 3D -space lattice

Types of unit cells:

There are two distinct types of unit cells: **primitive** and **non-primitive**.

1. Primitive cell:

- A primitive cell is the simplest type of unit cell which contains only one lattice point per unit cell (contains lattice points at its corner only).
- Primitive unit cells contain only one lattice point, which is made up from the lattice points at each of the corners.
- Ex: Simple cubic (SCC)

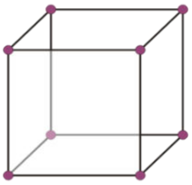
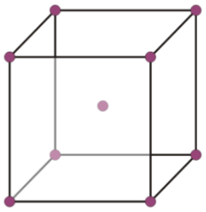


Fig: Simple Cubic

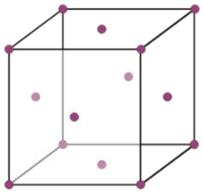
2. Non-primitive cell:

- If there are more than one lattice points in a unit cell, it is called a Non-primitive cell.
- Non-primitive unit cells contain additional lattice points, either on a face of the unit cell or within the unit cell, and so have more than one lattice point per unit cell.

Ex: BCC and FCC contain more than one lattice point per unit cell.



(a) BCC



(b) FCC

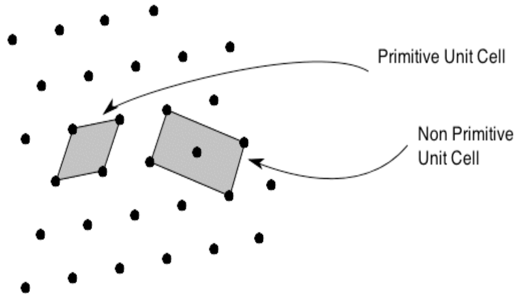


Fig: primitive and non- primitive unit cell in 2D-Spce lattice

Lattice parameters of unit cell:

Definition:

To represent a lattice unit cell, we require the six parameters i.e., *Axial lengths (a, b, c) and interfacial angles (α, β, γ)* these quantities are known as "Lattice Parameters".

i.e., Lattice parameters are

1. Axial lengths (a,b,c)
2. Interfacial angles (α, β, γ)

Explanation:

Consider a cubic unit cell with crystallographic axes X, Y, Z as shown in figure.

Let OA=a, OB=b, and OC=c be the intercepts made by the unit cell along the crystallographic axes. These quantities a, b and c are called translational vectors (or) axial lengths or primitives. The angles between the three crystallographic axes are known as interfacial angles. The angle between a and b is alpha (α) and b and c, is beta (β), and that between a and c is gamma (γ). These three angles (α, β, γ) are called **interfacial angles**.

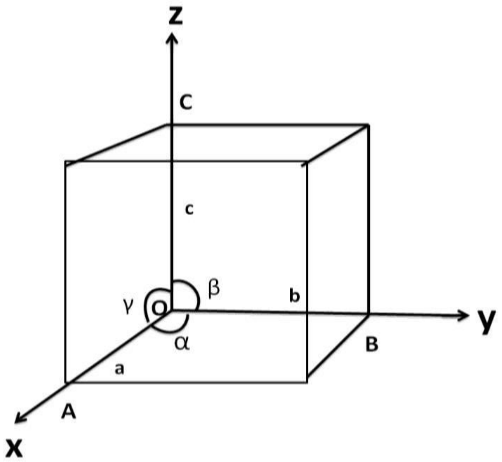


Fig: Cubic unit cell

The crystal systems and Bravias lattices:

Crystals are classified in to 7 crystal systems on the basis of lattice parameters viz:

(i) Axial lengths a ,b, c and
(ii) Interfacial (axial) angles α, β, γ.

The 7 basic crystal systems are

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

Bravais Lattices:

Bravais in 1880 showed that there are 14 possible types of space lattices in the 7 crystal systems as shown in table.

According to Bravais, there are only 14 possible ways of arranging points in space lattice from the 7 crystal systems such that, all the lattice points have exactly the same surrounding. Theses 14 space lattices are called the Bravais lattices.

The 7 crystal systems and Bravias lattices are discussed briefly one by one as follows.

1. Cubic crystal system:

In cubic crystal system, the three crystal axes perpendicular to each other and axial lengths are the same along the entire three axes as shown fig.

Lattice parameters:

All three sides equal, $a=b=c$
All three right angles, $\alpha=\beta=\gamma=90^0$

Examples: Pb, Hg, Ag, Po, Au, Cu, ZnS, diamond, KCl , CsCl , NaCl, Cu_2O , CaF_2 and alums etc.

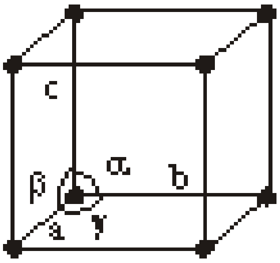
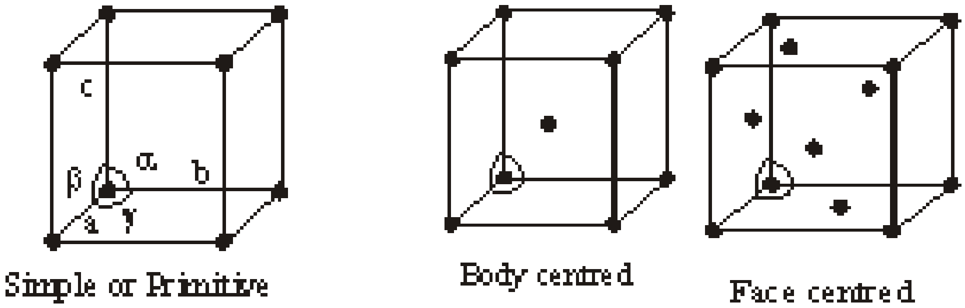


Fig: cubic system

Possible Bravais lattices:

- Primitive
- Body centered
- Face centered.



Simple or Primitive

Body centred

Face centred

Fig: Possible Bravias lattices of cubic system

2. Tetragonal System:

In tetragonal system, the three crystal axes are perpendicular to each other. Two of the three axis lengths are the same, but the third length is different, as shown in fig.

Lattice parameters:

- Two sides equal , $a=b \neq c$
- All three right angles; $\alpha = \beta = \gamma = 90^0$

Examples:

$NiSO_4$, SnO_2 and Indium

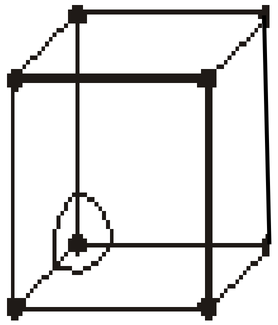


Fig: Tetragonal

Possible Bravais lattices:

- Primitive
- Body centered

Fig: Possible Bravais lattices of tetragonal system

3. Orthorhombic Crystal System:

In orthorhombic crystal system, the crystal axes are perpendicular to each other and all the three axial lengths are of unequal lengths (different), as shown in fig.

Lattice parameters:

- All the sides different $a \neq b \neq c$
- All three right angles; $\alpha = \beta = \gamma = 90^0$

Examples: KNO_3, $BaSO_4$ and $MgSO_4$ etc

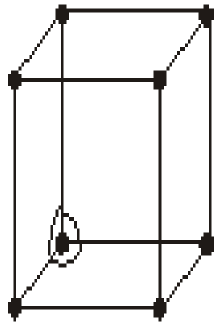


Fig: Orthorhombic

Possible Bravais lattices:

- Primitive
- Body centered
- Base centered
- Face centered.

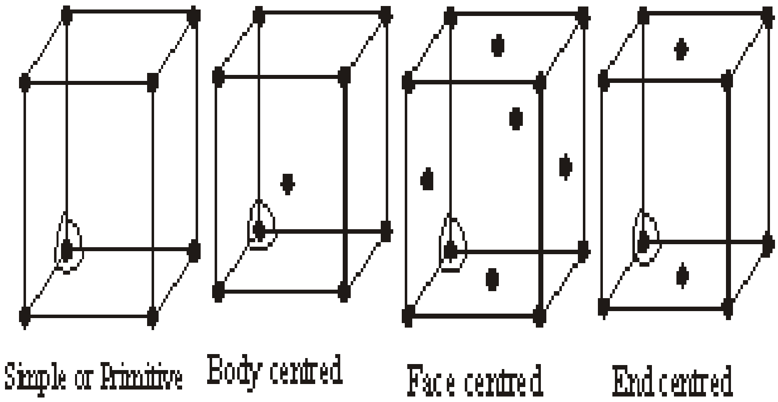


Fig: Possible Bravias lattices of orthorhombic system

4. Monoclinic Crystal system:

In monoclinic crystal system, two of the crystal axes perpendicular to each other, but the third obliquely
Inclined. The three axial lengths are different along the axes as shown in Fig.

Lattice Parameters:

- All the sides different $a \neq b \neq c$
- Two right angles, third arbitrary $\alpha=\beta=90^0$, $\gamma \neq 90^0$

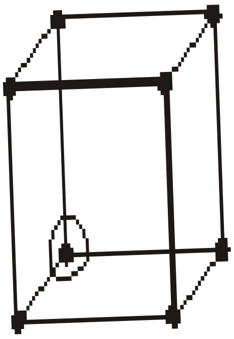


Fig: Monoclinic system

Examples: Na_2SO_4, $FeSO_4$, NO_2SO_3 etc

Possible Bravais lattices:

- Primitive
- Base centered

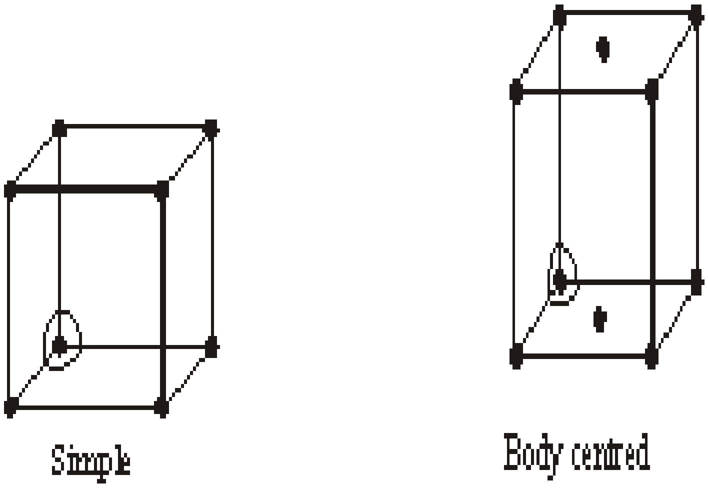


Fig: Possible Bravias lattice of monoclinic system

5. Triclinic crystal system:

In triclinic crystal system, all the three crystal axes are not perpendicular to each other. The axial lengths are also not equal (different) along the three axes, as shown in fig.

Lattice parameters:

- All three sides different $a \neq b \neq c$
- All three angles different $\alpha \neq \beta \neq \gamma \neq 90^0$

Examples: $CuSO_4$ and $K_2Cr_2O_7$

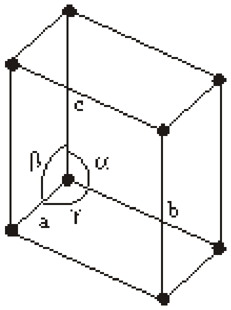


Fig: Triclinic system

Possible Bravais lattices:

- Primitive

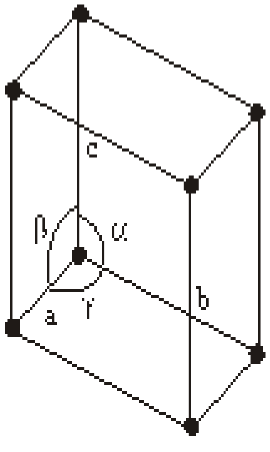


Fig: Possible Bravias lattice of triclinic system

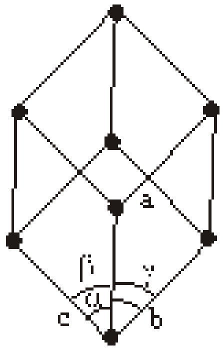
6. Trigonal (rhombohendral) crystal system:

In trigonal crystal system, the three axes are inclined to each other at an angle other 90^0. The three axial lengths are equal along three axes as shown in fig.

Lattice parameters:

- All the sides equal a=b=c
- All three angles equal, of arbitrary value $\alpha=\beta\neq 90^0$

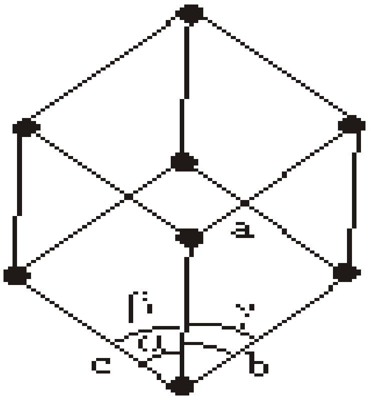
Examples: CaSO$_4$, Bi, Sb, Calcite etc



Rhombohedral **OR**
Trigonal system

Possible Bravais lattice:

- Primitive



Rhombohedral

Fig: possible Bravias lattice of rhombohedral system

7. Hexagonal system:

In hexagonal crystal system, two of the crystal axes are 90^0 apart, while the third is perpendicular to both of them. The axial lengths are the same along three axes that are 90^0 apart, but the axial length along the third axis is different as shown in figure.

Lattice parameters:

- Two sides equal, third arbitrary $a=b\neq c$
- Two right angles, third angles 120^0, $\alpha=\beta=90^0$; $\gamma=120^0$

Examples:

Tourmaline, Quartz, AgI and SiO_2

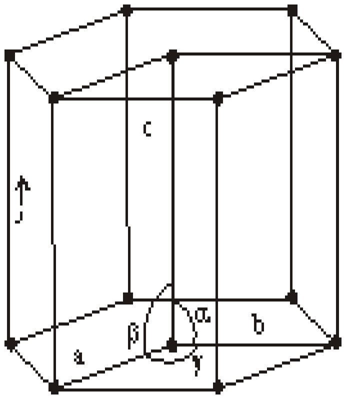


Fig: Hexagonal system

Possible Bravais lattices:

- Primitive.

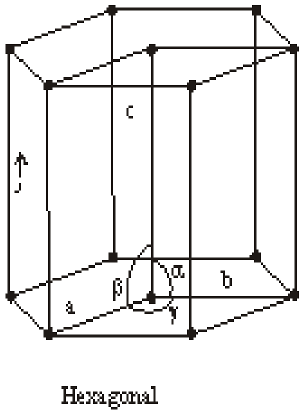


Fig: possible Bravias lattice of hexagonal system

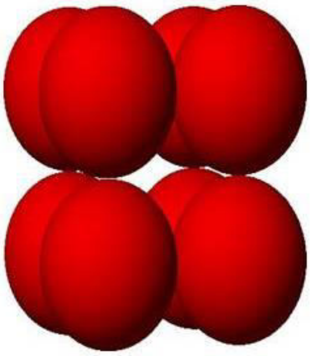
Structures of cubic system:

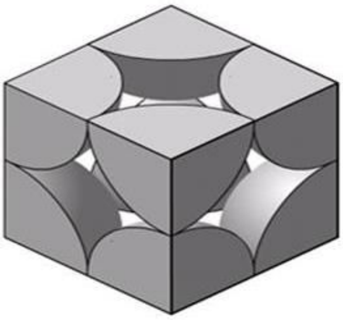
There are three types of structures possible in this system depending on the position of the lattice point (atoms) in the unit cell fig.

(1) Simple cubic (sc) (or) primitive
(2) Body centered cubic (BCC) and
(3) Face centered cubic (FCC)

1. Simple cubic (SCC) crystal structure:

- In this structure; there are only 8 atoms one at each corner of the cube.
- The corner atoms touch each other along the edges as shown in fig.
- Each and every corner atom is shared by 8 adjacent unit cells.





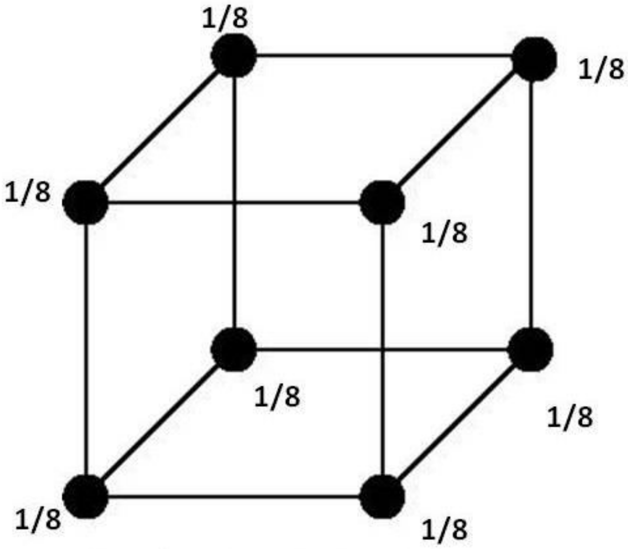


Fig: Simple cubic structure

(B) Body-centered cubic structure (BCC):

- In this case, we have two types of atoms fig,(i) corner atoms and (ii) Body centered atoms i.e., there are 8 corner atoms, one at each corner of the unit cell and one body centered atom at the centre of the unit cell as shown in fig.
- In this structure, the corner atoms do not touch each other. But each corner atom touches the body centered atom along the body diagonal as shown in fig.
- Each and every corner atom is shared by 8 adjacent unit cells and the body centered atom is shared by that particular unit cell alone and is not shared by any other unit cell.

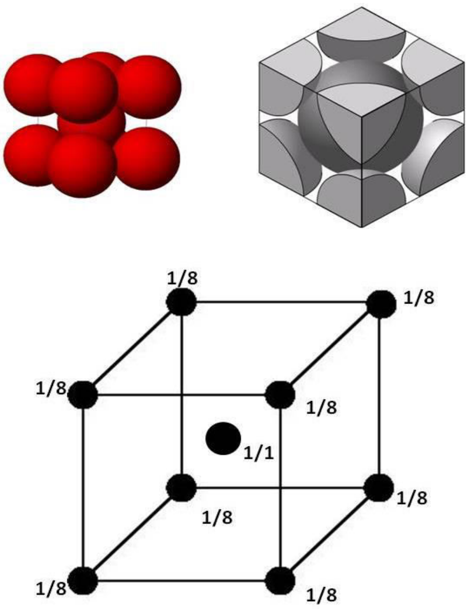


Fig: Body centered cubic structure

(C) Face-centered cubic structure (FCC):

- In this case, we have two types of atoms viz (i) Corner atoms and (ii) Face centered atoms, i.e. there are 8 corner atoms, one at each corner of the unit cell and six atoms at the centers of six faces of unit cell as shown in Fig.
- In this structure, the corner atoms do not touch each other. But each corner atom touches the face centered atoms along the diagonal of the face of the cube as shown in fig.
- Each and every corner atom is shared by adjacent unit cells, and each face centered atom is shared by only two unit cell, which lie on either side of the atom.

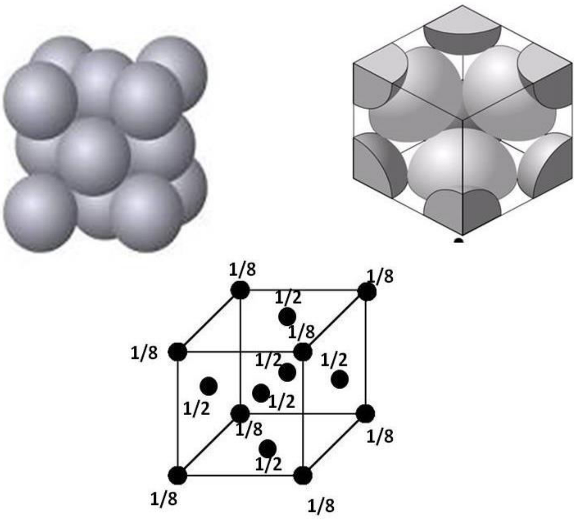


Fig :Face-centered cubic structure (FCC)

Parameters determing the crystal structure of materials:

Let is discuss some of the important parameters which are used to describe the crystal structure.

1. Number of atoms per unit cell (or) Effective number:

The total number of atoms present in (or) shared by an unit cell is known as number of atoms per unit cell.

2. Co-ordination number:

It is the number of nearest neighboring atoms to a particular atom.

3. Atomic radius:

Atomic radius is defined as half of the distance between any two nearest neighbor which have direct contact with each other, in a crystal of pure element. It is usually expressed in terms of cube edge ‘a’.

4. Atomic packing factor (packing density):

Atomic packing factor is defined as the ratio between the volume occupied by the total number of atoms per unit cell (v) to the total volume of the unit cell (V).

$$\text{i.e. APF} = \frac{\text{Volume occupied by the total no.of atoms per unitcell}}{\text{Total volume of the unit cell}} = v/V$$

$$= \frac{\text{No.of atoms per unit cell x volume of oneatom}}{\text{Total volume of the unit cell}}$$

5. Void space or interstitial space:

The void space in the unit cell is the vacant space left unutilized in the unit cell. It is equal to (1-APF). It is often expressed as percentage.

$$\text{Void space} = (1\text{-APF}) \times 100$$

6. Density of solid:

The density of a crystalline solid is defined as the ratio of the unit cell and the volume of a unit cell.

$$\text{Density } (\rho) = \frac{\text{Mass of unit cell}}{\text{volume of unit cell}}$$

Let us discuss all the above parameters one by one for a simple cubic structure.

Number of atoms per unit cell:

Definition:

The total number of atoms present in (or) shared by a unit cell is known as number of atoms per unit cell.

Note: This number depends on the number of corner atoms, body centered atom face centered atom, which varies from structure to structure.

Let us evaluate the number of atoms per unit cell for the three systems.

(a) Simple cubic structure:

Figure (1) shows the unit cell of simple cubic structure. In this case, there are only 8 atoms, one at each corner of the cube (or) the unit cell.
But in actual crystal, each and every corner atom is shared by 8 adjacent unit cells. In other words, we can say that each corner atom contributes only 1/8th of its part to a single unit cell.
i.e., total number of atoms per unit cell = $\frac{1}{8}$ x total number of corner atoms

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

Therefore, the number of atoms per unit cell in S.C is one. Thus, ***simple cubic is a primitive unit cell.***

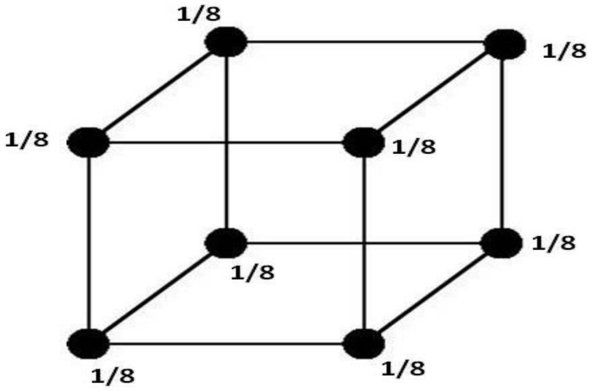


Fig: Simple cubic structure

(b) Body centered cubic structure:

In this case, we have two types of atoms namely
(i) Corner atoms (ii) Body centered atom

i.e., there are 8 corner atoms, one at each other corner of the unit cell and one body centered atom at the centre of the unit cell as shown in fig.

i) Number of corner atoms per unit cell:

Each and every corner atom is shared by 8 adjacent unit cells.
The total number of corner atoms per unit cell = $\frac{1}{8}$ x8=1

(ii) Number of body centered atoms per unit cell:

The body centered atom is shared by that particular unit cell alone and is not shared by any other unit cell.

The number of body centered atoms per unit cell =1/1 x1=1

Total no. of atoms = Total no. of corner atoms per unit cell in Bcc + Total no. of body centered atoms per unit cell.
=1+1 = 2

Therefore, the number of atoms per unit cell in BCC is two. Thus, *BCC is a non-primitive unit cell.*

(C) Face-centered cubic structure:

In this case, we have two types of atoms namely
(i) Corner atoms (ii) Face centered atoms.

i.e. there are 8 corner atoms, one at each corner of the unit cell and six atoms at the centers of six faces of unit cell as shown in fig.

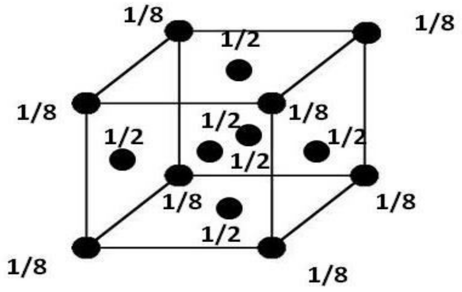


Fig :Face-centered cubic structure (FCC)

(i) Number of corner atoms per unit cell :

Each and every atom is shared by 8 adjacent unit cells.
The total number of corner atoms per unit cell= $\frac{1}{8}$ x 8=1

(ii) Number of face centered atoms per unit cell:

Each face centered atom is shared by only two unit cells, which lie either side of the atom (similarly we have six face centered atoms in an unit cells)
The total number of centered atoms per unit cell = (1/2) x6 = 3

The total no. of atoms per unit cell in FCC= Total number of corner atoms per unit cell + total no. of face centered atoms per unit cell =1+3 = 4

Therefore, the number of atoms per unit cell in FCC is four. Thus, ***FCC is a non-primitive unit cell.***

Coordination Number:

Definition:

Coordination Number is defined as the number of nearest neighboring atoms to a particular atom which are direct contact with each other.

The Coordination Number for the three types of cubic crystal structure can be calculated as follows.

(a) Simple Cubic Structure:

In this case, there are only 8 atoms, one at each corner of the cube (or) unit cell. For a particular atom say ‘C’ atom, there are 4 nearest neighboring atoms, i.e. atoms 1,2,3 and 4 on its own plane and there are 2 more nearest atoms i.e., atom-5 directly above the plane and atom-6 directly below the plane as shown in figure.

Therefore, The total Number of neighboring atoms to particular atom (C) =4+1+1=6

Hence, the coordination for SCC =6

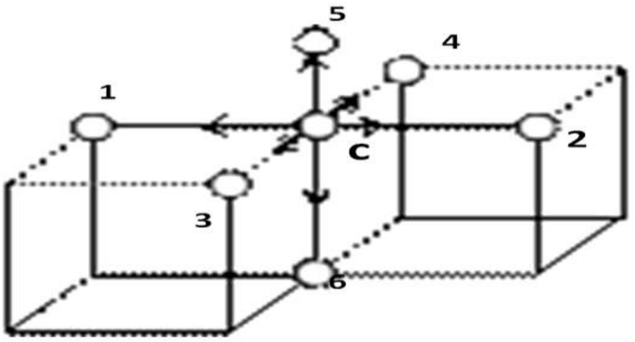


Fig: Co- ordination number in Simple cubic structure

(b). Body centered cubic Structure:

In this case, we have two types of atoms namely 1.Corner atoms 2. Body centered atoms i.e., there are 8 corner atoms, one at each corner of the unit cell and one body centered atom at the center of the unit cell as shown in figure.

The corner atoms do not touch each other. But each corner atom touches the body centered along the body diagonal. Thus for particular atom **‘C’** at the body centre obviously, there are 8 nearest neighbor (corner atoms).

Hence, the coordination for BCC =8

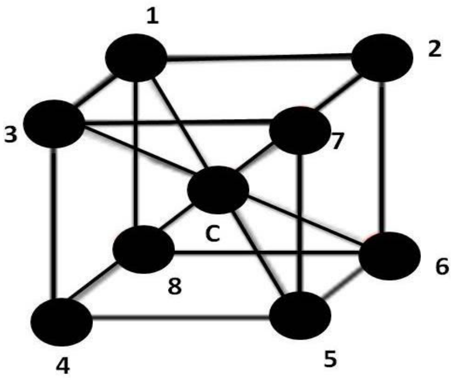


Fig: Co- ordination number in Base centered cubic structure.

(C). Face Centered Cubic Structure (FCC):

In this case, we have 2 types of atoms namely, 1.Corner atoms and 2. Face centered atoms. There are 8 corner atoms, one at each corner of the unit cell and six atoms at the centers of six faces of unit cells as shown in figure.

Let us consider 2 unit cells one above the other if the reference atom '**C**' taken as the face centered atom then it is surrounded by **4** corner atoms on the plane , and 4-face centered atoms above the plane and 4-face centered atoms below the plane as shown figure.

Therefore the coordination number for FCC=4+4+4=12

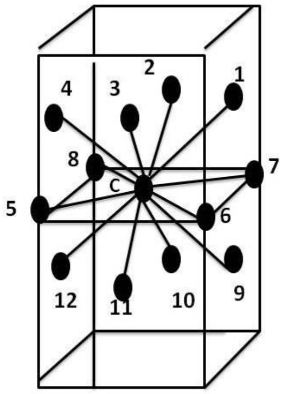


Fig: Co- ordination number in Face centered cubic structure.

Atomic Radius:

Definition:

Atomic radius is defined as half of the distance between any two nearest neighbor atoms which have direct contact with each other.

It can be expressed in terms of cube edge **a** and vice versa. All the atoms are assumed to be spherical in shape.

For the three cubic structures it can be calculated as follows.

(a) Simple Cubic Structure:

In simple cubic (SC) structure the corner atoms touch other along the edges as shown in fig.
Let us consider one of face of the simple cubic structure as shown in fig (2).
Hence the nearest neighbor distance is 2r = a

$$\therefore \quad \textbf{Atomic radius } r = \frac{a}{2}$$

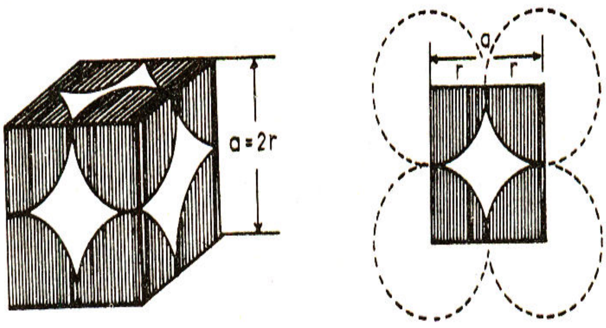


Fig: simple cubic structure

(b) Body centered cubic structure (BCC):

In BCC structure, the corner atoms do not touch each other. But each corner atom touches the body centered atom along the body diagonal as shown in fig. Therefore the two corner atoms **(A and D)** situated at the opposite ends can be joined by drawing a diagonal as shown in fig. Thus, the diagonal of the cube **AD** is 4r.

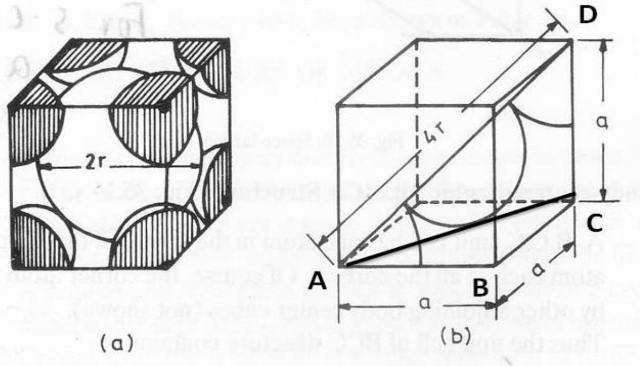


Fig :Body centered cubic structure (BCC)

But, from the geometry of the fig; we can write

$$(AD)^2 = (AC)^2 + (CD)^2$$
$$= (AB)^2 + (BC)^2 + (CD)^2$$

From fig ; $AC^2 = AB^2+BC^2$ and $AB=BC=CD=a$

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

$= 3a^2$

$AD=a\sqrt{3}$; But $AD = 4r$

$4r = a\sqrt{3}$

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

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

(C) Face-centered cubic structure (FCC):

In FCC structure the corner atoms do not touch each other. But each corner atom touches the face centered atoms along the diagonal of the face of the cube as shown in fig. Therefore, the two corner atoms (**A and C**) situated at the opposite ends of the same face can be joined by drawing a diagonal a shown in fig. Thus, the diagonal of the cube **AC=4r.**

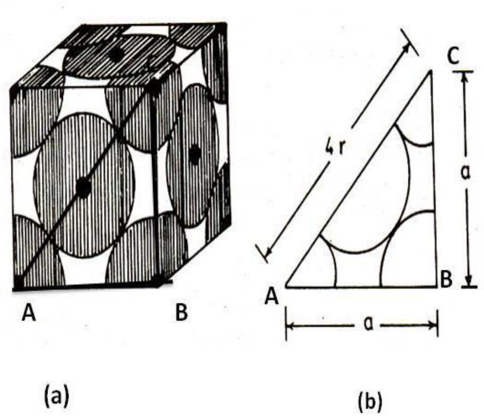


Fig :Face centered cubic structure (FCC)

From the geometry of the figure, we can write

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

$= a^2 +a^2$

$AC^2 = 2a^2$

$AC = a\sqrt{2}$; But **AC=4r**

$4r = a\sqrt{2}$

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

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

4. Atomic packing factor (APF) or packing density:

Definition:

Atomic packing factor is defined as the ratio of the volume occupied by the total number of atoms per unit cell to the total volume occupied by the unit cell.

$$APF = \frac{\text{Volume occupied by the total no.of atoms per unitcell}}{\text{Totalvolume of the unit cell}} = v/V$$

$$= \frac{\text{No.of atoms per unit cell x volume of one atom}}{\text{Total volume of the unit cell}}$$

The packing factor (or) packing density of the three cubic systems can be calculated as follows.

(a) Simple cubic structure (SCC):

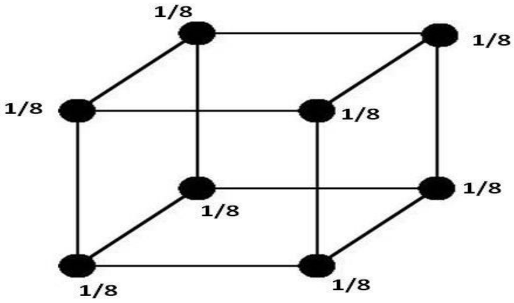
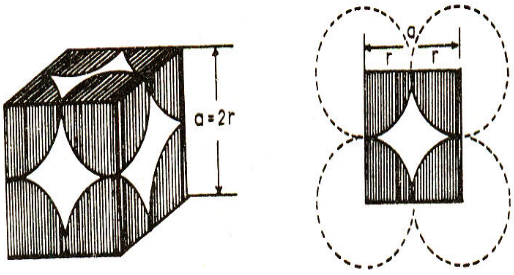


Fig: Simple cubic structure



In simple cubic,

The number of atoms per unit cell=1

Volume of 1 atom (spherical) = $\frac{4}{3}\pi r^3$

∴ Volume occupied by the total no. of atoms per unit cell (v)

= No. of atoms per unit cell x volume of one atom

$= 1x \ \frac{4}{3}\pi r^3$

We know the radius of atom in simple cubic $r = \frac{a}{2}$

$$=1x1x\ \frac{4}{3}\pi\left(\frac{a}{2}\right)^3$$

Volume of the unit cell (V) = length x breadth x height

We know that for a cubic system, length=breath=height=a

$$\therefore V=a\ x\ a\ x\ a$$
$$= a^3$$

$$APF = \frac{\text{Volume occupied by the total no.of atoms per unitcell}}{\text{Totalvolume of the unit cell}} = v/V$$

$$= \frac{\text{No.of atoms per unit cell x volume of one atom}}{\text{Total volume of the unit cell}}$$

$$= \frac{1\times\frac{4}{3}\pi(\frac{a}{2})^3}{a^3}$$

$$= \frac{\pi}{6}$$

$$= 0.052$$

$$\boxed{\therefore APF = \frac{\pi}{6} = 0.052}$$

And Void space = (1-APF) x 100

= (1-0.52) x 100

=48%

Therefore, we can say that 52% volume of the unit cell of sc is occupied by atoms and remaining 48% volume is vacant. Thus, the packing density 52%.
Since the packing density is very low, SC has loosely packed structure.

(b) Body-centered cubic Structure (BCC):

In body-centered cubic structure,

The number of atoms per unit cell=2

Volume of one atom (spherical) $=\frac{4}{3}\pi r^3$

$\therefore$ Volume occupied by the total no. of atoms per unit cell (v) = No.of atoms per unit cell x Volume of one atom.

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

$$=2\ x\frac{4}{3}\pi[a\sqrt{3}/4]^3$$

$$= \frac{8\pi}{3}\left[\frac{a^3 x\ 3\sqrt{3}}{4x4x4}\right]$$

$$\mathbf{v} = \pi a^3\ \sqrt{3}/8$$

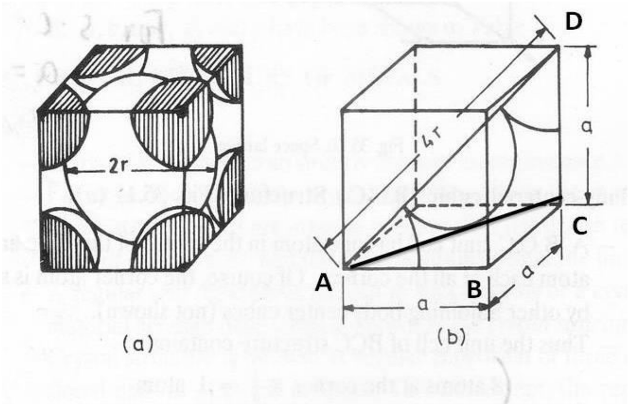


Fig :Body centered cubic structure (BCC)

Volume of the unit cell for a cubic system (V) $=a^3$

$$\therefore \text{APF} = \frac{\text{Volume occupied by the total no.of atoms per unitcell}}{\text{Totalvolume of the unit cell}}$$

$$= v/V$$

$$= \frac{\text{No.of atoms per unit cell x volume of one atom}}{\text{Total volume of the unit cell}}$$

$$= \pi a^3\sqrt{3}/8/a^3$$

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

$$= 0.68$$

$$\boxed{\therefore \ \text{APF}=\frac{\pi\sqrt{3}}{8}=0.68}$$

And Void space = (1-APF) x 100
= (1-0.068) x 100
=32%

Therefore, we can say that 68% volume of the unit cell of BCC is occupied by atoms and remaining 32% volume is vacant. Thus, the packing density 68%.
Since the packing density is very low, SC has loosely packed structure.

(C) Face-centered cubic structure:

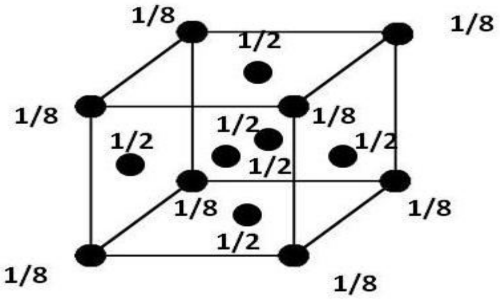
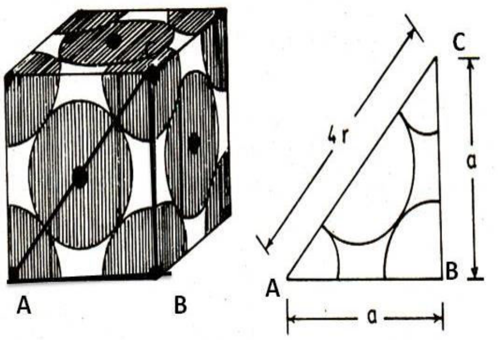


Fig :Face-centered cubic structure (FCC)

In face centered cubic structure,
The number of atoms per unit cell=4



(a) (b)

Fig :Face centered cubic structure (FCC)

Volume of one atom (spherical) = $\frac{4}{3}\pi r^3$

∴ Volume occupied by the total no.of atoms per unit cell (V) =No.Of atoms perunit cell x volume of one atom

$$=4 \text{ x} \frac{4}{3}\pi r^3$$

We know that the radius of atom in FCC is r =$\frac{a\sqrt{2}}{4}$

$$\therefore V = 4 \text{ x} \frac{4}{3}\pi\left(\frac{a\sqrt{2}}{4}\right)^3$$

$$= \frac{4\times4\pi}{3}(a^3 2\sqrt{2}/4\text{x}4\text{x}4)$$

$$= \frac{\pi a^3\sqrt{2}}{6}$$

Volume of the unit cell for a cubic system (V) =a^3

$$\text{APF} = \frac{\text{Volume occupied by the total no.of atoms per unitcell}}{\text{Totalvolume of the unit cell}}$$

$$= v/V$$

$$= \frac{\text{No.of atoms per unit cell x volume of one atom}}{\text{Total volume of the unit cell}}$$

$$= \frac{\frac{\pi a^3\sqrt{2}}{6}}{a^3}$$

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

$$= 0.74$$

$$\boxed{\therefore \ \text{APF}= \frac{\pi\sqrt{2}}{6} = 0.74}$$

And Void space = (1-APF) x 100

= (1-0.74) x 100

=26%

Therefore, we can say that 74% volume of the unit cell of FCC is occupied by atoms and remaining 26% volume is vacant. Thus, the packing density 74%.

Since the packing density is very high, FCC has closely packed structure.

Density of a crystalline solid:

The density of a crystalline solid is defined as the ratio of mass of the unit cell and the volume of a unit cell.

$$\text{Density } (\rho) = \frac{\text{Mass of unit cell}}{\text{Volume of unit cell}}$$

Expression for Lattice constant (a):

Let us consider a cubic unit cell of the following parameters.

- The lattice constant of the cell = a
- The number of atoms per unit cell= n
- The atomic weight of crystalline substance=M
- The density of unit cell= ρ
- The Avogadro's number =N_A
- The volume of unit cell =a^3

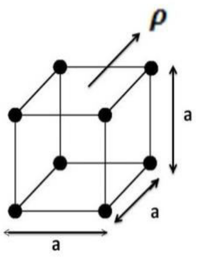


Fig:Cubic unit cell

$$\text{Mass of each atom in unit cell} = \frac{M}{N}$$

If there are 'n' no. of atoms in a unit cell, then the mass of the cubic unit cell = $\frac{nM}{N}$

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

$$\therefore \rho = \frac{nM}{N_A a^3}$$

$$\text{And} \quad a^3 = \frac{nM}{\rho N_A}$$

$$\boxed{a = \left(\frac{nM}{\rho N_A}\right)^{1/3}}$$

The above expression represents the expression for lattice constant.

The density for the three types of cubic crystal structure can be calculated as follows,

(a) Simple Cubic structure (SCC):

For SCC; n=1

$$\therefore \rho = \frac{M}{Na^3}$$

(b) Body-centered cube (BCC)

For BCC n=2

$$\therefore \rho = \frac{2M}{Na^3}$$

(c) Face centered cubic Structure (FCC)

For FCC; n=4

$$\therefore \rho = \frac{4M}{Na^3}$$

Miller indices-crystal planes:

Consider a two dimensional lattice with a periodic array of lattice points (fig 4.13).

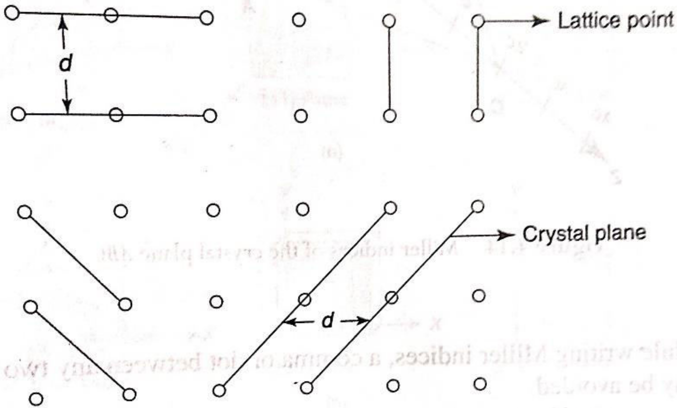


Figure 4.13 Crystal planes in two-dimensional lattice

Definition of Crystal plane:

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

Definition of interplanar spacing (d) :

The perpendicular distance between two adjacent crystal planes is called interplanar spacing (d).

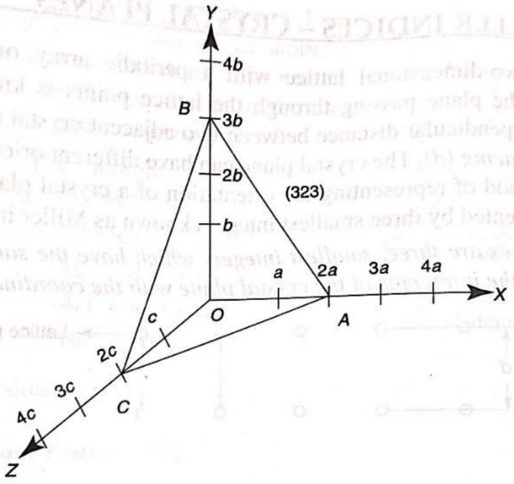


Figure 4.14 Miller indices of the crystal plane *ABC*

The crystal plane can have different orientations. Miller derived the method of representing the orientation of a crystal plane. The crystal plane is represented by three smallest integers known as Miller indices.

Definition of 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 :

1. The intercepts made by the crystal plane along x, y and z axes in terms of lattice parameters a , b , c are noted.
2. Express the intercepts as multiples of a, b, c .
3. Take the reciprocals of the intercepts.
4. Convert the reciprocals into integers by multiplying each one them with their LCM.
5. Enclose these integers in smaller parenthesis. This represents the Miller indices of the crystal plane.

For example, ABC is the crystal plane, which makes intercepts 2a,3b and 2c along the x,y and z axes respectively where a, b, c are the lattice parameters.

The intercepts as the multiples of a, b, c are 2, 3, 2.Reciprocals of the intercepts are $\frac{1}{2}$, $\frac{1}{3}$ and $\frac{1}{2}$ respectively.LCM is 6.Multiply the reciprocals by 6, so that they become integers 3,2,3.

The integers are written within the parenthesis as (323). (323) represents Miller indices of the crystal plane ABC.

Note :

1. While writing Miller indices, a comma or dot between any two numbers may be avoided.
2. The positive X-axis is represented as (100) , Y-axis is represented as (010) and Z axis as (001).Similarly the negative X-axis as ($\bar{1}00$), negative Y-axis as ($0\bar{1}0$) and negative Z-axis as ($00\bar{1}$).
3. The Miller indices for a plane (101) is read as ‘one zero one’, not as ‘one hundred and one’.

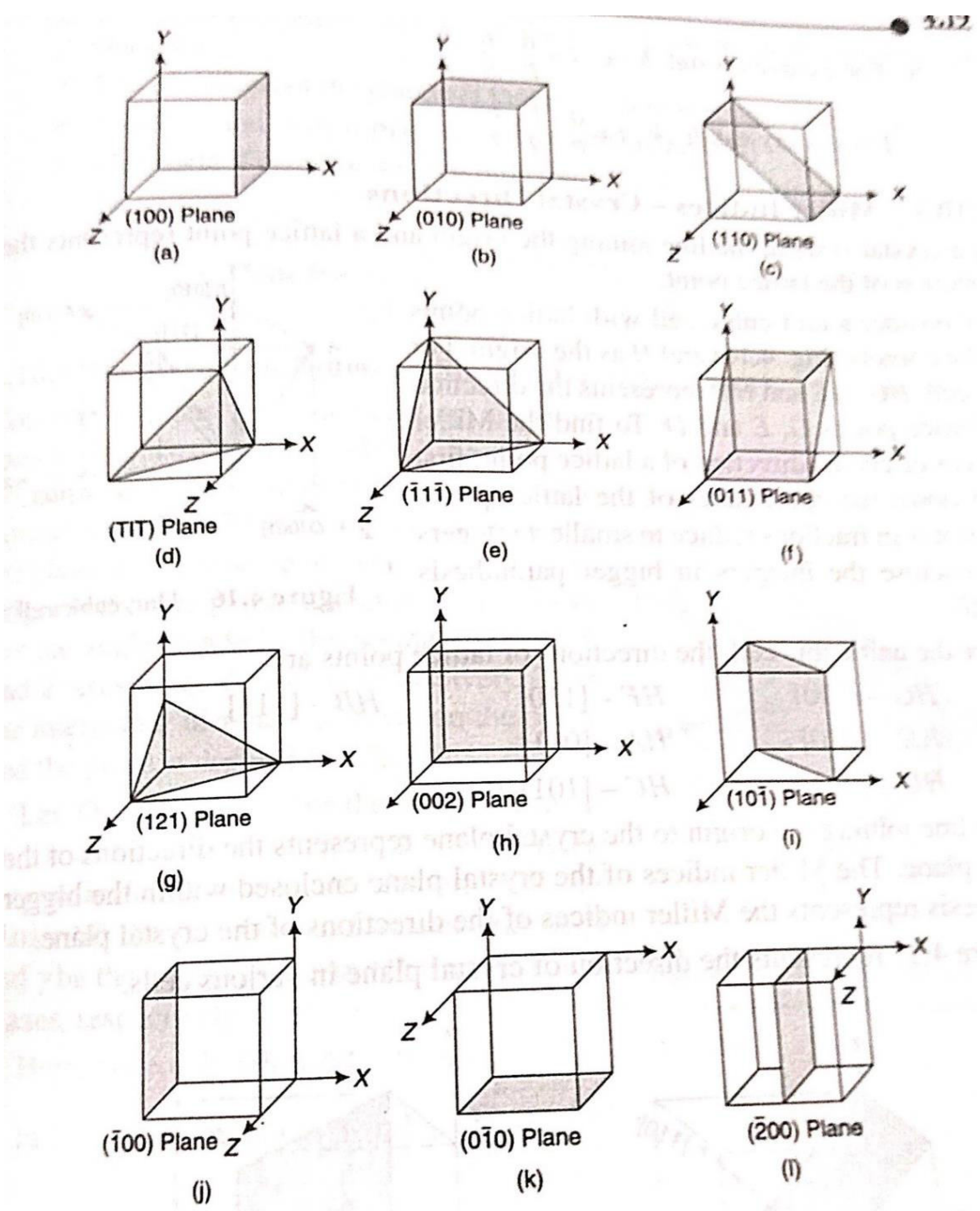


Figure 4.15 Miller indices of some crystal planes in unit cubic cell

Important features of Miller indices of Crystal planes:

1. Miller indices represent the orientation of crystal planes in a crystal lattice.
2. Any plane parallel to the one of the coordinate axes will have infinite intercept and the corresponding Miller index becomes zero.
3. A plane passing through the origin is defined in terms of a parallel plane having non zero intercepts.
4. If the Miller indices of the planes have the same ratio, then the planes are parallel to each other. Example is (211) and (422) etc.
5. Planes with negative intercepts are represented by a bar , i.e, $(\bar{1}00)$.The Miller indices $(\bar{1}00)$ indicates that the plane has an intercept in the negative X-axis.

6. If (hkl) is the Miller indices of a crystal plane , then the intercepts made by the plane with the coordinates are $\frac{a}{h}, \frac{b}{k}, \frac{c}{l}$ where a,b,c are lattice parameters or primitives.
7. For a cubic crystal, the interplanar spacing between the adjacent parallel planes is given by d = $\frac{a}{\sqrt{h^2+k^2+l^2}}$ where 'a' is lattice constant and (hkl) is the Miller indices of the crystal plane.
8. For a cubic crystal , h:k:l = $\frac{a}{p} : \frac{a}{q} : \frac{a}{r}$

For any crystal, h:k:l = $\frac{a}{p} : \frac{b}{q} : \frac{c}{r}$

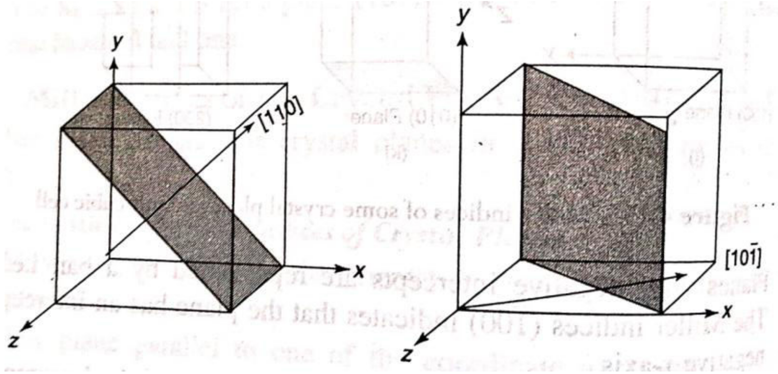


Figure: Directions of crystal planes

Miller indices – Crystal directions:

In a crystal system the line joining the origin and a lattice point is called direction of that the lattice point.

Consider a unit cubic cell with lattice points at the corners (Fig 5.18) and H as the origin. For the cell HG,HE and HD represents the direction of lattice points G , E and D. To find the Miller indices of crystal direction of a lattice point, first note down the coordinates of the lattice point and if it is in fractions, reduce it to smallest integers and enclose the indices in bigger parenthesis as [hkl].

For the cubic unit cell the directions of the lattice points are

HG-[100] , HF-[110] , HB-[111] , HE-[010], HA-[011] , HD-[001] and HC-[101] .

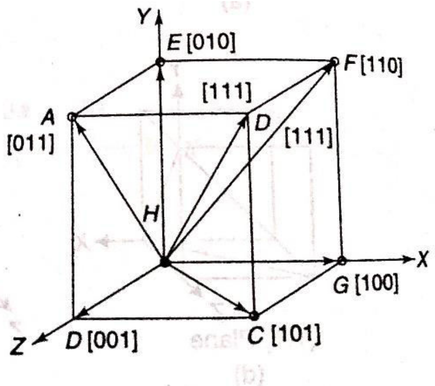


Figure : Cubic Unit Cell

Important features of Miller indices of crystal directions:

1. The line joining the origin to the lattice point represents the directions of the lattice point.
2. A normal line drawn from the origin to the plane gives the directions of the plane.
3. The directions of the plane are indicated by bigger parenthesis [hkl].
4. The direction [hkl] is perpendicular to the plane [hkl].
5. The angle θ between the two directions $[h_1,k_1,l_1]$ and $[h_2,k_2,l_2]$ is given by,

$$\text{Cos}\theta = \frac{h_1\,h_2+k_1k_2+\,l_1l_2}{\sqrt{h_1^2+k_1^2+l_1^2}\;\sqrt{h_2^2+k_2^2+l_2^2}}$$

Distances of separation between successive (hkl) planes :

Consider a plane ABC intercepting all three axes at distances OA, OB, and OC (a/h, b/k, and c/l respectively) as shown in figure. Let the normal to the plane from the origin intercept the plane at N. Distance of the normal from the origin is the interplanar distance 'd' (i.e., ON). Let the angles made by the normal to the X,Y, and Z axes be α, β, and γ respectively. Then the interplanar distance 'd' between the origin and the plane is derived as follows:

Let OA, OB, and OC be the intercepts made on the orthogonal axes OX, OY, and OZ; ON, the perpendicular distance from the origin to the plane; 'd' is the interplanar distance; α, β, and γ be the angles between ON and X,Y, and Z axes respectively.

Here, $OA = \frac{a}{h}$, $OB = \frac{b}{k}$, $OC = \frac{c}{l}$

In Δ ONA, $\cos\alpha = \frac{ON}{OA} = \frac{d}{(\frac{a}{h})} = d\,\frac{h}{a}$

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

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

We know from the law of direction cosines that

$\text{Cos}^2\alpha + \text{Cos}^2\beta + \text{Cos}^2\gamma = 1$

Therefore, $\left(\frac{dh}{a}\right)^2+\left(\frac{dk}{a}\right)^2+\left(\frac{dl}{a}\right)^2 = 1$

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

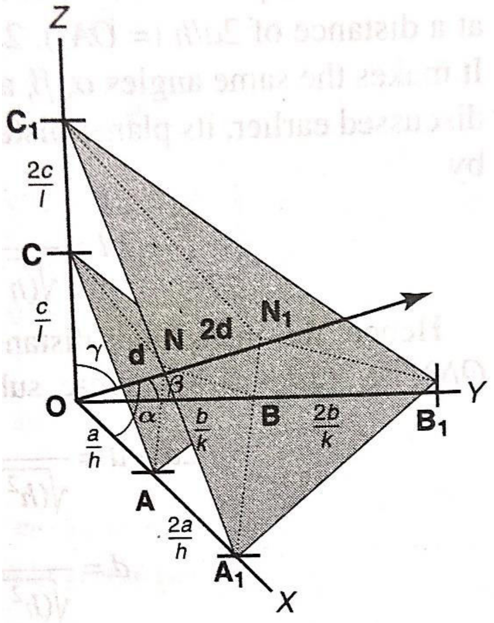


Figure. 4.18 Separation between successive (*hkl*) planes

For a cubic system, a=b=c, then the above equation becomes,

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

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

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

Consider a parallel plane intercepting the three axes at A_1, B_1, and C_1. Let it be at a distance of $\frac{2a}{h}$ $(= OA1), \frac{2b}{k}$ $(= OB1), and$ $\frac{2c}{l}$ $(= OC1)$ from the origin. It makes the same angle α, β, and γ with the X, Y, and Z axes respectively. Then, as discussed earlier, its planar distance from the origin 'O' is ON_1 (= 2d) and given by,

Therefore $ON_1 = 2d = \frac{2a}{\sqrt{h^2+k^2+l^2}}$

Hence the interplanar spacing between two adjacent planes = ON1-ON = 2d-d = d and given as,

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

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

The above equation represents expression for interplanar spacing between the two successive (hkl) planes.

X-Ray diffraction

Introduction:

- For diffraction to occur, the size of the obstacle must be comparable with the wavelength of radiation. In the crystal the regular arrangement of atoms in different planes results in diffraction of electromagnetic radiation passing through it.
- Since the interatomic spacing is only 2.3Å, X-rays whose wavelength is in the same range can be used for the crystal diffraction studies.
- Crystal acts as three dimensional space grating and the diffraction pattern thus produced reveals the internal arrangement of atoms in crystals. W.L. Bragg first derived a relation between interplanar spacing and angle of reflection.

Bragg's law:

- 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 an angle 'θ' with the plane I be reflected at atom A in the direction AR and another X-ray QC reflected at atom C in the direction CS. These diffracted X-rays will interfere constructively or destructively depending on the path difference between X-rays.
- To calculate the path difference, two normals AB and AD are drawn from A to QC and CS.

Path difference = BD

= BC+CD ----------→(1)

From ΔABC,

$$\text{Sin}\theta = \frac{CB}{AC}$$

CB = AC sinθ

CB = d Sinθ ------------→(2)

Similarly from ΔACD ,

$$\text{Sin}\theta = \frac{CD}{AC}$$

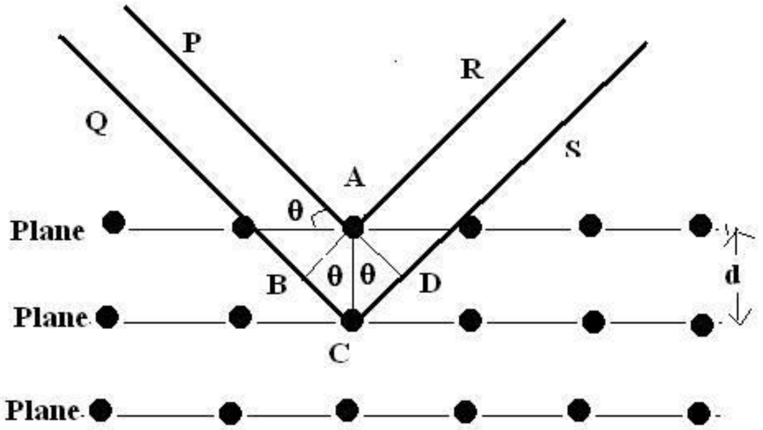
CD= AC Sinθ

CD= d Sinθ ----------------(3)

From (1), (2) & (3) we have,

Path difference = d Sinθ + d Sinθ

Path difference = 2 d Sinθ --------------(4)



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

Path difference= nλ -----------------------(5)

where n=1,2,3---

From (4) and (5) we have,

$$2\ d\ \mathrm{Sin}\theta\ = n\lambda \ \text{-------------}(6)$$

The above expression represents Bragg's law.

The above is according to which the diffracted X-rays interfere constructively and when the path difference is an integral multiple of the wavelength of X-rays. Corresponding to n=1,2,3---- we obtain first, second and third…order diffraction spots. Since maximum possible value of θ is one, we get

$$n\lambda = 2d$$

$$\lambda \leq 2d$$

Thus the wavelength λ should not exceed twice the interplanar spacing for diffraction to occur.

Importance of Bragg's law:

1. From Bragg's law, 2 d Sinθ = nλ we get $d = \frac{n\lambda}{2sin\theta}$.

Knowing wavelengths of X-rays (λ) and the glancing angle 'θ' , 'd' can be calculated.

2. Knowing'd', the lattice constant 'a' of the cubic crystal can be known.

3. Knowing a, ρ (density) and M (molecular weight), of the crystal, the number of atoms or molecules in the unit cell can be calculated.

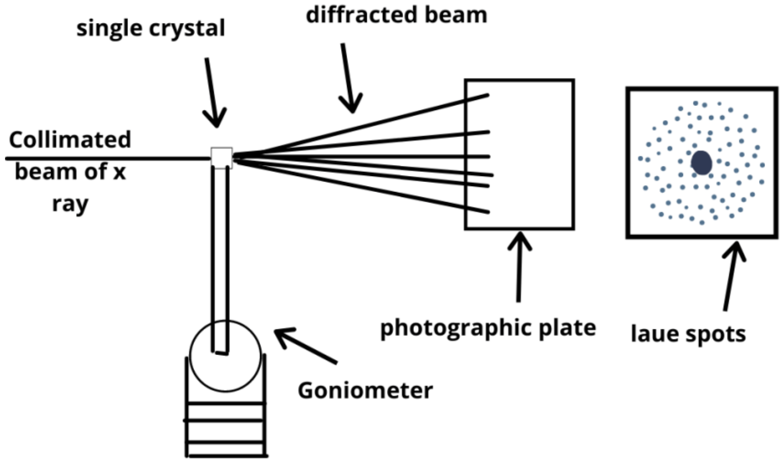
4. For a cubic crystal $d = \frac{a}{\sqrt{h^2+k^2+l^2}}$

Knowing d and a , the value of $h^2 + k^2 + l^2$ can be calculated.

5. Depending on the values of $h^2 + k^2 + l^2$, we can classify the crystals as BCC,FCC and SCC etc.

Laue Method

- It is one of the important methods. Used for the study of crystal structure and is mostly used for determination of Crystal symmetry.



- In this method, a beam of polychromatic X-rays of wavelengths ranging from 0.2**Å** to 2**Å** is allowed to fall on a small crystal of dimension 1 mm x 1mm x 1mm, placed on a goniometer.
- The goniometer can be rotated to change the orientation of the crystal with respect to the beam of X-rays. Generally, the beam is allowed to fall perpendicular to the plane of the crystal under study. While passing through the crystal.
- The X-ray falls on different Bragg's planes having a spacing d. And making different angles '**θ**' with the incident direction of X-rays.
- For some value of d, **λ** and **θ,** which satisfy the Bragg's condition, $2d \sin\theta = n\lambda$. constructive interference takes place and increase in intensity takes place at certain directions producing a diffraction pattern.
- This diffraction pattern may be observed by placing a photographic plate on the other side of the crystal.
- The diffraction pattern obtained on the photographic plate. Consists of a symmetrical arrangement of spot depending upon the symmetry property of the crystal lattice. The Laue method is generally used to determine the symmetry.
- For example, for a crystal with four-fold symmetry and axis parallel to the beam of X-ray, four-fold rotation of the crystal would produce identical Laue patterns.

Conclusion of Laue method

It may be noted that the Laue method cannot be used for the determination of crystal structure. It is because that out of the continuous range of wavelengths. A number of wavelengths may be reflected in different order. From a single plane producing and overlapping of certain reflections at a single spot. Thus, a number of reflections may be missing in the Laue pattern.

Powder method (or) Debye Scherrer method :

- The powder method is an X-ray Diffraction technique used to study the structure of microcrystals (tiny crystallites) in the form of powder.
- This method gives information regarding to the size and orientations of the Crystallites in the powder. Experimental arrangement is shown in figure.
- The powder is prepared by crushing the polycrystalline material so that they make all possible angles with the incident X-rays. Thus all orders of reflections from all possible atomic planes are re-ordered at the same time.
- The experimental arrangement consists of a cylindrical camera, called Debye-Scherer camera consisting of a film in the inner portion.
- The finely powdered sample is filled in a capillary tube made of nondiffracting material.
- The incident X-rays after passing through the filter and pin holes of lead diaphrgrams produce a fine beam of monochromatic X-rays.
- The fine beam after passing through the entry hole falls on the capillary tube containing the powdered crystals.
- Since the powder consists of randomly oriented crystallites, all possible 'θ' and'd' values are available for diffraction of incident X-rays.
- The diffraction takes place for these values of d and θ which satisfy the Bragg's relation $2d\sin\theta=n\lambda$, where λ is constant for monochromatic X-rays.
- For a particular value of θ , various orientations of a particular set of planes are possible. The diffracted X-rays corresponding to fixed values of θ and d lie on the surface of a cone with it's apex at tube P and the semi vertical angle 2θ.
- Different cones are observed for different sets of d and θ for a particular order of n and also for different combinations of 'θ' and' n' for a particular value of d.
- The transmitted X-rays come out through the exit hole. The diffracted X-ray cone make impressions on the film in the form of arcs on either side of the exit and entry holes with their centres coinciding with the hole.

The angle θ corresponding to a particular pair of arcs is related to the distance's' between the arcs as,

$$4\theta \text{ (radians)} = \frac{S}{R} \qquad \text{(since angle}= \frac{arc}{radius} \text{)}$$

Where 'R' is the radius of the camera.

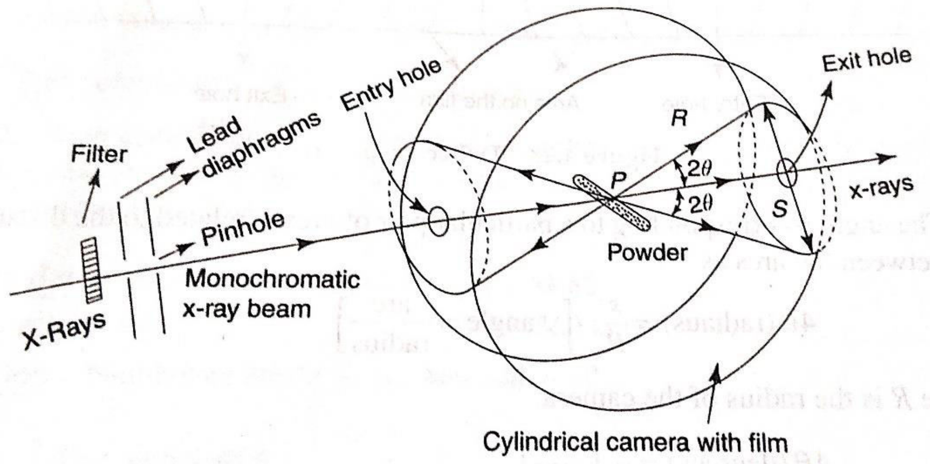


Figure 4.22 Powder method

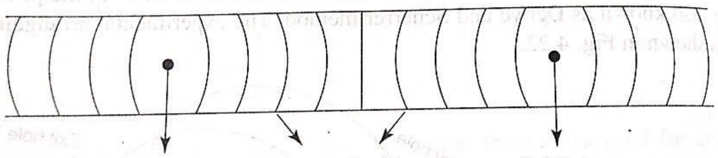


Figure 4.23 Diffraction pattern

$$4\theta \text{ (degrees)} = \frac{S}{R}\left(\frac{180}{\pi}\right)$$
$$= \frac{57.296\, S}{R}$$

From the above expression, θ can be calculated.
The interplanar spacing for first order diffraction is,

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

Knowing all the parameters, the crystal structure can be studied.

Merits:

1. Using filter, we get monochromatic X-rays. (λ Remains constant)
2. All crystallites are exposed to X-rays and diffractions take place with all available planes.
3. Knowing all parameters, crystal structure can be studied completely.

UNIT-III: DIELECTRIC & MAGNETIC MATERIALS

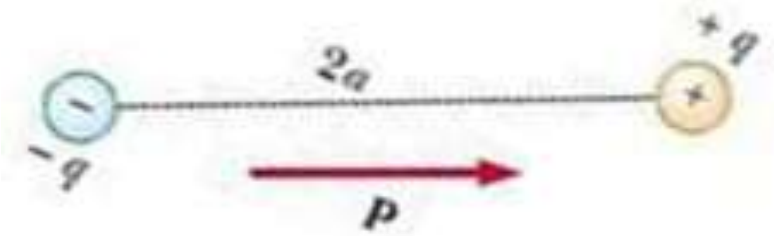
DIELECTRICS: Introduction - Dielectric polarization - Dielectric polarizability, Susceptibility and Dielectric constant - Types of polarizations -Electronic (Quantitative), Ionic (Quantitative) and Orientation polarizations (Qualitative) - Lorentz internal field - Clausius-Mossotti equation - Piezoelectricity.

BASIC Definitions

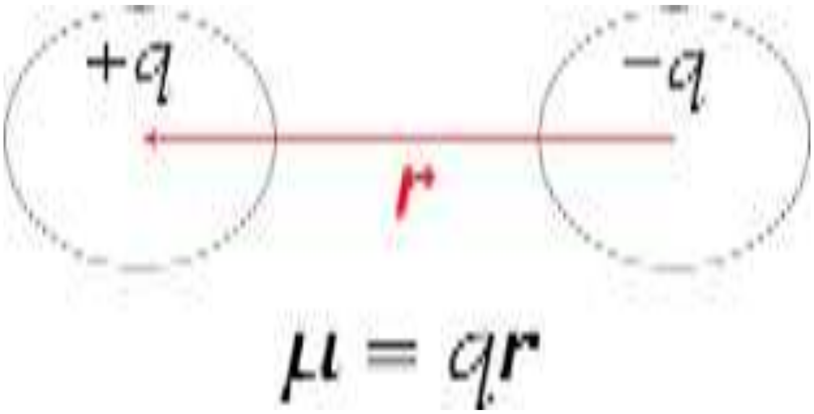
(1) ***Non-Polar dielectrics**:* If center of gravity of positive charges and negative charges coincide at a point that are called non polar dielectrics.

(2) ***Polar dielectrics:*** If center of gravity of positive charges and negative chargesdo not coincide at a point that are called non polar dielectrics.

(3) ***Electric Dipole:*** Two opposite charges of equal magnitude separated by a finite distance is called electric dipole.



(4) **Dipole moment (μ):** It is the product of the charge and the distance between two charges.



$$\mu = qr$$

(5) **Permittivity (ε):** The ability of a material allow polarization.

(6) *Relative Permittivity/Dielectric constant (εr):* $\varepsilon r = \varepsilon/\varepsilon o$

The ratio of permittivity of the material to the permittivity of free space.

ε_o= permittivity of free space (8.854×10^{-12} F/m)

(7) **Dielectric Polarization:** The displacement of negatively charged electrons andpositively charged nucleus in the presence of electric field is called polarization.

Displacement of charges produce local dipoles in the material. The induced diploe moment (μ) is directly proportional to the electric field (E).

$\mu \infty E$

$\mu = \alpha E$ here, α is polarizability

(8) **Dielectric polarizability (α)**: The ratio of average dipole moment (μ) to theapplied electric field (E). $\alpha = \mu / E$ **Unit:** Fm^2

(9) ***Polarization Vector (P):***

The average dipole moment (μ) per unit volume (v).

$P = \mu/v P = N \mu$ (since N=1/V)

$P = N \alpha E$

(10) **Electric susceptibility (χ):** Polarization is directly proportional to the productof 'ε_o' and applied electric field (E).

$P \alpha \varepsilon_o$

$E P = \chi$

$\varepsilon_o E$

$\chi = P / \varepsilon_o E$

(11) ***Dielectric displacement (D):***

The displacement of charges in the presence of electric field. $\therefore D \alpha E$.

Relation between Electric susceptibility (χ) and Relative Permittivity (ε_r)

Dielectric displacement directly proportional to Electric field applied.

$D = \varepsilon_o E + P$

$\varepsilon E = \varepsilon_o E + P$

(since, $D = \varepsilon E$)

$\varepsilon_o \varepsilon_r E = \varepsilon_o E + P$

(since, $\varepsilon = \varepsilon_o \varepsilon_r$)

$P = \varepsilon_o E(\varepsilon_r - 1)$

$P/\varepsilon_o E = (\varepsilon_r - 1)$

$$\boxed{\chi = (\varepsilon_r - 1)}$$

TYPES OF POLARIZATION:

1. <u>ELECTRONIC POLARIZATION</u>: -

If positively charged nucleus and negatively charged electrons displaced bythe application of electric field is called an electronic polarization.

It is independent of temperature.

The displacement of charges produces local dipoles.

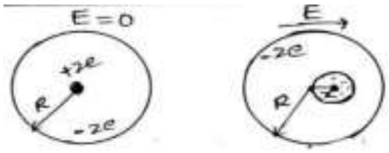
The induced dipole moment is directly proportional to the applied electric field.

$\mu_e \infty E$

$\therefore \mu_e = \alpha_e E$ ------ (1) here, α_e is Electronic Polarizability

<u>Electronic Polarisability</u> (α_e):-

Consider an atom of dielectric which contains the number of electrons ofcharge '-ze' and nucleus of charge +ze. R is radius of atom.



1) Charge density of the atom, $\rho = \dfrac{-ze}{{}^{4}/{}_{3}\pi R^3}$ ------ (2)
2) By the application of electric field, electron cloud and nucleus separated by X.
3) When they are separated the coulomb attractive force and Lorentz repulsiveforces develop between them.

Lorentz force = - Ze E ---------------- (3)

Coulomb force = Ze × $\left[\dfrac{charge\ enclosed\ in\ sphere\ of\ radius\ x}{4\pi\varepsilon_o\ .R^2}\right]$ -------(4)

4 Charge enclosed in sphere of radius

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

From equ. (2) $$= \frac{4}{3}\pi x^3 . \left(-\frac{Ze}{({}^{4}/{}_{3})\pi R^3}\right)$$

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

Hence Coulomb force is $= \dfrac{Ze}{4\pi\varepsilon_{0\,R^2}} X - \dfrac{ZeX^3}{R^2}$

$$= -\frac{Z^2\, e^2 X}{4\pi\varepsilon_0\, R^3}$$

At equilibrium Position, from equations (3) & (5),

Lorentz force = Coulomb force

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

$$X = \frac{4\pi\varepsilon_0\, R^3 E}{Ze}$$

1) Induced dipole moment, $\mu_e = Zex$

$$\mu_e = Ze\{\frac{4\pi\varepsilon_0\, R^3 E}{Ze}\}$$

$\mu_e = 4\pi\varepsilon_0 R^3 E$ ------(6)

$\mu_e \alpha E$

$\mu_e = \alpha_e E$

from equations (1) and (6),

Electronic Polarizability $\alpha_e = 4\pi\varepsilon_0 R^3\ Fm^2$

2. IONIC POLARISATION: -

If ions (anions and cations) are displaced by the application of electric fieldis called ionic polarization.

It is independent of temperature.

The displacement of charges produces local dipoles.

The induced dipole moment is directly proportional to the application electric field.

$\boldsymbol{\mu_i \propto E}$

$\therefore \boldsymbol{\mu_i = \alpha_i E}$ ------ (1) here, α_i is Ionic Polarizability

Ionic Polarizability(α_i):-

Consider an ionic material and assume that each unit cell contains one positiveion and one negative ion.

1) When an electric field is applied, positive ions displaced by 'x_1' and negative ions displaced by 'x_2'.
2) The resultant dipole moment per unit cell is

$\mu_i = [x_1 + x_2]$------ (2)

3) In the presence applied field, the force acting on positive ion $F = \beta_1 x_1$

$x_1 = \frac{F}{\beta_1}$

since $F = e\,E$, β_1 is restoring force constant = $m\omega_o^2$, m is mass of positive ion

$x_1 = \frac{e.E}{m\omega_o^2}$ ------ (3)

4) Similarly, the force acting on the negative ion $F = \beta_2 x_2$

$x_2 = \frac{F}{\beta_2}$

since $F = e\,E$, β_2 is restoring force constant = $M\omega_o^2$, m is mass of negative ion

$x_2 = \frac{e.E}{M\omega_o^2}$ ------ (4)

5) from equations (2), (3) & (4), dipole moment $\mu = e\,[\frac{e.E}{m\omega_o^2} + \frac{e.E}{M\omega_o^2}]$

$$\mu_i = \frac{e^2}{\omega_o^2}\left[\frac{1}{m} + \frac{1}{M}\right].E \text{-----------(5)}$$

6) from equations (1) and (5),

Ionic Polarizability $\boxed{a_i = \frac{\boldsymbol{e^2}}{m_o^2}\left[\frac{\mathbf{1}}{\boldsymbol{m}} + \frac{\mathbf{1}}{\boldsymbol{M}}\right]}$ F-m^2

3. ORIENTATION POLARISATION: -

Already existing dipoles orient in the field direction by the application ofelectric field is called Orientation Polarization.

Orientation Polarization depends on temperature.

Polarization $P = N\mu_0$

since, $\mu_0 = \boldsymbol{\alpha_0} E$

$\mathbf{P = N\,\alpha_0\,E}$ ------- (1) here, α_0 = Orientational Polarisability.

Orientational Polarisability(α_0):-

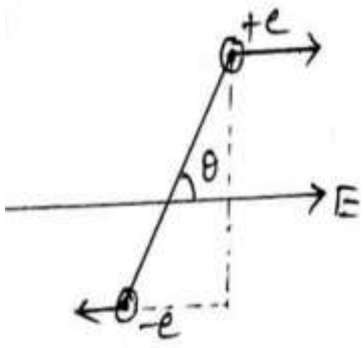
Consider a dielectric contains number of dipoles.

1) In the presence of electric field, already existing dipoles orient in the fielddirection.
2) The polarization vector, $P = N\mu$ -----------(2)

   Here, 'N' is number of atoms per unit volume,

   μ is average dipole moment.
3) By solving we get the average dipole moment,

$$\mu = \frac{\mu^2 E}{3KT} \text{ ------- (3)}$$



Here 'K' is Boltzmam constant and 'T' is temperature.

4) From equations (2) & (3), we have that $P = N.\,\frac{\mu^{2}E}{3KT}$

$$P = N\left[\frac{^{2}}{3KT}\right]E \text{----------------(4)}$$

5) from equations (1) and (4),

   Orientation Polarizability $\boxed{a_{\boldsymbol{o}} = \frac{\boldsymbol{\mu^2}}{\mathbf{3KT}}}$ *Fm^2*

4.SPACE CHARGE POLARISTION: -

"Space charge polarization occurs due to the accumulation of charges atelectrodes or interfaces in multiphase dielectrics.

It is found in ferrites and semi-conductors.Space charge polarization is very small.

TOTAL POLARIZATION:

The total polarizability of a dielectric material is the sum of electronic, ionic,orientational and space charge polarizabilities.

$$a_{\mathbf{total}} = a_{\mathbf{e}} + a_{\mathbf{i}} + a_{\mathbf{o}} + a_{\mathbf{s}}$$

Total Polarization of a dielectric material is $\boldsymbol{P} = \boldsymbol{N}\alpha\,\mathbf{E}$

$$P_{total} = N\left[4\pi\varepsilon_0 R^3 + \frac{e^2}{\omega_o^2}\left[\frac{1}{m} + \frac{1}{M}\right] + \frac{\mu^2}{3KT}\right]\mathbf{E}$$

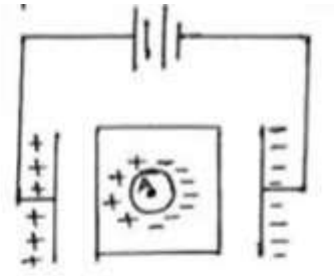
This equation is called as ***Langevin-Debye*** *equation.*

INTERNAL FIELD / LOCAL FIELD / LORENTZ FIELD

Definition – The field acting at a point Space in dielectric by application of electric field.

Consider a di-electric material placed in between two plates of parallel plate capacitor. Let a point ‘P’ in the spherical cavity 'A' in dielectric as shown in the figure.

The internal field acting at a point ‘P’ is



$$\mathbf{E_i = E_1 + E_2 + E_3 + E_4}$$

Proof:-

Field E₁:

E_1 is the field acting in between two parallel plates ofthe capacitor.

$$\boxed{E_1 = E + \frac{P}{\varepsilon_o}}$$

Field E2:

E_2 is the field intensity at a point ‘P’ due to the induced charges on surfacesof dielectric.

$$\boxed{E_2 = -\frac{P}{\varepsilon_o}}$$

Field E3:

E_3 is the field intensity at a point ‘P’ due to neighboring atoms (or all thedipoles) in the spherical cavity.

$$\boxed{E_3 = 0}$$

Field E4:

E_4 is the field intensity at a point ‘P’ due to polarized charges on the surfaceof spherical cavity.

$$\boxed{E_4 = \frac{P}{3\varepsilon_o}}$$

The internal field acting at a point ‘P’,

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

$$E_i = \left[E + \frac{P}{\varepsilon_o}\right] + \left[-\frac{P}{\varepsilon_o}\right] + [0] + \left[\frac{P}{3\varepsilon_o}\right]$$

$$E_i = E + \frac{P}{\varepsilon_o} - \frac{P}{\varepsilon_o} + \frac{P}{3\varepsilon_o}$$

∴ Internal field $\boxed{E_i = E + \frac{P}{3\varepsilon_o}}$

CLAUSIUS MOSOTTI RELATION

Consider a dielectric and assume there is no ions and permanent dipoles. Hence the ionic polarizability (α_i) and orientational polarizability (α_0) are zero.

$$\alpha_i = \alpha_0 = 0$$

polarization $P = N\,\alpha_e\,E_i$

$$P = N\,\alpha_e\left[E + \frac{P}{3\varepsilon_o}\right] \qquad \left(\text{since, } E_i = E + \frac{P}{3\varepsilon_o}\right)$$

$$P = N\alpha_e E + \frac{N\alpha_e P}{3\varepsilon_o}$$

$$P - \frac{N\alpha_e P}{3\varepsilon_o} = N\,\alpha_e\,E$$

$$P\left[1 - \frac{N\alpha_e}{3\varepsilon_o}\right] = N\,\alpha_e\,E$$

$$\left[1 - \frac{N\alpha_e}{3\varepsilon_o}\right] = \frac{N\,\alpha_e\,E}{P}$$

$$\left[1 - \frac{N\alpha_e}{3\varepsilon_o}\right] = \frac{N\,\alpha_e\,E}{\varepsilon_o E(\varepsilon_r - 1)} \qquad \left(\textit{since, } P = \varepsilon_o E(\varepsilon_r - 1)\right)$$

$$1 - \frac{N\alpha_e}{3\varepsilon_o} = \frac{N\alpha_e}{\varepsilon(\varepsilon_r - 1)}$$

$$1 = \frac{N\alpha_e}{3\varepsilon_o} + \frac{N\alpha_e}{\varepsilon(\varepsilon_r - 1)}$$

$$1 = \frac{N\alpha_e}{3\varepsilon_o}\left[1 + \frac{3}{(\varepsilon_r - 1)}\right]$$

$$\frac{N\alpha_e}{3\varepsilon_0}\left[\frac{(\varepsilon_r - 1) + 3}{\varepsilon_r - 1}\right] = 1$$

$$\frac{N\alpha_e}{3\varepsilon_0}\left[\frac{(\varepsilon_r + 2}{\varepsilon_r - 1}\right] = 1$$

$$\boxed{\frac{N\alpha_e}{3\varepsilon_0} = \left[\frac{(\varepsilon_r - 1}{\varepsilon_r + 2}\right]}$$

This is called Clausius Mosotti equation.

APPLICATIONS OF DIELECTRICS

Dielectrics widely used as insulating materials.

1) **Plastic or Rubber:** **U**sed as outer jackets of electrical conductors.
2) **Ceramics:** Ceramics widely used as insulators for switches, plug holders etc...
3) **PVC Materials:** Used as wires and cables, PVC films, tapes....
4) **Mica:** Mica used as an insulator in the form of paper, tape, cloth and boards....
5) **Mineral Insulating Oil:** Used as Transformer oil, cable oil, capacitor oil etc.
6) **Inert gases:** Used in electronic tubes and discharge tubes as insulators.
7) **Air:** Air condensers. It is the most important insulating material.

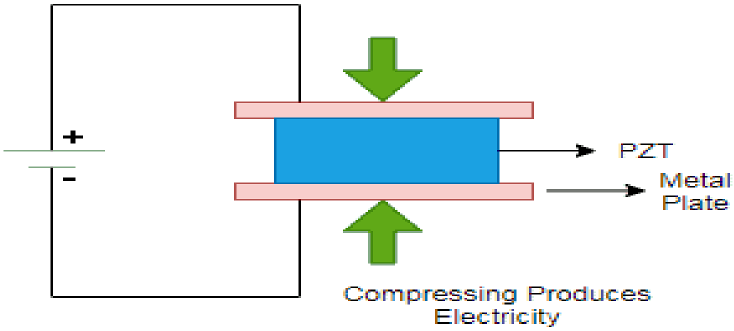
8) **<u>Capacitors</u>:** Dielectric materials used in capacitors to store the energy.
9) **<u>High Voltage Applications</u>:** Used in high voltage applications.
10) **<u>Asbestos</u>:** Asbestos insulation is providing to prevent the flow of electric current.

PIEZO ELECTRICIT

When mechanical stress is applied to the material (crystal), it can electrically have polarized. This is called piezo electric effect. Or

The materials exhibit electronic polarization when the mechanical stress is applied.

When a piezo electric crystal like quartz is subjected to compressions, an opposite kinds of charges developed at the end faces perpendicular to the directionof applied force.



<u>Applications of Piezo electric materials</u>

1) Piezo electric materials exhibit piezo electricity
2) Piezo electric materials used for high voltage generators
3) Piezo electric materials used as amplifiers
4) Piezo electric materials used as filters
5) Microphones.
6) Piezoelectric Motors.
7) Actuators in Industrial Sector.
8) Sensors in Medical Sector.
9) Actuators in Consumer Electronics (Printers, Speakers)
10) Piezoelectricity Buzzers
11) Piezo electric materials used to produce ultrasonic.

Unit-3 - Chapter-2
Magnetic materials

Magnetism

A substance that attracts pieces of iron (or) steel is called “Magnet”. This property of a substance is called “magnetism.

Basics of Magnetism

Magnet:

The magnets are materials which produces a magnetic field. The magnets are materials which attract the ferromagnetic materials like iron, Co, Ni etc.

Properties of Magnets:

1. Magnets attract ferromagnetic objects.
2. The magnetic field at the poles of a magnet is greater than at the middle of magnet.
3. The like poles of magnet repel each other while the opposite poles attract eachother.
4. The magnet has a property that when it is suspended freely it’s South Pole and North Pole moves to the earth’s North and South Pole, respectively.

Magnetic Poles:

When a bar magnet is dipped in a heap of iron filings and taken out, it is seen that maximum amount of iron filings are seen to cling to the magnet at the two ends of the magnet. Practically no iron filings cling in the middle. The regions of the magnet at which maximum amount of iron filings cling are called poles of the magnet. ***Poles of magnet are regions near the two ends of a magnet with maximum power of attraction.*** The strength of the pole is called **pole strength** denoted by ***m*****.** The **S.I. unit of pole strength is *Ampere Meter.***
The distance between two magnetic poles is called “magnetic length” ($2l$).

Magnetic Dipole:

- Magnetic dipoles are found to exist in magnetic materials, analogous to electric dipoles.
- Two equal and opposite charges separated by a small distance is called an electric dipole. Similarly a north pole and south pole separated by a small distance $2l$ (**magnetic length***)* constitute a magnetic dipole.

- ***For example:*** A bar magnet, a compass needle etc. are the magnetic dipoles. And also a current loop behaves as a magnetic dipole.

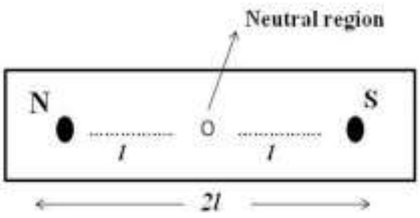


Fig : Magnetic dipole

Magnetic Dipole Moment:

The behavior of magnetic dipole is described by the magnetic dipole moment.

(a)In the case of bar magnet:

It is defined as the product of pole strength (m) and magnetic length (2*l*).

$$\boxed{\vec{\mu}_m = m\,(2l)}$$

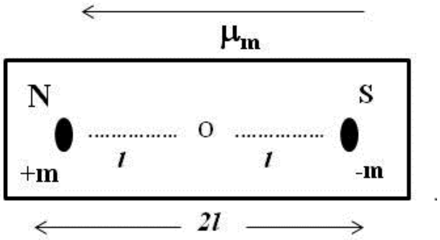


Fig : Magnetic dipole moment

It is a vector quantity. It is directed from South Pole to North Pole.
The S.I.Unit of magnetic dipole moment: Ampere – meter ^{2} (A-m^2).

(b) In the case of current loop:

A current carrying loop behaves as a magnetic dipole. Consider a current carrying conductor loop of wire as shown fig.
The current (I) establishes a magnetic field around the loop. By right hand palm rule, the upper face of the loop acts a N- pole and the lower face act as S- pole.

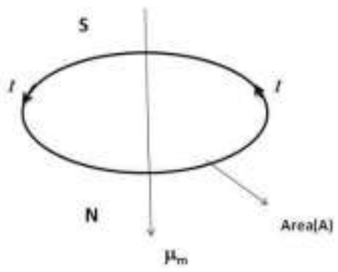


Fig : Current carrying conductor loop

The magnitude of dipole moment of current loop (μ_m) is

(i) Directly proportional to current (I) through the loop.

(ii) Directly proportional to the area of cross –section (A).

$$\mu_m \,\alpha\, I.A$$

$$\mu_m = K\, IA$$

$$\boxed{\mu_m = IA}$$

Where K is a proportionality whose value is one

Magnetic Field:

.The space surrounding a magnet upto which it’s influence can be felt is called Magnetic field .

A magnetic field can be represented by drawing lines called “magnetic lines of force”. The lines go from North to South on the magnet.

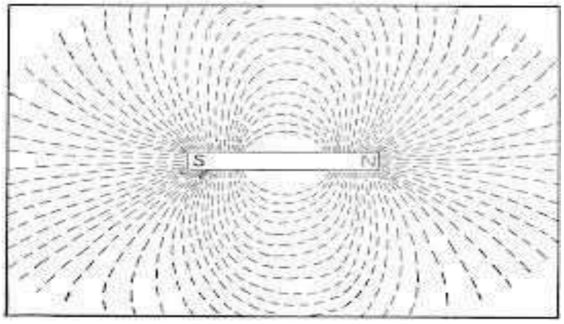


Fig: Magnetic field.

Magnetic Flux:

A group of magnetic lines of force is called “magnetic flux”.

The symbol for magnetic flux is Φ (phi).

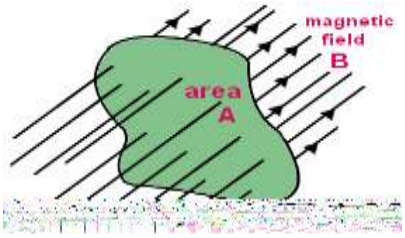
The SI unit of magnetic flux is the Weber (Wb).

One Weber is equal to 1 x 10^8 magnetic field lines.

Magnetic Flux Density:

Magnetic flux density is the amount of magnetic flux per unit area of a section, perpendicular to the direction of flux.

$$\text{Magnetic flux density (B)} = \frac{\text{Magneticflux (Weber)}}{\text{Area } (m^2)}$$



$$\boxed{B = \frac{\emptyset}{A} \text{ Tesla}}$$

Magnetization:

The process of converting a non-magnetic material into a magnetic material is known as "magnetization".

Intensity of Magnetization (I or M)

When a material medium is placed in a magnetic field, it gets magnetized. To magnetize the material medium is to create the magnetic dipole moments.

The magnetic dipole moment per unit volume of the material is called the intensity of magnetization I (or simply magnetization).

$$I = \frac{\text{Magnetic dipole moment}(\mu_m)}{\text{Volume (V)}} = \frac{\text{Length of magnet }(2l)\ \text{X}\ \text{Pole Strength (m)}}{\text{Length of Magnet }(2l)\ \text{X Area of cross –section (A)}}$$

$$= \frac{\text{Pole Strength (m)}}{\text{Area of Cross Section (A)}}$$

The S.I. Unit of magnetization is ampere / meter

Magnetic Field Strength (H):

The ability of magnetic field to magnetize a material medium is called its magnetic intensity or field strength. It is denoted by **H**.

The S.I. Unit of magnetic field strength is ampere / meter.

Magnetic Susceptibility (χ_m):

The word Susceptibility comes from the Latin word "susceptible" means the easily affected

The magnetic susceptibility of a material medium indicates how easily a material medium can be magnetized in the presence of magnetic field..

The intensity of Magnetization is directly related to the applied field strength H.

$$M \alpha H$$

$$M = \chi_m H$$

$$\boxed{\text{Magnetic Susceptibility } (\chi_m) = \frac{M}{H}}$$

Therefore; the magnetic susceptibility of a material is defined as the ratio of intensity of magnetization (I) developed in the material to the applied magnetic field (H).

Magnetic Permeability (μ):

- It is the natural property of material.
- In Latin, *per* means *through* and *meare* means *to pass.*
- It is defined as the ability of the material to permit the passage of magnetic lines of force through it.
- The Magnetic induction B is proportional to the applied Magnetic field intensity H.

$$B \alpha H$$

$$B = \mu H$$

$$\boxed{\text{Magnetic Permeability } (\mu) = \frac{B}{H}}$$

Where "μ" is the permeability of a medium.

For vacuum:,

$$\boxed{B = \mu_0 H}$$

Where is the proportionality constant and is also called permeability of the free space and its value is $4\pi \times 10^{-7}$ H m^{-1}.

Relative permeability (μ_r):

The ratio of permeability of medium to the permeability of free space is called relative permeability μ_r of the medium

$\mu_r = 1$ for vacuum. It has no units.

$$\boxed{\mu_r = \frac{\mu}{\mu_o}}$$

The Relation between Relative Permeability and Magnetic Susceptibility:

When a magnetic material is magnetized by placing it in a magnetic field, the resultant field inside the material is the sum of the field due to the magnetization of the material and the original magnetizing field. The resultant field is called magnetic induction or magnetic flux density **B.**

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

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

$$\mu H = \mu_0(H+M) \qquad (\because B=\mu H \text{ and } \mu = \mu_0\mu_r)$$

$$\mu_0\mu_r H = \mu_0\left(1+\frac{M}{H}\right)$$

$$\boxed{\mu_r = (1+\chi_m)}$$

Where $\chi_m = \frac{M}{H}$

This is the relation between Relative Permeability and Magnetic Susceptibility.

Origin of Magnetism:

An electron is a good traveler because it has no fixed planes.
It has no desire to revolve around the nucleus, and yet it revolves and creates magnetism…
It revolves in the state of wei-wu-wei (action of non action).

- Magnetism is one of the manifestations of ultimate matter-energy.
- Magnetism is an intrinsic property of every charged particle.
- Every moving charged particle creates magnetic field in the creation.
- Magnetism manifests by itself in the material.
- Magnetism is an interdependence

Science says:

Magnetism originates from magnetic dipole moment. This magnetic dipole moment arises due to the rotational motion of charged particles.

According to modern view;

- All substances are made of atoms or molecules. An atom which consists of ‘+’ vely charged nucleus at the centre and negatively charged electrons revolving around the nucleus in different orbits. This motion of electrons is called orbital motion as shown in fig. The orbiting elections constitute tiny current loops. These loops behave as the magnetic dipoles.
- The orbital motion of electrons around the nucleus gives rise to the orbital magnetic dipole moment (μ_{orbit}).
- The electrons also rotate around their own axes. This motion of electrons is called spin motion as shown fig.
- The spinning motion of electrons around their axes gives rise to the spin magnetic dipole m oment (μ_{spin}).
- The motion of the protons and neutrons within the nucleus also contributes to the total magnetic moment (($\mu_{nucleus}$). But the magnitude of the nuclear magnetic moment is (about 10^{-3} times) very small compared with the magnetic moment of electron and is usually neglected.

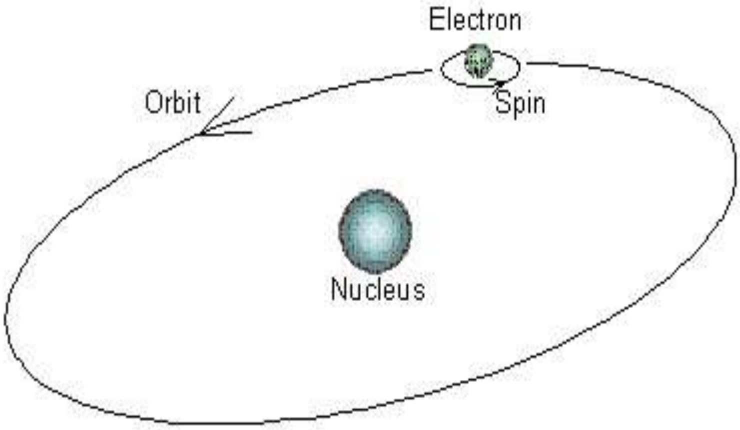


Fig: Motion of electron

(1) Orbital magnetic dipole moment of electron (μ_{orbit}):

Let us consider an electron of mass **‘m’** and charge e revolving around the nucleus in a circular orbit o radius **‘r’** with linear velocity **‘v’** as shown in fig.

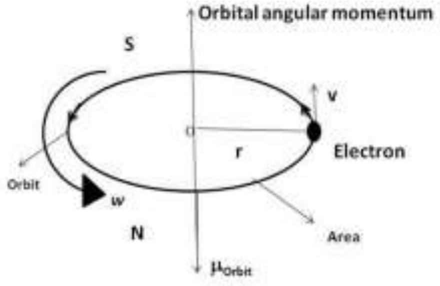


Fig : Orbital motion of electron

The revolving electron in circular orbit establishes a current is given by

$$I = \frac{\text{Charge of electron}}{\text{time period}} = \frac{-e}{T} \longrightarrow (1)$$

Where 'T' is the time taken by the electron to make one revolution around the nucleus

$$\text{i.e., } T = \frac{2\pi}{w} \longrightarrow (2)$$

Where *'w'* is the angular frequency of the electron

But relation between linear velocity 'v' and angular velocity can be written as

$$v = r\,w$$

$$\text{and } w = \frac{v}{r} \longrightarrow (3)$$

Substituting the equation (3) in (2),

$$T = \frac{2\pi r}{v} \longrightarrow (4)$$

Further, substituting the equation (4) in (1),

$$I = \frac{-ve}{2\pi r} \longrightarrow (5)$$

The current 'I' establishes a magnetic field around the circular orbit, so that the upper surface acts as South Pole and the lower surface acts as North Pole.

The Area of the orbit is $\mathbf{A} = \pi r^2 \longrightarrow (6)$

Then the corresponding magnetic dipole moment is given by

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

$$= \frac{-ve}{2\pi r} X \pi r^2$$

$$= \frac{-evr}{2} \longrightarrow (7)$$

Dividing and multiplying the equation (7) by the mass "m' of electron.

$$\mu_{\text{Orbit}} = \frac{-evr}{2} X \frac{m}{m}$$

$$= \frac{-e(mvr)}{2m}$$

$$= \frac{-e(\vec{L})}{2m} \qquad (\text{But } \vec{L} = mvr)$$

$$\boxed{\mu_{\text{Orbit}} = \frac{-e}{2m}\vec{\mathbf{L}} \text{ (Orbital angular momentum)}}$$

The – ve sign indicates that the orbital angular momentum and orbital magnetic dipole moment are in opposite directions.

Let us assume that the component of orbital magnetic dipole moment (μ_{Orbit}) of electron is measured along the z- axis of a coordinate system. Then the measured component μ_{orbit}, z can have only the two values is given by

$$\mu_{\text{Orbit},z} = \frac{-e}{2m}\mathbf{L_z}$$

$$\mu_{\text{Orbit},\,z} = -\left(\frac{e}{2m}\right) \mathbf{m}_{\boldsymbol{l}} \frac{\boldsymbol{h}}{\boldsymbol{2\pi}}$$

$$\mu_{Orbit,\,z} = -\left(\frac{eh}{4\pi m}\right) m_l$$

$$\boxed{\mu_{Orbit,z} = -\mu_B \cdot m_l}$$

Where $\mu_B = \frac{eh}{4m\pi}$ is known as Bohr magneton and its value is 9.27x 10^{-24} A-m^2.

Spin magnetic dipole moment of electron (μ_{spin}):

The electrons also rotate around their own axes. This motion of electrons is called spin motion as shown fig.

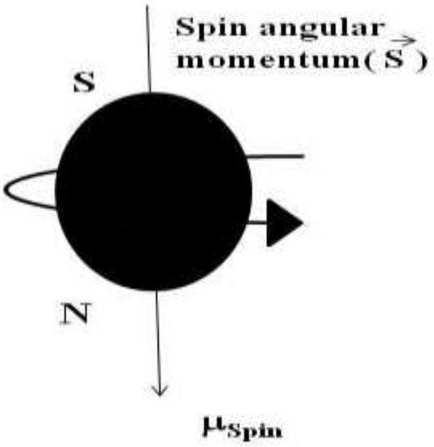


Fig: Spin motion of electron

The spinning electron constitutes a tiny current loop. This loop behaves as a magnetic dipole.

The magnetic dipole moment arises due to its spin motion is called spin magnetic moment (μ_{spin}) and is given by

$$\mu_{Spin} = -g\left(\frac{e}{2m}\right)\vec{S} \text{ (Spin angular momentum)}$$

The – ve sign indicates that the spin angular momentum and spin magnetic dipole moment are in opposite directions.

Let us assume that the component of spin angular momentum ($\vec{S}$) is measured along the z-axis of a coordinate system. Then the measured component S_Z can have only the values is given by

$$S_Z = m_s \frac{h}{2\pi}$$

Where m_s is called magnetic spin quantum number = $\pm\frac{1}{2}$

$m_s = +\frac{1}{2}$ for spin up and

$m_s = -\frac{1}{2}$ for spin down

Let us assume that the component of spin magnetic dipole moment ((μ_{Spin}) of electron is measured along the z- axis of a coordinate system. Then the measured component $\mu_{spin, z}$ can have only the two values is given by

$$\mu_{Spin,\ z} = -g\,(\frac{e}{2m})\,S_z$$

$$\mu_{Spin,\ z} = -g\,(\frac{e}{2m})\,\mathbf{m_s}\,\frac{\boldsymbol{h}}{\boldsymbol{2\pi}}$$

$$\mu_{Spin,\ z} = -2\,(\frac{eh}{4\pi m})\,\mathbf{m_s}$$

$$\boxed{\mu_{Spin,\ z} = -2\,(\mu_B)\,\mathbf{m_s}}$$

Where $\mu_B = \frac{eh}{4m\pi}$ is known as Bohr magneton and its value is 9.27x 10-^{24} A-m^2.

Nuclear spin magnetic dipole moment ($\mu_{Nuclear}$):

The atomic nucleus contains protons and neutrons. They have intrinsic spin.

The spin motion of the protons and neutrons within the nucleus also contributes to the total spin magnetic dipole moment and is given by

$$\mu_{nuclear,\ spin} = \frac{eh}{4\pi M_n} = 5.525X1O^{-27}\ A\text{-}m^2$$

Where M_n is the Mass of the proton

But the magnitude of the nuclear magnetic dipole moment is(about 10^{-3} times) very small compared with the magnetic dipole moment of electron and is usually neglected.

Therefore, the magnetism mainly arises due to the orbital and spin magnetic dipole moments of electron.

Classification magnetic materials:

Magnetic materials are classified based on presence or absences of the permanent magnetic dipoles in a material. They are

1. Dia magnetic material
2. Para magnetic material
3. Ferro magnetic material
4. Anti Ferro magnetic material and
5. Ferri magnetic material

1.Diamagnetic materials:

Those materials which when placed in a magnetic field are weakly or feebly magnetized in a direction opposite that of the applied magnetic field are called diamagnetic materials

Examples:

Bismuth, Copper, Zinc, Gold, Water, etc

Cause of diamagnetism:

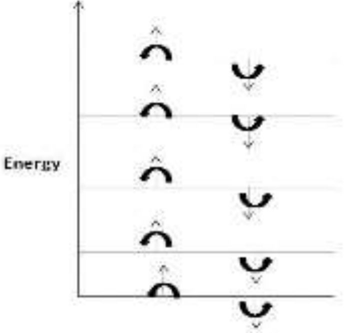
In the Diamagnetic materials, there exist paired electrons, so the spins in two opposite directions are equal and hence magnetic dipole moments cancel with each other i.e., the resultant magnetic dipole moment is equal to zero.

Therefore, most of these materials do not have magnetism in the absence of magnetic field.

Effect of external magnetic field:

a) In the absence of external magnetic field, the atoms/molecule/ions of the diamagnetic substance have no net magnetic dipole moment. Hence, the material does not exhibit diamagnetism

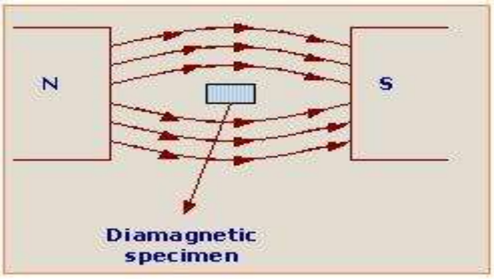
b) When a diamagnetic material is placed in an external magnetic field, currents are induced in the current loops of atom/molecule/ion according to Faraday's law of electromagnetic induction. According to Lenz's law, these currents give rise to a magnetic field which opposes the applied magnetic field. Hence, the induced magnetic moments of atoms/molecule/ions are opposite to the applied magnetic field.



Properties:

- They don't possess permanent magnetic dipole moment.

- When a diamagnetic material is placed in a magnetic field, it is feebly magnetized in a direction opposite to that of the applied magnetic field.
- When a diamagnetic material is placed in a magnetic field, the magnetic lines force prefers to pass through the surroundings air rather than through the diamagnetic magnetic material.



- The magnetic flux density inside is small than that in the free space. Hence the relative permeability $\mu_r < 1$.
- The magnetic susceptibility (χ_m) is negative and small.
- The magnetic susceptibility (χ_m) is independent of temperature.
- When a rod of diamagnetic material is suspended freely in a uniform magnetic field, the rod comes to rest with its axis perpendicular to the direction of the applied field.

2.Para magnetic materials:

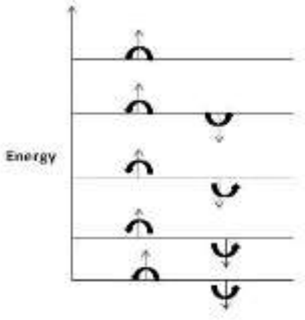
Those materials which when placed in a magnetic field are weakly or feebly magnetized in the direction of the applied magnetic field are called Para magnetic materials.

Examples:

Aluminum, platinum, copper sulphate($CuSo_4$),manganese, chromium etc.

Cause of paramagnetism:

In the case of paramagnetic materials, the spins in two opposite directions will not be equal. There exist some unpaired electrons which gives rise to spin magnetic dipole moment. Hence the resultant magnetic dipole moment will not be equal to zero. i.e., they possess permanent magnetic dipole moment.



Effect of external magnetic field:

c) In the absence of external magnetic field ,the dipoles of the paramagnetic material are randomly oriented and ,therefore, the net magnetic dipole moment of the material is zero. Hence, the material does not exhibit paramagnetism.

d) When a paramagnetic material is placed in an external magnetic field,the magnetic dipoles are partially aligned in the direction of the applied magnetic field. Therefore, the material is weakly or feebly magnetized in the direction of the applied magnetic field.

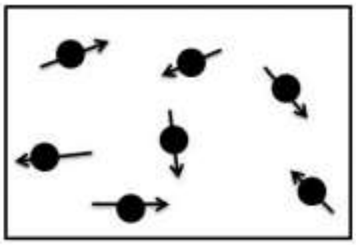


Fig: In the absence of external magnetic field (H=O)

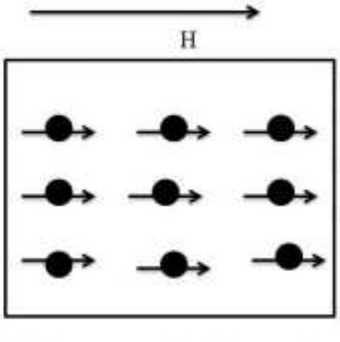
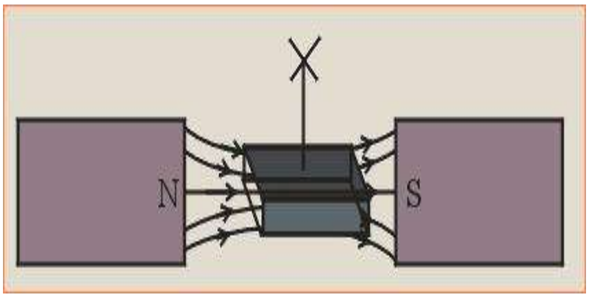


Fig: In the presence of external magnetic field

Properties:

- They possess permanent magnetic dipole moment.
- When a paramagnetic material is placed in a magnetic field, it is feebly or weekly magnetized in the direction of applied magnetic field.
- When a paramagnetic material is placed in a magnetic field, the magnetic lines force prefers to pass through the paramagnetic magnetic material rather than air.

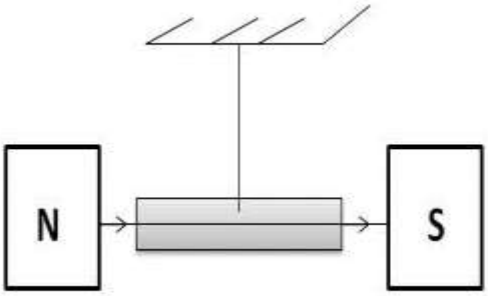


- The magnetic flux density inside is greater than that in the free space. Hence the relative permeability $\mu_r > 1$.
- The magnetic susceptibility (χ_m) is positive and small.
- The magnetic susceptibility (χ_m) is inversely proportional to the temperature.

$$\chi_m = \frac{C}{T-\theta_C} \text{ (Curie-Weiss law)}$$

Where C → Curie constant
T → Absolute temperature and
θ_C → Curie temperature

- When the temperature is less than the Curie temperature, paramagnetic materials becomes diamagnetic material.
- When a rod of paramagnetic material is suspended freely in a uniform magnetic field, the rod comes to rest with its axis parallel to the applied field.



3.Ferro magnetic materials:

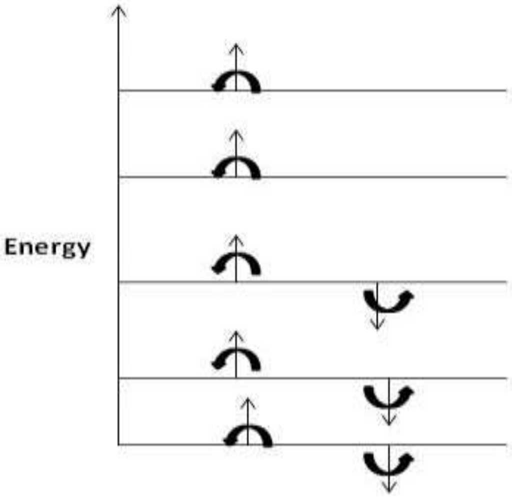
Those materials which when placed in a magnetic field are strongly magnetized in the direction of the applied magnetic field are called Ferro magnetic materials.

Examples:

Iron, Steel, Nickel, Cobalt, etc

Cause of Ferro magnetism:

- In a Ferro magnetic material, the number of unpaired electrons is more and most of the magnetic dipole moments align parallel to each other even in the absence of magnetic field..Hence they possess permanent magnetic dipole moment even in the absence of magnetic field.



- In Ferro magnetic materials, atoms grouped into regions called *domains*, instead of acting independently like paramagnetic materials.

The region of space over which the magnetic dipole moments are aligned is called domain.A typical domain contains 10^{17} to 10^{21} atoms and occupies a volume of 10^{-12} to 10^{-8} m^3.

Effect of external magnetic field:

a) In the absence of external magnetic field, the domains of a ferromagnetic material are randomly oriented. In other words, within the domain, all magnetic dipole moments are aligned, but the direction of alignment varies from domain to domain. The result is that there is no net magnetic dipole moment. Therefore, a Ferro magnetic material does not exhibit magnetism in the normal state.

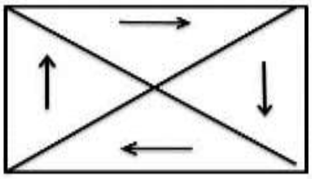


Fig: Without field

zzz

b) When a Ferro magnetic material is placed in an external magnetic field, a net magnetic dipole moment develops. This can occur in two ways:

i) By the movement of domain walls

ii) By the rotation of domain walls.

i) By the movement of domain walls:

- The movement of domain walls takes place in weak magnetic fields.
- Due to weak magnetic field applied to the material the magnetic dipole moments increases and hence the boundary of domains displaced, so that the volume of the domains changes as shown in fig.

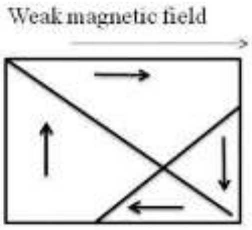


Fig: Displacement of domain walls With weak magnetic field

ii) By the rotation of domain walls

- The rotation of domain wall takes place in strong magnetic fields.
- Due to strong magnetic field applied to the material the magnetic dipole moments increases enormously and hence the domains rotate, so that the magnetic dipole moments are aligned in the direction of applied magnetic field as shown in fig..

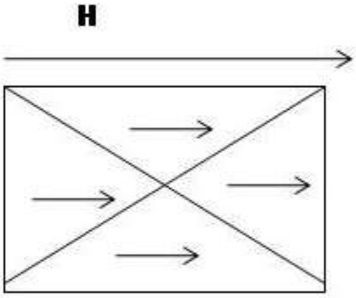
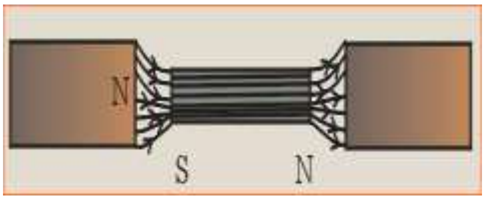


Fig : Rotation of domain walls in strong magnetic field

Properties:

- They possess permanent magnetic dipole moment.
- When a Ferro magnetic material is placed in a magnetic field, it is strongly magnetized in the direction of applied magnetic field.
- When a Ferro magnetic material is placed in a magnetic field, the magnetic lines force tend to crowed into the Ferro magnetic material.

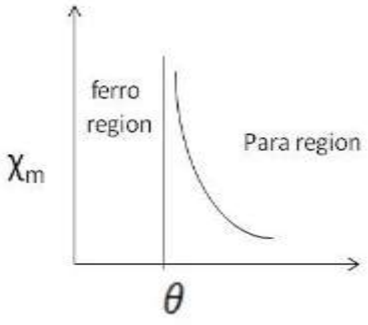


- The magnetic flux density inside is very greater than that in the free space. Hence the relative permeability $\mu_r >> 1$.
- The magnetic susceptibility (χ_m) is positive and very high.
- The magnetic susceptibility (χ_m) is inversely proportional to the temperature.

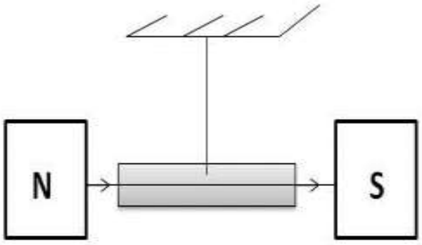
$$\chi_m = \frac{C}{T-\theta_C} \text{ (Curie-Weiss law)}$$

Where C → Curie constant
T → Absolute temperature and
θ_C → Curie temperature

- When the temperature is greater than the Curie temperature, ferromagnetic materials becomes Para magnetic material.



- When a rod of Ferro magnetic material is suspended freely in a uniform magnetic field, it quickly aligns itself in the direction of the applied magnetic field.



Classification of Ferro magnetic materials:

Depending upon the spin orientation of the electrons, ferromagnetic materials are classified into two types, they are 1.Antiferromagnetic materials 2. Ferri magnetic materials

Antiferromagnetic materials:

The materials which consist of anti parallel spin magnetic dipole moment with same magnitudes are known as anti ferromagnetic materials.

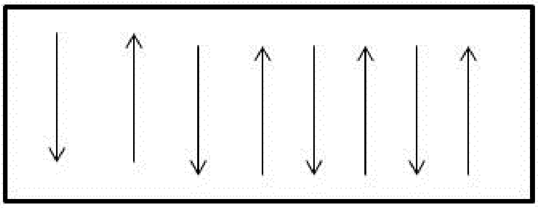
Examples:

Ferrous oxide (FeO),
Manganese oxide (MnO_4),
Manganese sulphide MnS),

Chromium Oxide (Cr_2O_3),
Ferrous Chloride ($FeCl_2$) etc

Properties:

- In this materials spin magnetic dipole moments are aligned in anti parallel manner.

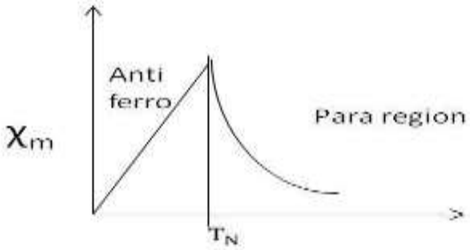


- The magnetic susceptibility is very small and positive
- The magnetic susceptibility is inversely proportional to temperature. The variation of susceptibility with temperature is shown in fig.

$$\chi_m = \frac{C}{T \pm \theta_C}$$

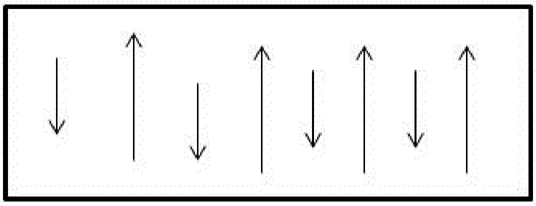
C is → Curie constant
T → Absolute temperature and
θ_C → Curie temperature

χ_m is increases gradually with temperature and attains a maximum value at Neel temperature(T_N) and then decreases with increase in temperature.



Ferrimagnetic materials:

The materials which consist of anti parallel magnetic dipole moments of different magnitudes are known as ferrimagnetic materials.



Examples:

Ferrites-general formula: Me^{+2} $Fe^{2}O_4$

Where Me^{+2} =divalent metal ions(Zn,Cu,Ni).

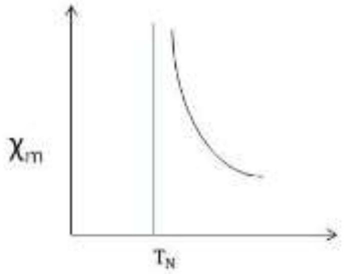
Properties:

- In this materials spin magnetic dipole moments of different magnitudes are aligned in anti parallel manner.

- The magnetic susceptibility is very high and positive
- The magnetic susceptibility is inversely proportional to temperature. The variation of susceptibility with temperature is shown in fig.

$$\chi_m = \frac{C}{T \pm \theta_C}$$

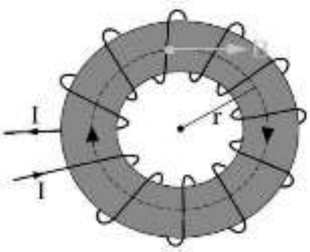
C → Curie constant
T → Absolute temperature and
θ_C → Curie temperature



HYSTERISIS:-

When a Ferro magnetic substance (e.g. iron) is subjected to a cycle of magnetization (i.e. it is magnetized first in one direction and then in the other), it is found that flux density B in the material lags behind the applied magnetizing force H. This phenomenon is known as hysteresis.

Definition of Hysteresis: *The phenomenon of lagging of flux density (B) behind the magnetizing force (H) in a ferromagnetic material subjected to cycles of magnetization is known as hysteresis*.



Explanation :

The term hysteresis is derived from the Greek word hysteresis meaning to lag behind..If a piece of ferromagnetic material is subjected to one cycle of magnetization ,the resultant B-H curve is a closed loop a b c d e f a Called hysteresis loop.

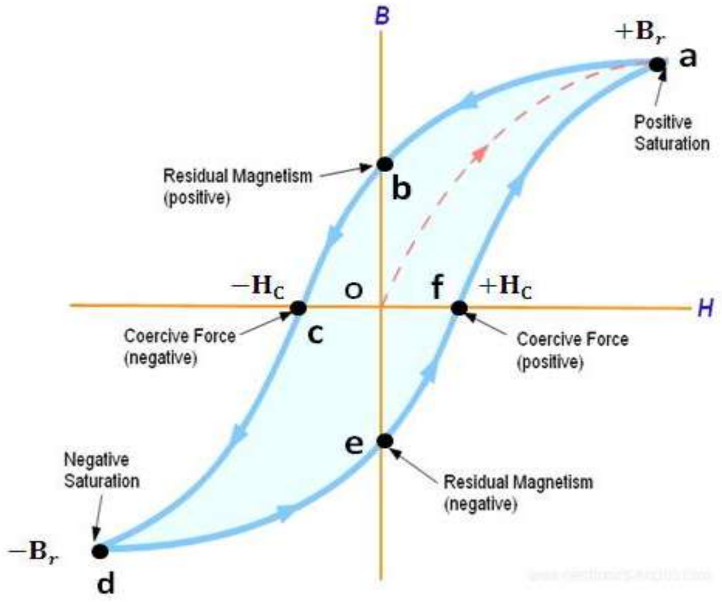


Fig: B-H Curve

(i) To start with, the toroid is unmagnetised and its situation is represented by point O in fig. As H is increased (by increasing current I), B increases along **oa** and reaches its saturation value B_{max} at a .At this stage, all the domains are aligned.

(ii) If now H is gradually reduced by decreasing the current in the toroid, it is found that curve follows the path **ab** instead of **ao** .At point **b**, H=0 but flux density in the material has a finite value $+B_r$ (=**ob**) called *residual flux density*. It is also called **remanence** or **retentivity.** Note that *B* lags behind H. This effect is called *hysteresis.*

(iii) In order to reduce flux density in the material to zero, it is necessary to apply *H* in the reverse direction. This can be done by reversing the current I the toroid .When *H* is gradually increased in the reverse direction, he curve follows the path **bc**. At point c, B=0 and $H= -H_C$ .The value of *H* needed to wipe out residual magnetism is called coercive force (H_C).

(iv) Now *H* is further increased in the reverse direction until point d is reached where the sample is saturated in the reverse direction ($-B_{max}$).If *H* is now reduced to zero point **e** is reached and the sample again retains magnetic flux density ($-B_r$).The remaining part of the loop is obtained by increasing current to produce *H* in the original direction. The curve "*a b c d e f a"* is called hysteresis loop. Thus hysteresis loop results because the domains do not become completely unaligned when *H* is made zero. The area enclosed by the hysteresis loop represents loss in energy. This energy appears in the material as heat.

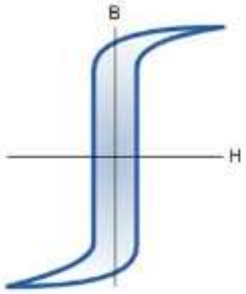
Based on the area of the hysteresis loop, the magnetic materials are classified into soft and hard magnetic materials.

Soft magnetic materials:-

The materials which can be easily magnetized and demagnetized are called Soft magnetic materials.

Properties:

- They can be easily magnetized and demagnetized and hence they show high values of susceptibility and permeability.
- Movement of domain wall is easy and hence even for small applied field large magnetization occurs.
- The nature of hysteresis loop is very narrow
- The hysteresis loop area is very small hence the hysteresis loss is also small as shown in fig.



- The coercivity and retentivity values are small
- These materials are free from irregularities or impurities or imperfections

Examples:

Fe- Si alloys, Ni-Fe alloys, Fe-Co alloys, Ferrities and Garnets etc

Applications:

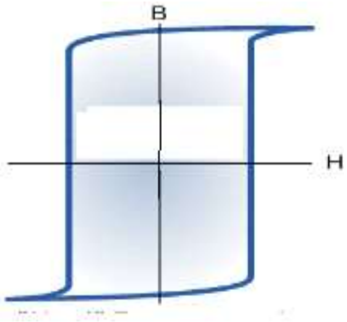
- ➢ They are used in switching devices, electromagnets,
- ➢ They are used in matrix storage of computers.
- ➢ They are used in motors, relays and sensors
- ➢ They are used to make the temporary magnets.

Hard magnetic materials:-

The materials which can’t be easily magnetized and demagnetized are called hard magnetic materials.

Properties:

- They can’t be easily magnetized and demagnetized and hence they show low values of susceptibility and permeability.
- Movement of domain wall is not easy due to presence of impurities and hence large magnetic field is required for magnetization
- The nature of hysteresis loop is very broad.
- The hysteresis loop area is large hence the hysteresis loss is also large as shown in fig.



- The coercivity and retentivity values are high
- These materials are have irregularities or impurities or imperfections
- **Examples:**

Carbon steel, tungsten steel, chromium steel,
Cu-Ni-Fe alloys
Cu-Ni-Co alloys
Al-Ni-Co alloys

- **Applications:**

- ➢ They are used in magnetic detectors ,
- ➢ They are used in microphones.
- ➢ They are used in magnetic separators.
- ➢ They are used to make the permanent magnets.

Unit: IV

Chapter I&II : Quantum Mechanics and Nanomaterials

Chapter I: Quantum mechanics :

INTRODUCTON:

In the late seventeen century, Isaac Newton discovered classical mechanics, the law of motion of macroscopic objects.

In the early twentieth century, physicists found that classical mechanics does not correctly describe the behavior of very small particles such as the electrons nuclei (protons & neutrons etc.) and molecules. The behavior of such particles is described by a set of laws called **Quantum mechanics.**

i.e. Classical mechanics applies only to macroscopic particles. For microscopic "particles" .We require a new form of mechanics, called **Quantum mechanics.**

Classical mechanics:

- Classical mechanics deals with the motion and behavior of **macroscopic particles**.

Ex: Motion of planets.

- Classical mechanics is expressed in the language of un-probabilities, certainties.

Quantum mechanics:

- Quantum mechanics deals with the motion and behavior of **microscopic particles**

Ex: Motion of Electrons

- Quantum mechanics is expressed in the language of probabilities, not certain.

DUAL NATURE OF UNIVERSE:

de-Broglie hypothesis:

According to de-Broglie

1. The entire universe is consists of matter and radiation only.
2. **Nature loves symmetry:** Things in nature exists in two forms -- matter and radiation. With experimental evidences, like interference, diffraction, photo electric effect etc., it is proved that radiation can have two forms: (i) wave form and (ii) particle form. If radiation can take two forms, then matter can also have two forms.
3. Every moving particle has always associated with a wave. The particle is controlled by this wave.

The wave associated with moving particle of matter (like electrons, protons etc) are known as matter wave or pilot waves or de-Broglie waves.

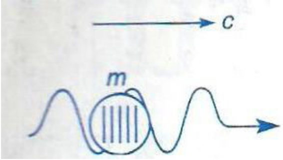


Figure .1 Motion of particle (Photon)

If a particle of mass *m* moving with velocity *v*, then the wavelength of matter wave is given by

$$\boxed{\lambda = \frac{h}{mv}}$$

Where

h→ Planck's constant,
m → mass of particle,
V→ velocity of the particle

Derivation of de – Broglie's wave length:

According to Planck's quantum theory of radiation (light) the energy of photon is given by

$$E = h\nu \quad \text{-------} \quad (1)$$

Where ' h' is Planck's constant,
'ν' is frequency of radiation

According to Einstein's energy-mass relation, the energy of photon is given by

$$E = mc^2 \quad \text{--------} \quad (2)$$

Where
' m' is mass of photon
'c' is velocity of light or photon

From the above equations (1) and (2); we can write

$$h\nu = mc^2 \qquad [\because C = \nu\lambda]$$

$$\frac{hc}{\lambda} = mc^2 \qquad [\because \nu = \frac{c}{\lambda}]$$

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

$$\lambda = \frac{h}{mc} = \frac{h}{p} \quad \text{-------------} \quad (3)$$

Where p = mc is the momentum of photon having mass *m* and travelling with velocity *c*.
de - Broglie suggested that equation (3) can be applied both for photons and material particles. If m is mass of the particle and v is the velocity of the particle, then Momentum (p) = mv

$\therefore$ de – Broglie wave length $\lambda = \frac{h}{mv}$ **-------** (4)

This equation represents that the de-Broglie wave length associated with a particle and also known as de –Broglie's wave equation.

OTHER FORMS OF de –Broglie's WAVE LENGTH:

1.de –Broglie's wave length in terms of energy:

If m is mass of the particle and v is the velocity of the particle, then the kinetic energy of the particle;

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

Multiplying by 'm' on both sides; we get

$$m E = \frac{1}{2} m^2v^2$$

$2 m E = m^2v^2$

$$\text{(Or) } m v = \sqrt{2 m E}$$

$\therefore$ de – Broglie wave length $\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2 m E}}$ **-----------------** (5)

2.de –Broglie's wave length in terms of voltage:

If a charged particle of charge 'q' is accelerated through a potential difference 'v', then

$$E = q v \quad \text{------} \quad (6)$$

Also we know that the K.E of the particle $E = \frac{1}{2} mv^2$ ----- (7)

Equating equations (7) and (6) we get

$$\frac{1}{2} mv^2 = q v$$

Multiplying by 'm' on both sides we get

$$\frac{1}{2} m^2v^2 = m q v$$

$$\therefore m^2v^2 = 2 m q v$$

$$m\,v = \sqrt{2\,m\,q\,v} \quad \text{-------} \quad (8)$$

Substituting equation (8) in equation (4) , we get

$$\therefore \text{ de – Broglie wave length } \lambda = \frac{h}{mv} = \frac{h}{\sqrt{2\,m\,q\,v}} \quad \text{-----} \quad (8)$$

de –Broglie's wave length for electron

Substituting the values of m, q and h in equation 9 we get

$$\lambda = \frac{6.626 \text{ X } 10^{-34} \text{ JS}}{\sqrt{2 \text{ X} 9.1 \text{ X } 10^{-31} \text{ Kg X } 1.6 \text{ X} 10^{-19} \text{ C X V}}}$$

$$= \frac{12.27 \text{ X } 10^{-10} \text{ m}}{\sqrt{V}} \qquad [\because 1 \text{ A}^0 = 10^{-10} \text{ m}]$$

$$\lambda = \frac{12.27}{\sqrt{V}} \text{A}^0$$

This equation represents the de – Broglie wave length associated with an electron.

Wave velocity:

We know that

$E= h\nu$ and $E = mc^2$

$$h\nu = mc^2$$

$$\nu = \frac{mc^2}{h}$$

The wave velocity is given by

$$\omega = \nu\,\lambda$$

$$\omega = \frac{mc^2}{h} \cdot \frac{h}{mv}$$

$$\therefore \omega = \frac{c^2}{V}$$

Thus matter waves travel faster than velocity of light.

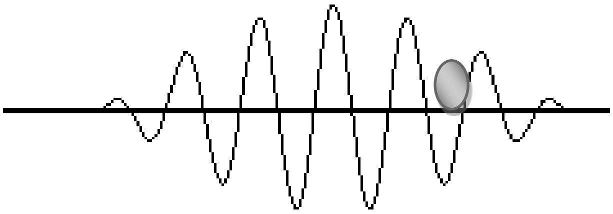
Properties of de-Broglie waves:

The following are the properties of matter waves.

The de-Broglie wavelength of particle of mass (m) moving with a velocity (v) is given by

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

If v = 0, $\lambda \rightarrow \infty$ and if $v \rightarrow \infty$, $\lambda \rightarrow 0$.
This implies that matter waves are associated with material particles only if they are in motion.
2. Lesser the velocity of the particle, larger the wave length associated with it.
3. Smaller the mass of the particle, the greater the length associated with it.
4. The matter wave of particle is independent of charge (or) nature of the particle.
5. de-Broglie waves are pilot waves. The word, pilot means that these waves pilot (or) guide the particle.
6. Matter waves travel faster than velocity of light, i.e., $\omega = \frac{c^2}{V}$.
7. Mater waves are not electromagnetic waves.
8. The wave nature of matter introduces an uncertainty in the location of the position of the particle because a wave cannot be set exactly at this position (or) at that position. 9. de-Broglie waves are called probability waves. The amplitude of the wave tells us about the probability of finding particle in space at a particular instant. Large wave amplitude means large probability of finding the particle at that position.



NOTE:

1. Mention an application of matter waves?

A. The electron microscope is an application of matter waves, associated with electrons

2. Why cannot we experience the existence of matter waves in our day to day life?

A. $\lambda = \frac{h}{mv}$, if m is large, λ will be small, thus the wave length will be very small, compared to the size of the particle, hence it is not observable.

The universe is an inherently uncertain. Mind cannot know all of existence of creation (or) universe...
Benediction Muni

Matter Wave	Electromagnetic (EM) wave
1. Matter wave is associated with moving particle. 2. Wavelength depends on the mass of the particle and its velocity. $\lambda = \frac{h}{mv}$ 3. Matter wave can travel with a velocity greater than the velocity of light. 4. Matter wave is not electromagnetic wave.	1. Oscillating charged particle gives rise to electromagnetic wave. 2.Wavelength depends on the energy of photon $\lambda = \frac{hc}{E}$ 3. Electromagnetic wave travels with velocity of light. i.e, $c = 3x10^8$ m/s. 4. Electric field and magnetic field oscillate perpendicular to each other.

Heisenberg uncertainty principle:

In 1927, Heisenberg proposed a very interesting principle, which is direct consequence of the dual nature of matter, known as uncertainty principle.

According to classical mechanics, it is possible to determine accurately and simultaneously the values of position and momentum of a particle at any time.

Consider a particle of mass ‘m’ moving with velocity ‘v’ along X-direction as shown in fig.

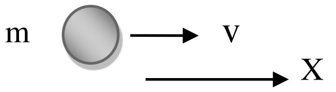


Fig: Motion of classical particle

The position of particle is given by $x = vt \longrightarrow (1)$

The momentum of particle is given by $p = mv \longrightarrow (2)$

$$\text{And } v = \frac{p}{m} \longrightarrow (3)$$

Substituting equation (3) in eq (1),we get

$$X = \frac{p}{m} t \longrightarrow (4)$$

From the above equation, it is clear that the position and momentum of a particle can be determine accurately.

But, According to Heisenberg uncertainty principle, it is impossible to determine accurately and simultaneously the values of position and momentum of a particle at any time.

If Δx is the error (uncertainty) in measuring position, Δp is the error (uncertainty) in measuring momentum; then according to this principle

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

NOTE: Similarly such relations are $\Delta E.\ \Delta t \geq \frac{h}{4\pi}$ and $\Delta J.\ \Delta\theta \geq \frac{h}{4\pi}$, Where ΔE and Δt are the uncertainties in determining the energy and time, while ΔJ and $\Delta\theta$ are uncertainties in determining the angular momentum and angle.

Application of uncertainty principle:

1. It is also verified Existence of protons and neutrons inside the nucleus
2. It is calculated binding energy of electron in an atom
3. It is also calculated Mass of Π -meson
4. Emitted radiation of excited atom is confirmed by this principle.

Significance of Uncertainty principle:

- This principle is significant only for motion of microscopic objects and is negligible for that of macroscopic objects
- According to classical mechanics (macroscopically) it is possible to predict exactly the position and momentum of particle. But, according to uncertainty principle, or quantum mechanics (microscopically), it is not possible to determine accurately and simultaneously the values of position and momentum of a particle at any time.
- This principle actually tells us that we cannot detect the particle nature and wave nature of matter at the same time.

Physical significance of wave function:

The wave nature of matter introduced an uncertainty in the location of the position of the particle because a wave cannot be set exactly at this position (or) at that position.

According to Heisenberg uncertainty principle tells us that we cannot detect the particle nature and wave nature at the same time.

To resolve this uncertainty, Eddington once upon a time humorously suggested that the primordial entity is neither particle nor wave but a ‘wavicle’. Thus, de-Broglie waves are called probability waves.
The amplitude of the wave tells us about the probability of finding particle in space at a particular instant. A large wave amplitude means a large probability of finding the particle at that position.

Mathematically, to explain it, scientists introduced a new physical quantity called wave function.

Wave function: -

it is a mathematical tool used in quantum mechanics to describe any physical system, and it is denoted by 'ψ'.

It is variable quantity i.e., associated with a moving particle at any position (x,y,z) and at any time t and it relates probability of a finding the particle at that point and at that time.

It must be well behaved, that is single valued and continuous everywhere.

It usually complex quantity and individually it has no meaning.

To explain it, Max born suggested a new idea about the physical significance of ψ which is generally accepted now a days.

According Max born $\psi\ \psi^* = |\psi|^2$ is a real and positive, it has physical meaning. It represents the probability of finding the particle in the state ψ.

The probability of finding the particle in a volume $dv = dx.dy.dz$ is given by

$$\text{Probability (P)} = |\psi|^2$$

For the total probability of finding the particle somewhere is (space).

$$P\ dv = \iiint |\psi|^2\ dx\ dy\ dz = 1$$

A wave function ψ satisfying the above relation is called a normalized wave function.

For motion of a particle in one dimensional, the quantity

$$Pdx = |\psi|^2 dx$$

is the probability of finding the particle over a small distance dx at position x.

Explanation:-

Consider a particle having three dimensional motions along x,y,z co-ordinates (as shown in figure).wave function

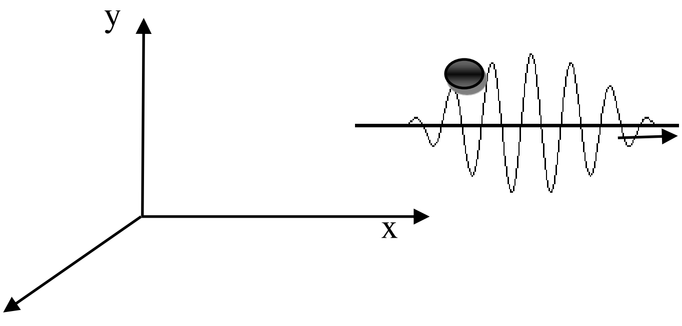


Fig: Probability of finding particle in space

The values of the wave function (ψ) associated with a moving particle, at a point x,y,z in a space is related to finding of the particle there.

Since the wave function is a complex quantity, it may be expressed in the form of

$$\psi_{(x,y,z)} = (a+ib)$$

Where a,b are real function of the variables (x,y,z,t) and $i=\sqrt{-1}$.

The complex conjugate of ψ is given by

$$\psi^{*}_{(x,y,z)} = (a-ib)$$

Multiplying the above two equations, we have

$$\psi\psi^{*} = (a+ib)\,(a-ib) = a^2+b^2$$

According to Max born

$$P = \psi\psi^{*} = |\psi_{(x,y,z)}|^2 = a^2+b^2$$

Thus the product of ψ and ψ^{*} is real and positive if $\psi \neq 0$ and is known as probability density of the particle associated with the de-Broglie wave.

Schrodinger wave equation:-

Introduction: -

Schrodinger wave equation is one of the basic equations in quantum mechanics, this equation can be applied for both microscopic and macroscopic particles.

Schrodinger derived a mathematical equation to describe the dual nature of matter waves.

Definition: -

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

Schrodinger connected the expression for the de-Broglie wave length into the classical wave equation for a moving particle and obtained a new wave equation.

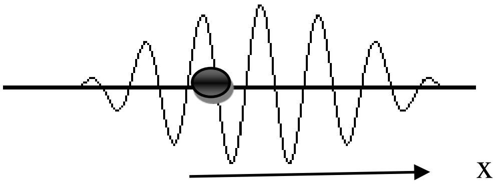
Classical wave equation +de- Broglie wave equation = Schrodinger wave equation.

There are two types of Schrodinger wave equations they are

1) Time independent wave equation
2) Time dependent wave equation

Schrodinger one dimensional Time independent wave equation :-

Let us consider a particle of mass m moving with a velocity v. Let ψ be the wave function of a particle along X-direction at any time (as shown in figure).



The classical differential equation of wave motion is given by

$$\frac{\partial^2\psi}{\partial x^2}=\frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} \quad \text{--------} \quad (1)$$

The solution for equation (1) is assumed to be

$$\psi = \psi_0 e^{-i\omega t} \quad \text{-------} \quad (2)$$

Where ψ_0 is the amplitude of the wave at any point..

Differentiating equation (2) partially with respect to'‘t’; we get

$$\frac{\partial\psi}{\partial t} = \psi_0 e^{-i\omega t} \times (-i\omega) \quad \text{-------} \quad (3)$$

Differentiating once again equation (3) partially with respect to ‘t’; we get

$$\frac{\partial^2\psi}{\partial t^2} = \psi_0\, e^{-i\omega t} \times (-i\omega) \text{ x } (-i\omega)$$

$$= \psi_0 e^{-i\omega t} (-\omega^2) \qquad [\text{ from eq (2)}]$$

$$\frac{\partial^2\psi}{\partial t^2} = -\ \omega^2\psi \quad \text{-------} \quad (4)$$

Substituting equation (4) in (1) we get

$$\frac{\partial^2\psi}{\partial x^2} = \frac{1}{v^2}(-\omega^2\psi)$$

$$= -\ \frac{\omega^2}{v^2}\psi \quad \text{-------} \quad (5)$$

But $\omega = 2\pi\nu = 2\pi\, v/\lambda$ $\quad$ ($v = \nu\lambda$

$\nu = v/\lambda$)

(or) $\frac{\omega}{v} = \frac{2\pi}{\lambda} \rightarrow$ (6)

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

$$\frac{\partial^2\psi}{\partial x^2} + \frac{4\pi^2\psi}{\lambda^2} = 0 \quad \text{--------} \quad (7)$$

This is the classical wave equation in terms of wavelength.

Schrodinger connected the expression for the de Broglie wave the length in to the classical wave equation in terms of wavelength for a moving a particle and obtained a new wave equation.

We know that debroglie wavelength is given by

$$\lambda = \frac{h}{mv} \quad \text{--------} \ (8)$$

Substituting equation (8) in (7), we get

$$\frac{\partial^2\psi}{\partial x^2} + \frac{4\pi^2 m^2 v^2}{h^2}\psi = 0 \quad \text{------} \ (9)$$

If E is the total energy of a particle, ‘V’ is the potential energy and $\frac{1}{2}mv^2$ is the kinetic energy; then

Total energy (E) =P.E+K.E

$$E = V + \frac{1}{2}mv^2$$

(Or) $\quad E - V = \frac{1}{2}mv^2$

$$2(E-V) = mv^2$$

Multiplying by ‘m’ on both sides in the above equation, we get

$$2m\,(E-V) = m^2\,v^2 \quad \text{--------} \ (10)$$

Substituting equation (10) in (9) we get

$$\frac{\partial^2\psi}{\partial x^2}+\frac{8\pi^2 m}{h^2}(E-V)\,\psi = 0 \text{ -------- } (11)$$

(Or) $$\frac{\partial^2\psi}{\partial x^2}+\frac{2m}{\hbar^2}(E-V)\,\psi=0 \quad \text{--------} \quad (12)$$

Where $\hbar = \frac{h}{2\pi}$ is called plank's reduced constant.

This equation is known as Schrodinger time independent one-dimensional wave equation.

Note:

For 3dimensional:

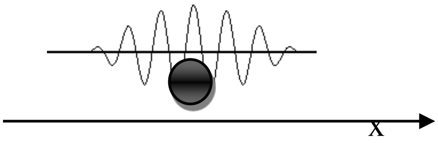
$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{8\pi^2 m}{h^2}(E-V)\,\psi=0$$

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

$\nabla^2 = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$ is called Laplace operator

Schrodinger's Time dependent wave equation:

Let us consider a particle of mass m moving with a velocity v. Let ψ be the wave function of a particle along x-direction at any time (as shown in figure).



The classical differential equation of wave motion is given by

$$\frac{\partial^2\psi}{\partial x^2}=\frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} \quad \text{----} \quad (1)$$

The solution for equation (1) is assumed to be

$$\psi = \psi_0 e^{-i\omega t} \quad \text{-----} \quad (2)$$

Where ψ_0 is the amplitude of the wave at any point..

Differentiating equation (2) partially with respect to't'; we get

$$\frac{\partial\psi}{\partial t} = \psi_0 e^{-i\omega t} \times (-i\omega)$$

$$= -i\omega\psi \quad \text{-----} \quad (3)$$

$$\text{But } E = h\nu = h\frac{\omega}{2\pi}$$

$$= \frac{h}{2\pi}\,\omega \qquad (\omega = 2\pi\nu \rightarrow \nu = \frac{\omega}{2\pi})$$

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

And $\omega = \frac{E}{\hbar}$ ----- (4)

Substituting equation (4) in eq (3), we get

$$\frac{\partial\psi}{\partial t} = -\,i\frac{E}{\hbar}\psi$$
$$= \frac{E}{i\,\hbar}\psi$$
$$E\,\psi = i\,\hbar\frac{\partial\psi}{\partial t} \qquad \text{-----} \qquad (5)$$

Substituting equation (5) in Schrodinger time independent one-dimensional wave equation, we get

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E\text{-}V)\,\psi = 0 \qquad \text{-----} \qquad (6)$$

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

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

Multiplying $\frac{\hbar^2}{2m}$ on both sides, we get

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

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

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

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

This equation is known as Schrodinger time dependent one-dimensional wave equation.

(Or) $$H\,\psi = E\psi$$

Where $H = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$ is called Hamilton operator.

$E = i\,\hbar\frac{\partial}{\partial t}$ is called energy operator.

Particle in an infinite potential well (or) potential box:

Consider a particle of mass 'm' moving back and forth between the walls of a one dimensional box separated by a distance 'a' as shown in figure 6.6.Let the particle travel along the x axis and confined between $x = 0$ *and* $x = a$ by two infinitely hard walls so that the particle has no chance of penetrating them.

Thus, it doesn't lose energy when it colloids walls and its total energy remains constant. This box can be represented by a potential box of width 'a' with potential walls of infinite height at $x = 0$ *and* $x = a$ so that the potential energy 'V' of the particle is infinitely high on both sides of the box inside it, 'V' is uniform.

Let us assume that V=0 inside the box.

$$V(x) = 0 \qquad for\ 0 < x < a$$

$$V(x) = \infty \qquad for\ x \le 0\ and\ x \ge a\,.$$

Then the wave function ψ(x) of the particle in the region $0 < x < a$ where V=0 is described by Schrodinger's one dimensional time independent wave equation i.e.,

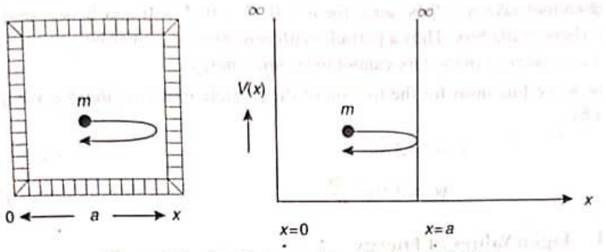


Figure 5.5 Particle in one-dimensional potential box

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

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

$$\frac{\partial^2\psi}{\partial x^2} + K^2\ \psi(x)\ = 0$$

Where $K^2 = \frac{2m}{\hbar^2} E$ (or) $K = \sqrt{\frac{2m}{\hbar^2}\ E}$

The solution of above equation is given by,

$$\psi(x)\ = A\,SinKx\ +\ B\,CosKx$$

Where A and B are arbitrary constants.

Applying the first boundary condition, i.e., $at\ x = 0\ , \psi(x) = 0$ we get

$B = 0$

Applying the secondary boundary condition, we have $x = a\ , \psi(x)\ =\ \psi(a)\ = 0$

$\therefore\ \psi(a) = A\ SinKa = 0$

$A \neq 0$ since there will not be any solution. Hence we have

$SinKa = 0$

$Ka = n\pi$

$K = \frac{n\pi}{a}$ where n=1,2,3,…..

We cannot take n=0 because for n=0 , K= 0 , E=0 and hence $\psi(x) = 0$ everywhere in the box. Thus the particle with zero energy cannot be present in the box. i.e., a particle in the box cannot have zero energy.

The wave functions for the motion of the particle in the region $0 < x < a$ are given by,

$$\psi_n(x) = A\ SinKx$$

$$\psi_n(x)\ = A\ Sin(\frac{n\pi x}{a})$$

Eigen values of energy:

We know that $K^2 = \frac{2m}{\hbar^2} E$

$$E = \frac{K^2\hbar^2}{2m}$$

Substituting the value of 'K' we get,

$$E = [\frac{n^2\pi^2}{a^2}]\frac{\hbar^2}{2m}$$

$$= [\frac{n^2\pi^2}{a^2}][\frac{h^2}{8\pi^2 m}] \qquad (\because \hbar = \frac{h}{2\pi})$$

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

From the above equation it is clear that

1.The lowest energy of the particle obtained by putting n=1

i.e, $E_1 = \frac{h^2}{8ma^2}$ and $E_n = n^2E_1$

This is known as zero point energy of the system.

2. For n=1, 2, 3 we get discrete energy values of the particle in the box.

$$E_1 = \frac{h^2}{8ma^2}$$
$$E_2 = 2^2\frac{h^2}{8ma^2} = 4\ E_1$$
$$E_3 = 3^2\frac{h^2}{8ma^2} = 9\ E_1$$

The spacing between the nth energy level and next higher level increases as

$$(n+1)^2 E_1 - n^2 E_1 = (2n+1) E_1$$

3. These values of E_n are known as Eigen values of energy and the corresponding wave functions ψ_n as Eigen functions of the particle. The integer 'n' is the quantum number of energy level E_n .Figure 6.7 shows the energy level diagram for the particle.

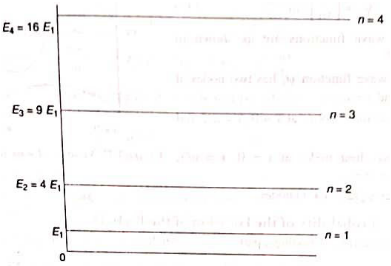


Figure 5.6 Energy-level diagram of particle in a one-dimensional box

<u>Eigen functions or Normalisation of the wave function:</u>

The eigen wave function for the motion of the particle are

$$\psi_n(x) = A\,Sin(\frac{n\pi x}{a}) \quad in\ the\ region\ 0 < x < a$$
$$\psi_n(x) = 0 \quad \text{in the region} \quad x \leq 0\ and\ x \geq a$$

The total probability that the particle is somewhere in the box must be unity.

$$\int_0^a P_x\,dx = \int_0^a |\psi_n\ (x)|^2\,dx = 1$$

$$\int_0^a A^2\,Sin^2(\frac{n\pi x}{a})\,dx = 1$$

$$A^2\int_0^a \frac{1}{2}\left[1\text{-}\cos\frac{2\pi nx}{a}\right]dx = 1$$

$$\frac{A^2}{2}\left[x - \frac{a}{2\pi n} Sin\frac{2\pi n x}{a}\right]_0^a = 1$$

The second term becomes zero at both the limits

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

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

The normalized wave function is,

$$\psi_n(x) = \sqrt{\frac{2}{a}}\ \mathrm{Sin}\frac{n\pi x}{a}$$

The wave functions are shown in figure 5.7.

The wave function ψ_1 has two nodes at $x = 0\ and\ x = a.$

ψ_2 has three nodes at $x = 0, x = a/2\ and\ x = a.$

ψ_3 has three nodes at $x = 0, x = a/3, x = 2a/3\ and\ x = a.$

Thus $\psi_n(x)$ has (n+1) nodes.

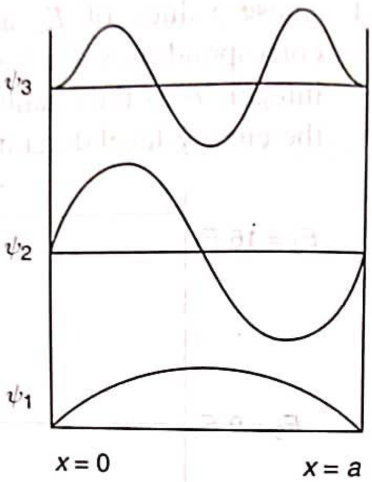


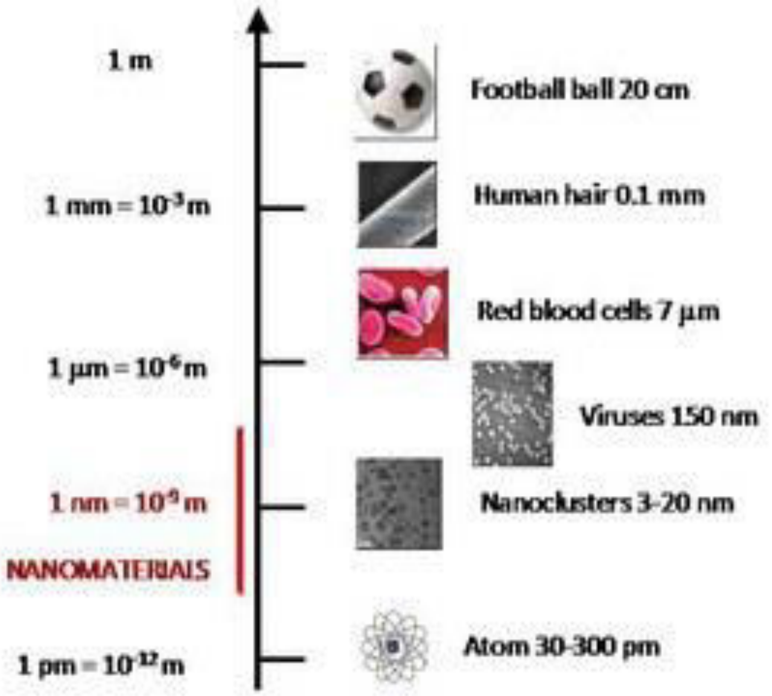
Figure 5.7 Variation of wave function

Chapter-2
Nanomaterials

Introduction:-

All materials are composed of grains, which in turn comprise many atoms. The visibility of these grains depends on their size. The materials possessing grains of size ranging from 1 to 100 nm, are known as **“Nanomaterials”** and the developed technology is called nano technology. This was first discovered by Feynman in 1959.

- Nano technology deals with the design, manufacturing and application of devices (or) materials which lie in the sizes of 1 to 100 nm.
- Nano means 10^{-9} (one-billionth)
- A nanometer 1nm = 10^{-9} m(one-billionth of meter)
- Nano materials are found in both biological systems and man-made structures.
- Nature has been using nano materials for millions of years.



Nano materials:-

All materials are composed of grains, which in turn comprise many atoms. The visibility of these grains depends on their size. The materials possessing grains of size ranging from 1 to 100 nm, are known as **“Nanomaterials”.**

Examples: zno, cu-Fe alloys, Ni, Pd, Pt etc.

Classification of Nanomaterials:

According to Siegel, Nanostructured materials are classified as Zero dimensional, one dimensional, two dimensional, three dimensional nanostructures.

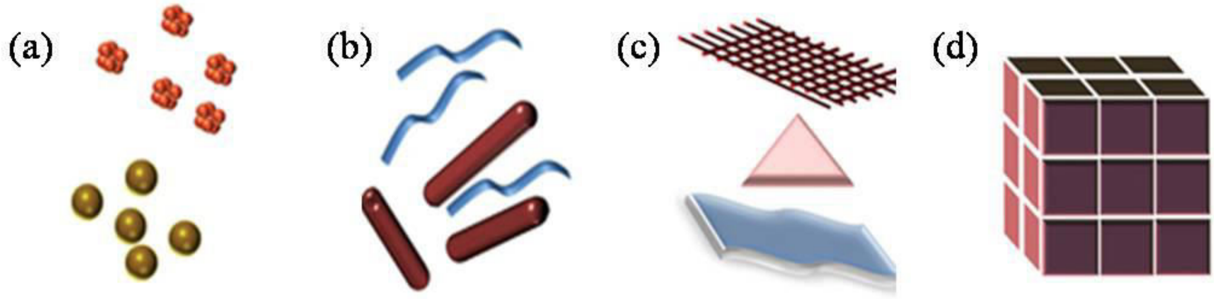


Fig: Classification of Nanomaterials (a) 0D spheres and clusters, (b) 1D nanofibers, wires, and rods, (c) 2D films, plates, and networks, (d) 3D nanomaterials.

- **One-dimensional Nanomaterial: -** In these Nanomaterial, grains will be layered in the form of multi-layers such as thin films or surface coatings.
- **Two dimensional Nanomaterials: -** This consists of ultrafine grains layered over layers or buried layers, which include nano wires and nano tubes.
- **Three dimensional Nanomaterials**: - This consists of nano meter sized grains.

Examples: precipitates, colloids and quantum dots.

Why the properties of nano materials are different?
(Or)
Basic principles of Nanomaterials:-

Two principle factors cause the properties of nano materials to differ significantly from other materials increased in surface area to volume ratio , and quantum confinement . These factors can change or enhance the properties such as reactivity, strength and electrical characteristics.

(1) INCREASE IN SURFACE AREA TO VOLUME RATIO :-

Nanomaterials have a relatively larger surface area when compared to the larger form of the material of same volume. Let us consider a sphere of radius ‘r”.

Its surface area = $4\pi r^2$

Its volume = $\left(\frac{4}{3}\right)\pi r^3$

Surface area to its volume ratio = $\frac{4\pi r2}{\frac{4}{3}\pi r3} = \frac{1}{\frac{r}{3}} = \frac{3}{r}$

Thus, when the radius of the sphere decreases, its surface area to volume ratio increases. Let us consider another example. For a one cubic volume shown in fig .4.The surface area is $6m^2$.When it is divided in to eight pieces its surface area becomes $12m^2$.When the same volume is divided in to 27 pieces its surface area becomes $18m^2$ .Thus we find that when the given volume is divided in two smaller pieces ,the surface area increases. Hence as particle size decreases a greater proportion of atoms are found at the surface compared to those in-sides.

For example, a particle of size 30 nm has 5% of atoms its surface, at 10nm 20% of its atoms, and at 3nm has 50% of its atoms.

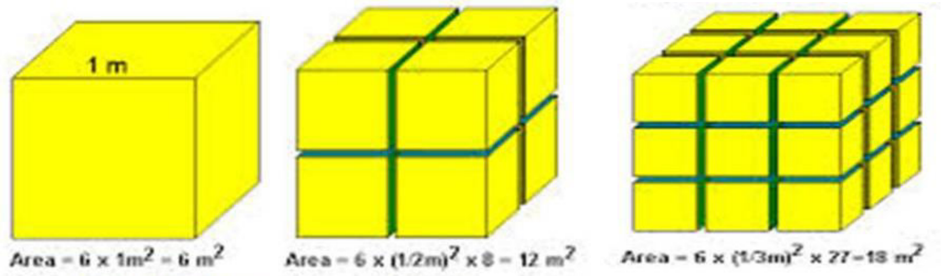
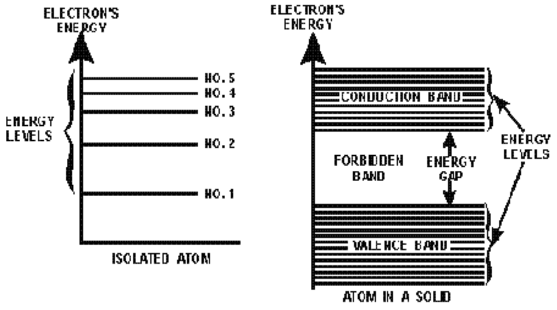


Fig: when the given object divided into smaller particles, the surface area increases.

(2) QUANTUM CONFINEMENT: -

The properties of materials can be studied based on their energy levels. When atoms are isolated, their energy levels are discrete. When very large number of atoms closely packed to form a solid, the energy levels split and form bands. .Nanomaterial is intermediate to the above cases. As a result, the energy levels change, when the material size is reduced to nano scale, energy levels of electrons changes. This effect is called **"Quantum confinement ".** This affects the optical, electrical and magnetic properties of nano materials.



Fabrication of Nanomaterials:-

Nano materials can be generally fabricated in two broad ways, namely

- (i) Top-down approach
- (ii) Bottom – up approach

i) Top-down approach: - In which, the bulk solid materials are breaked in to nano sizes.

(ii) Bottom – up approach: - In which, the nano materials are build up from the bottom: atom by atom, molecule by molecule or cluster by cluster..

The schematic representation of the synthesis and building of nano structured materials are shown in fig (1) and fig (2) respectively.

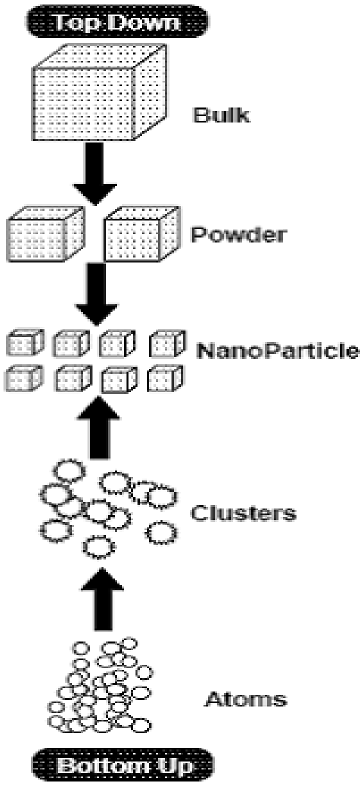


Figure: Schematic representation of the building up of Nanostructure.

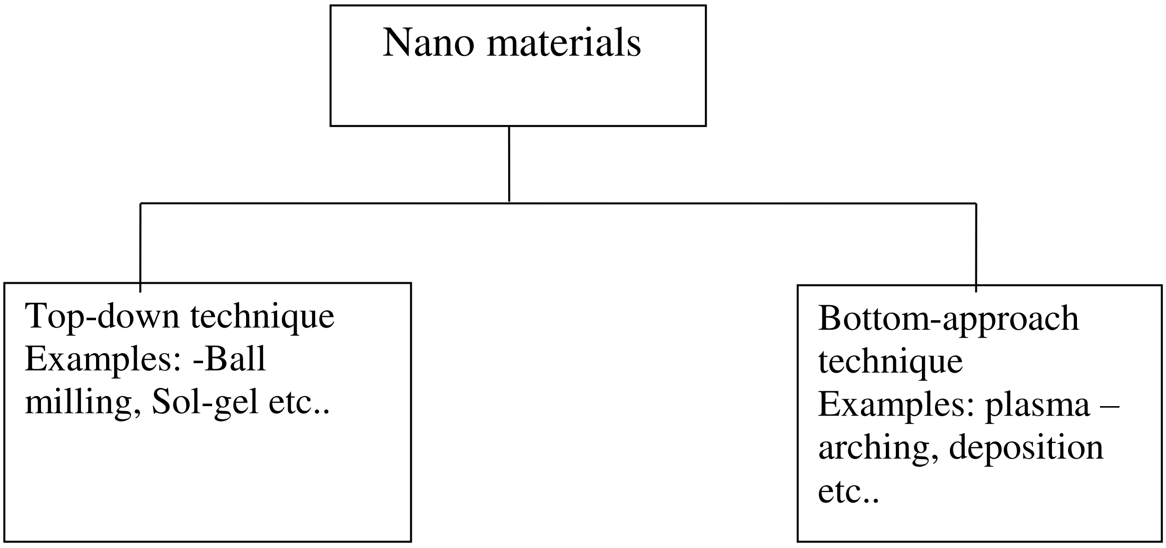


Fig:-Synthesis of nano materials.

1. **Ball milling (or) Mechanical crushing**:-

- The ball milling method is a typical example of top-down method of fabrication of nano materials.

- A ball mill is a type of grinder used to grind materials into extremely fine powder in order of nm.
- In this method, small balls of the material are allowed to rotate around the inside of a drum and then fall on a solid with gravity force. The balls are broken in to nano crystallites. This is also known as mechanical crushing.
- This method is used to prepare a wide range of elemental powders.For example iron nano particles of sizes 13 to 30nm can be formed.
- This method is used for produce metal oxide nano crystals (cerium oxide CeO_2 and Zinc oxide ZnO_2 .

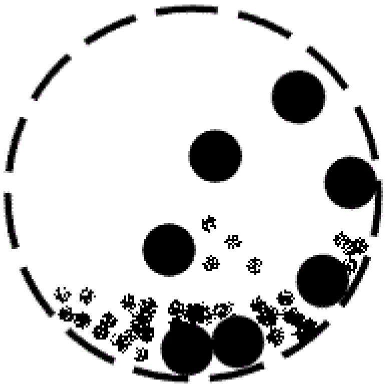


Fig: Ball milling method

Properties of Nano particles: - As the size of the nano particle is very less, these materials exhibits peculiar physical, electronic, magnetic, mechanical and chemical properties.

1) **Physical properties** :-

- Since the size of the particle is very less, the particles are very close to each other and hence the inter particle spacing is very less in nano materials.
- Because of its very less size, these nano materials cannot be further divided into smaller particles and it does not have any dislocation in it. Thus we can say that they have high strength, hardness and toughness.
- The melting point of nano materials will be very less.

(2) **Electronic properties: -**

- The energy bands in these materials will be very narrow.
- The electrical conductivity and energy band width of same materials change when they pass from bulk phase to nano particle phase. For example, bulk silicon is an insulator; it becomes a conductor in nano phase.
- Nano material semiconductors such a Ge and Si do not snow semi conducting property.

(3) Magnetic properties: - The nano materials shows variation in their magnetic property, when they change from bulk state to nano phase state. Some of the examples are listed in table (1).

S.No	Material	Bulk state	Nano-phase state
1	Iron, Ni,Co	Ferro-magnetic	Super Para-magnetic
2	Sodium, Potassium	Para-magnetic	Ferro magnetic
3	Chromium	Anti-ferromagnetic	Para-magnetic

(4) Mechanical properties :-

- Mechanical properties such as hardness, toughness, elastic modulus varies from material to material.
- They exhibit super plastic behavior.

(5) Chemical properties:-

- The nano structures in chemistry are collides and these are formed in a condensed phase having size in the range from 1 to 100 nm.
- The chemical reactivity of a cluster depends on the cluster size. This is useful in the preparation of catalytic agents. Some chemically inert bulk materials become good chemical catalyst in the nano phase, for example: Platinum and gold.
- In chemical reactions, the rate of increase in mass transport increases as the particle size decreases.

Applications of Nanomaterials:-

(i) Mechanical Engineering:-

- Since they are stronger, lighter etc; they are used to make hard metals.
- Nano-MEMS (Micro-Electro Mechanical Systems) are used in ICS, optical switches, pressure sensors, mass sensors etc

(ii) Electrical Electronics and Communication Engineering:-

- Orderly assembled nano materials are used as quantum electronic devices and photonic crystals.
- Some of the nano materials are used as sensing elements. Especially the molecular nano materials are used to design the robots, assemblers etc.
- They are used in energy storage devices such as hydrogen storage devices, magnetic refrigeration and in ionic batteries.
- Dispersed nano materials are used in magnetic recording devices, rocket propellant, solar cells, fuel cells etc.
- Recently nano robots were designed which are used to remove the damaged cancer cells and also to modify the neuron network in human body.

(iii) Computer Science Engineering and IT:-

- Nano materials are used to make CD’s and Semiconductor laser.
- These materials are used to store the information in smaller chips.
- They are used in mobiles, lap-tops etc.
- Further they are used in chemical/ optical computer.

- Nano-dimensional photonic crystals and quantum electronic devices plays a vital role in the recently developed computers.

(iv) Bio-Medical and Chemical Engineering:-

- Consolidated state nano particles are used as catalyst, electrodes in solar and fuel cells.
- Bio-sensitive nano particles are used in the production of DNA-chips, bio- sensors etc.
- Nano-structured ceramic materials are used in synthetic bones.
- Few nano materials are also used in adsorbents, self-cleaning glass, fuel additives, drugs, Ferro fluids, paints etc.
- Nano-metallic colloids are used as film precursor.

Semiconductors

Semiconductors:

A Semiconductor is a substance whose conductivity or resistivity (10^{-4} to 0.5 ohm –m) lies in between conductors and insulators.

Examples: Si, Ge, GaAs etc.

Properties:

- They have crystalline structure.
- They are formed by covalent bonds.
- They have negative temperature of coefficient of resistance.
- At T=0K, they behaves as insulators.
- When the impurities (III group or V group elements) added to the pure semiconductor, then electrical conductivity increases.

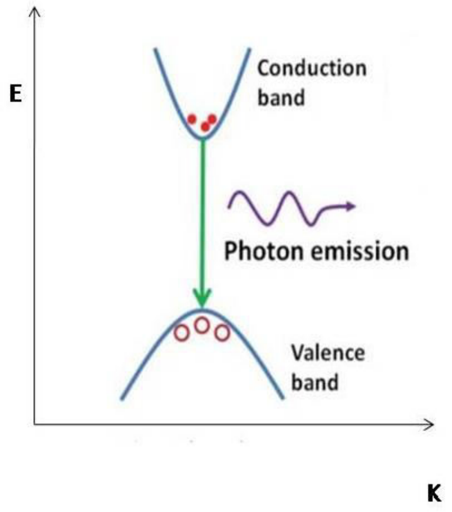
Direct Band Gap And Indirect Band Semi Conductors:

Based on the type of energy emission the semiconductors can be of two groups.

1. Direct band gap semiconductors
2. Indirect band gap semiconductors

Direct Band Gap Semi Conductors:

The semiconductor, in which the minimum of the conduction band lies directly above the maximum of the valance band in the E-K space diagram(as shown in fig), is known as direct band gap semiconductor.



In a direct band gap semiconductor such as GaAs, ARAS and INP, when an excited electron falls back into the valence band, the electrons and holes recombine to produce light energy.

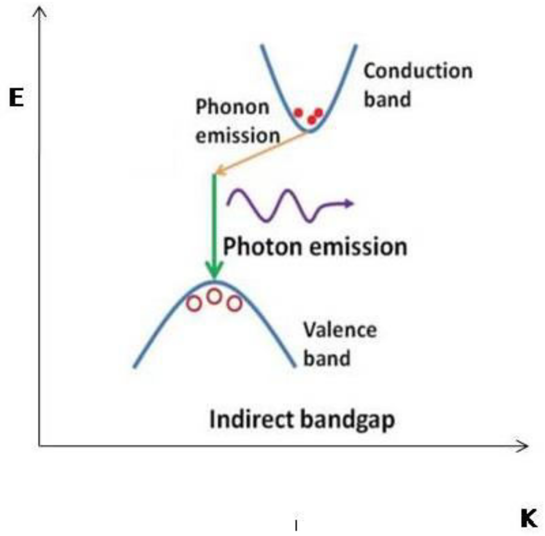
$$i.e.,\ \bar{e} + hole \longrightarrow hv\ (photon)$$

This process is known as radiative recombination and also called spontaneous emission.

These direct band gap semiconductors are used to make LED's and lasers of different colours.

Indirect Band Gap Semi Conductors:

The semiconductor, in which the minimum of the conduction band does not lies directly above the maximum of the valance band in the E-K space diagram(as shown in fig), is known as indirect band gap semiconductor.



In an indirect gap semiconductor such as Si, Ge and Gap, when an excited electron falls back into the valance band, the electrons and holes recombine to generate heat and is dissipated within the material.

$$i.e.,\ \bar{e} + hole \longrightarrow phonon$$

This process is known as non-radiative recombination.

Intrinsic semiconductors and extrinsic semiconductors

Based on purity semiconductors are classified into types,

1. Intrinsic semiconductors
2. Extrinsic semiconductors

Intrinsic semiconductor:

A semiconductor in an extremely pure form is known as intrinsic semiconductor.

Examples: Si, Ge etc.

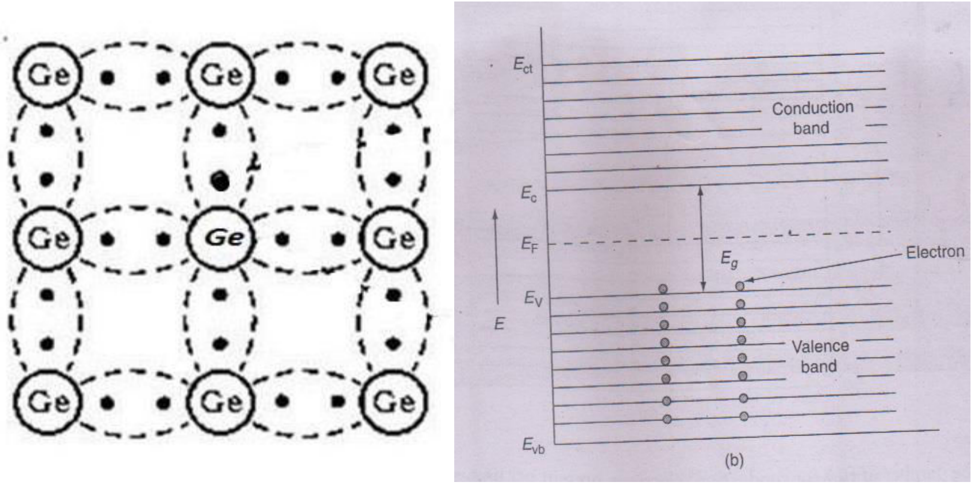
Explanation:

Consider a pure (semi conductor) Si or Ge Crystal. We know that Ge is a forth group element, i.e., it has four valence electrons; to get stability each silicon atom will make four covalent bonds with neighboring Silicon atoms as shown in fig.

Effect of temperature on intrinsic semiconductor:

i) At absolute zero temperature(0K):

At absolute zero temperature, all he electrons are tightly bound by the semi conductor atoms. The inner orbit electrons are bound to the nucleus where as the valence electrons are engaged in covalent bonding. At this temperature, the covalent bonds are very strong and there are no free electrons. *Therefore, the semi conductor crystal behaves as a perfect insulator at absolute zero temperature.*



a) Structure b) Energy band diagram

Fig: At absolute zero temperature (0K)

ii) Above absolute zero (> 0 k)

When the temperature is raised, some of the covalent bonds in the semi conductor break due to the thermal energy supplied. The breaking of bonds set those electrons free, at the same time vacant site produced in the covalent bond called “hole”. The result is that a few free electrons exist in the semi conductor. These free electrons can constitute a tiny electric current if potential difference is applied across the semi conductor as shown in fig(c)

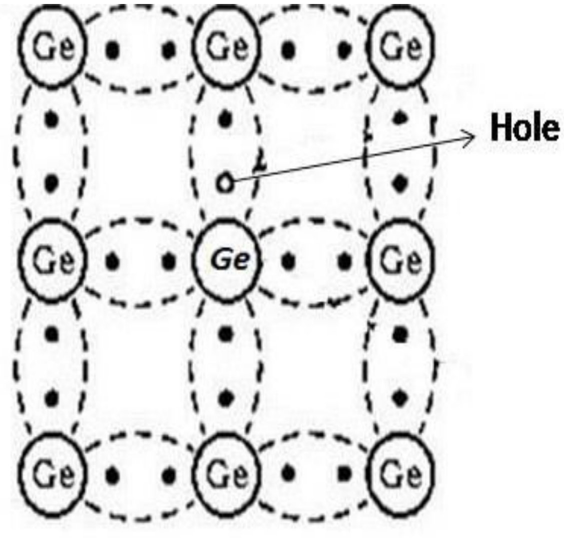
Fig (d) shows the energy band diagram. As the temperature is raised, some of the valence electrons acquire sufficient energy to enter into the conduction band and thus become free electrons. Under the influence of electric field, these free electrons will constitute electric current. It may be noted that each time a valence electron enters into the conduction band; a hole is created in the valence band, which acts a positive charge. For one electron set free one hole is created. Therefore, thermal energy creates hole- electron pairs;

In an intrinsic semi conductor, even at room temperature electron-hole pairs are created. Every free electron creates one hole in the valence band. *Therefore the number of electrons in the conduction band and the number of holes in the valence band become equal.*

.

When electric field is applied across an intrinsic semi conductor, the current conduction takes place by two processes namely: by free electrons and holes. Therefore the total current inside the semiconductor is the sum of currents due to free electrons and holes.

$$\boxed{I = I_{Electron} + I_{Hole}}$$



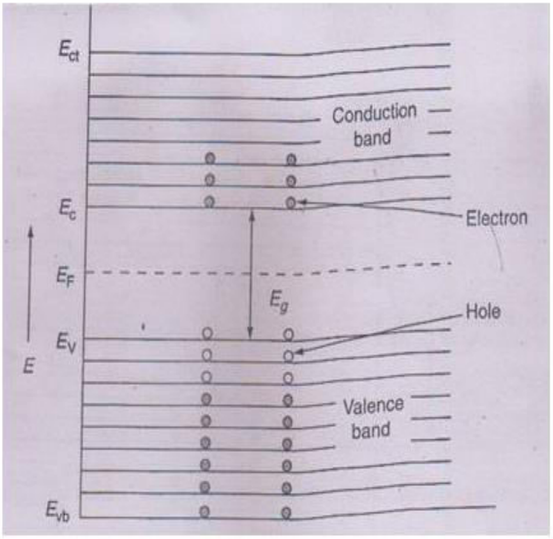


Fig: At T >0K

Extrinsic Semi Conductor:

The electrical conductivity of a pure semiconductor is very small. To increase the conductivity, impurities are added. The impurity added semi conductor is called **“Extrinsic Semi Conductor”.**

(OR)

The conductivity of intrinsic semiconductor can be increased enormously by adding small amounts of impurity atoms [such as III or V group atoms]. This impure semiconductor is called **“Extrinsic Semi Conductor”.**

Doping:

The process of adding impurities to a semiconductor is called doping and the impurity added is called **“Dopant”.**

Depending upon the type of impurity added, Extrinsic Semiconductors are classified into two types.

1. N - Type Semi Conductor.
2. P - Type Semi Conductor.

N – Type Semi Conductor:

When a small quantity of pentavalent impurity is added to a pure semi conductor, it is known as ‘n – type semi conductor’.

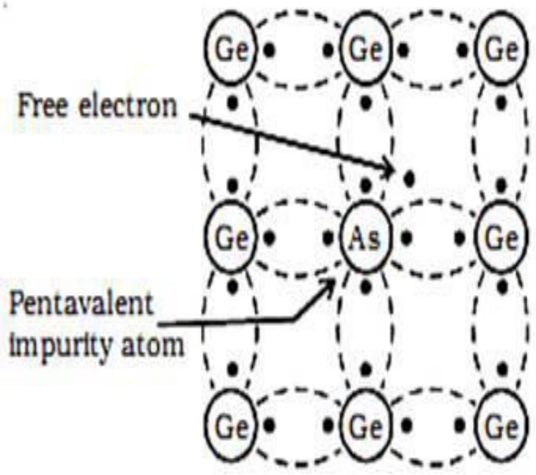
The logical relation is

Pure Semi Conductor + V Group Element = n – type Semi Conductor

Explanation:

- To explain the formation of n-type semi conductor, consider a pure (semi conductor) Germanium Crystal.

- We know that germanium atom has four valence electrons, when a small amount of pentavalent impurities like arsenic (As) is added to a germanium crystal, a large number of free electrons available in the crystal.
- The reason is simple. Arsenic is pentavalent i.e., its atom has five valance electrons. The four of the five valence electrons of Arsenic will make covalent bonds with four germanium atoms. The fifth valence electron of arsenic atom finds no place in covalent bonds and is thus free as shown in fig.
- Therefore for each arsenic atom is added, one free electron will be available in the germanium crystal.
- Thus, a small amount of arsenic impurities (As) are added to a germanium crystal, a large number of free electrons available in the crystal.
- Pentavalent impurities are also known as donor impurities because they donate free electron to semi conductor crystal.

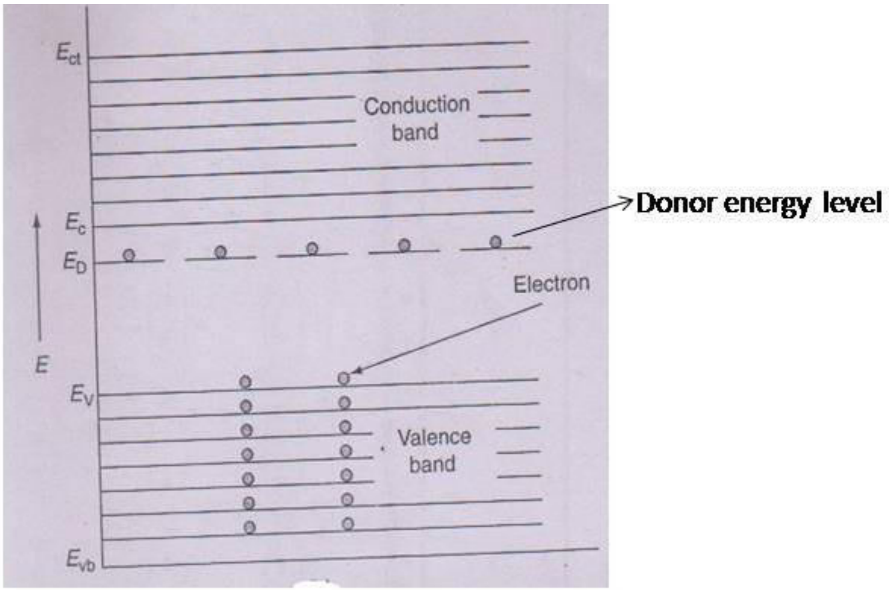


<u>Energy Band Description:</u>

Fig (2) shows the energy band description of n-type semi conductor.

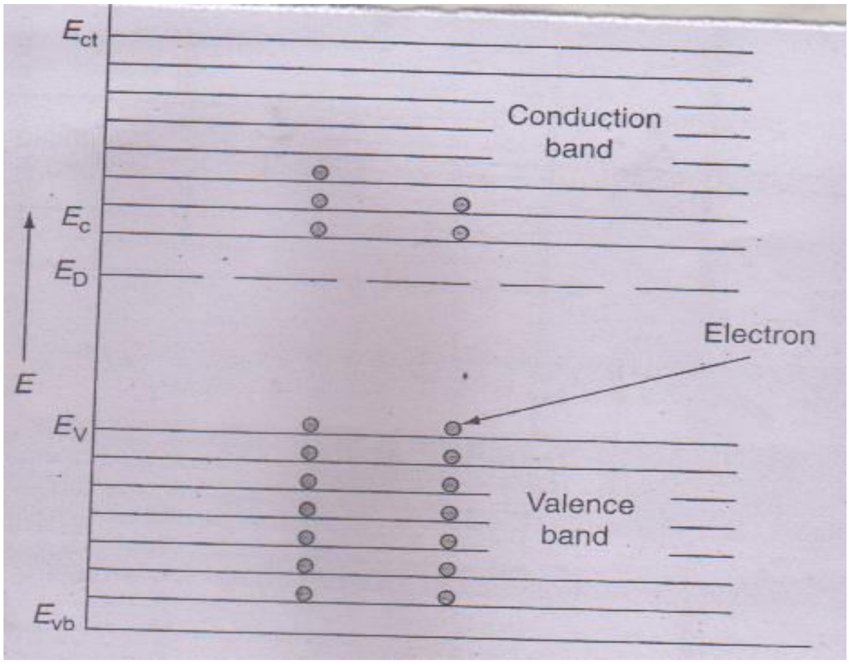
The addition of donor impurity to an intrinsic semi conductor creates extra energy level (called donor energy level) just below the bottom of conduction band.

1. **At Absolute Zero:**
   At absolute zero temperature the fifth electrons of arsenic atoms occupy the donor level (represented by dashed lines) as shown in fig.



2. **<u>At above Absolute Zero:</u>**

   Even room temperature provides enough thermal energy to push the electrons sitting at donor energy level to conduction band. (The result is that at room temperature, there are a large number of free electrons in the conduction band as shown in fig) and also few of the covalent bonds in the semi conductor break due to the thermal energy applied. Due to the breaking of covalent bond, there will be a few holes formed in the valance band at this temperature. The result is that at room temperature, there are a large number of free electrons in the conduction band compared to the holes in valence band, i.e., Electrons are majority carriers and holes are minority carriers. So this material is called n-type semi conductor.



P-Type Semi Conductor:

When a small quantity of trivalent impurity (such as indium (In) Boron (B), aluminum (Al) etc. is added to a pure semi conductor, it is called P-type semi conductor.

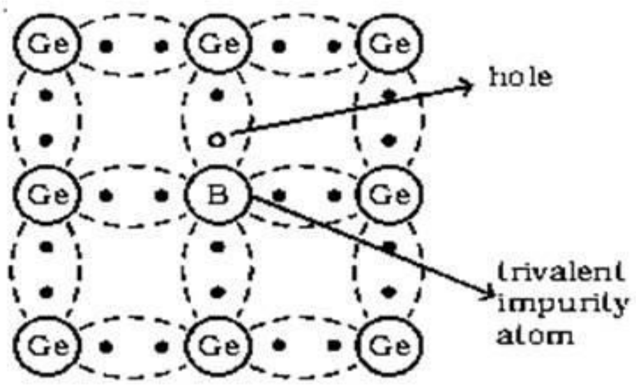
The logical relation is

Pure Semi Conductor + III Group Element = P – type Semi Conductor

Explanation:

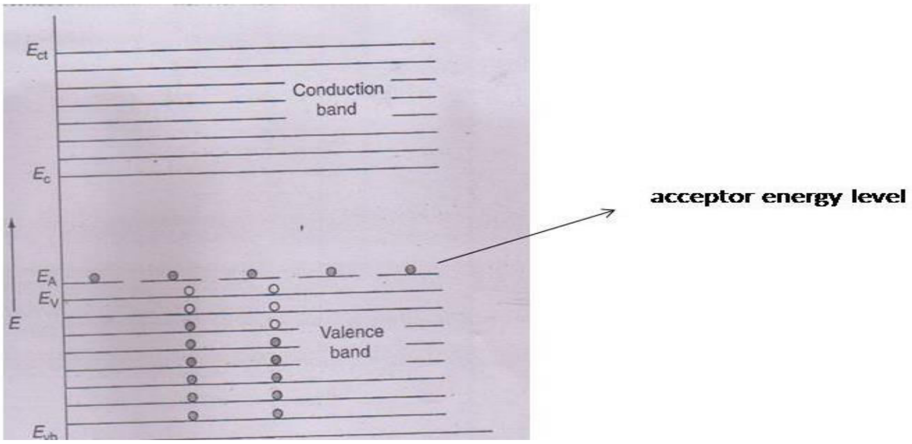
- To explain the formation of p-type semi conductor, consider a pure (semi conductor) Germanium Crystal.
- We know that germanium atom has four valence electrons, when a small amount of trivalent impurities like boron atoms (B) are added to a germanium crystal, a large number of holes available in the crystal.
- The reason is simple. Boron is trivalent i.e., its atom has thee valence electrons. The three valence electrons of Boron atom will make three covalent bonds with surrounding Ge atoms.
- The fourth bond is incomplete because short of one electron. This missing electron is called a “hole”.

- Therefore for each arsenic atom is added, one free electron will be available in the germanium crystal.
- Thus, a small amount of boron impurities (B) are added to a germanium crystal, a large number of free holes available in the crystal.
- Trivalent dopant impurities also called acceptors. Because they have need of extra electrons to complete their fourth covalent bonds formation with Ge atoms.

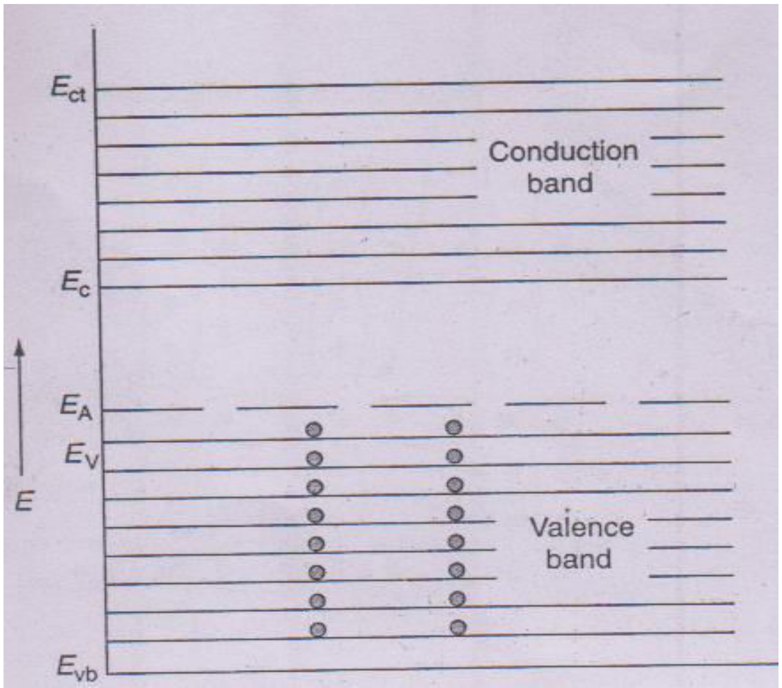


Energy Band Description:

Fig(2) shows the energy band description of p-type semi conductor.
The addition of acceptor impurity to an intrinsic semi conductor creates extra energy level (celled acceptor energy level) just above the top of the valance bond [see fig].



Since the energy difference between acceptor level and valence band energy level is very small so even at low temperature the valence band electrons gain sufficient thermal energy to occupy the acceptor energy level states as shown in fig.



After receiving an electron the, Boron atom becomes a negative ion.

But at room temperature provides enough thermal energy t push the electrons in the valence band to the acceptor energy level and also due to thermal agitation a few electrons jumps from B to C.B. The result is that at room temperature there are a large number of holes in the V.B compared to the electrons in the C.B. i.e., holes are majority carriers and electrons are minority carries. So, this material is called P-type semi conductors.

Carrier concentration:

In general, the number of charge carriers (free electron or holes) per unit volume of a semi conductor material is called “carrier concentration or density.”

We know that, in the semiconductors, free electron and holes are the charge carriers. So, the carrier concentration can be divided into two types.

1. Electrons carrier concentration and
2. Holes carrier concentration.

Electrons carrier concentration :

The number of free electrons present per unit volume of conduction band of the semi conductor is called “electros carrier concentration or density.”

Let ‘n’ be the electron carrier concentration in the conduction band and is given by

$$n = 2\left(\frac{2me^{*}\pi K_B T}{h^2}\right)^{3/2} \quad \exp^{-}{}^{(E_C - E_F)}/_{K_B T}$$

$$\text{(Or)} \quad n = N_c \exp^{-}{}^{(E_C - E_F)}/_{K_B T} \qquad \longrightarrow (1)$$

$$\text{Where} \quad N_c = 2\left(\frac{2me^{*}\pi kB^{T}}{h^2}\right)^{3/2} \quad \text{is called Pseudo constant}$$

and m_e* is called effective mass of electron.

Holes carrier concentration:

The number of holes present per unit volume of valence band of the semi conductor is called “holes carrier concentration or density.”

Let P be the holes – carrier concentration in the valence band and is given by

$$p = 2\left(\frac{2mh^{*}\pi K_B T}{h^2}\right)^{3/2} \quad \exp^{-}{}^{(E_F - E_v)}/_{K_B T}$$

$$\text{(Or)}\ P = N_V \exp^{-(E_F - E_V)}/_{K_B T} \qquad \longrightarrow (2)$$

$$\text{Where } N_V = 2\left(\frac{2mh^{*}\pi K_B T}{h^2}\right)^{3/2} \text{ is a Pseudo constant.}$$

andm_h* is called effective mass of hole.

Carrier concentration in an intrinsic semi conductor:

We know that, at OK in an intrinsic semi conduct, the valence bond is completely filled and conduction band is completely empty. The Fermi level is exactly mid way between the valance band and conduction band as shown in fig.

As the temperature of intrinsic semi conductor is increased, electrons from the valence band get thermally excited to the conduction band. These electrons in the conduction band behave like a free particle with an effective mass m_e*.

Similarly, the holes created by these electrons in the valance bond also behave like a free particle with an effective mass m_h^*.

Therefore, at any temperature, the number of free electron (electron carrier concentration) in the conduction band is equal to the number of holes (holes carrier concentration) in the valence band.

$$\text{i.e.,}\quad n = p = n_i$$

where n_i is called intrinsic carrier concentration.

$$\text{Also the product } n.p = n_i^2 \longrightarrow (3)$$

This is known as law of mass action.

Let ‘n’ be the electron carrier concentration in the conduction band and is given by

$$n = 2\left(\frac{2m_e^*\pi K_B T}{h^2}\right)^{3/2} \exp^{-(E_C - E_F)}/_{K_B T}$$

$$\text{(Or)}\quad n = N_c \exp^{-(E_C - E_F)}/_{K_B T} \longrightarrow (1)$$

$$\text{Where}\quad N_c = 2\left(\frac{2m_e^*\pi kB^T}{h^2}\right)^{3/2} \quad \text{is called Pseudo constant}$$

and m_e^* is called effective mass of electron.

Let P be the holes – carrier concentration in the valence band and is given by

$$p = 2\left(\frac{2m_h^*\pi K_B T}{h^2}\right)^{3/2} \exp^{-(E_F - E_v)}/_{K_B T}$$

$$\text{(Or)}\ P = N_V \exp^{-(E_F - E_V)}/_{K_B T} \longrightarrow (2)$$

$$\text{Where } N_V = 2\left(\frac{2m_h^*\pi K_B T}{h^2}\right)^{3/2} \text{ is a Pseudo constant.}$$

and m_h^* is called effective mass of hole.

Substituting equations (1) and (2) in (3) gives

$$n_i^2 = \left[N_c \exp^{-(E_C - E_F)}/_{K_B T}\right]\left[N_V \exp^{-(E_F - E_V)}/_{K_B T}\right]$$

$$= N_C\, N_V \exp\left[\frac{-E_C+E_F-E_F+E_V}{K_B T}\right]$$

$$= N_C\, N_V \exp^{(-E_C + E_V)}/_{K_B T}$$

$$= N_C\, N_V \exp^{-(E_C - E_V)}/_{K_B T}$$

But $E_C - E_V = E_g$

$$ni^2 = N_C\, N_V \exp^{-(E_g)}/_{(K_B T)}$$

$$n_{i} = (N_C\ \ N_V)^{1/2} \exp^{-(E_g)}/_{(K_B T)} \longrightarrow (4)$$

This equation represents the intrinsic carrier concentration.

Fermi level in an intrinsic semiconductor :- .

At temperature T k, the electrons concentration (n) is equal to the holes concentration ‘P’ in the intrinsic semiconductor

i.e. $n = P$

Therefore [from equations (1) and (2)]

$$N_c \exp^{-}\, {}^{(E_C - E_F)}/_{K_B T} \quad = \quad N_V \exp^{-(E_F - E_V)}/_{K_B T}$$

$$\frac{\exp^{-(E_C-E_F)}/_{K_B T}}{\exp^{-(E_F-E_V)}/_{K_B T}} \quad = \quad \frac{N_V}{N_c} \exp^{-}\, {}^{(E_C - E_F)}/_{K_B T} \times \exp^{(E_F - E_V)}/_{K_B T} = \frac{N_V}{N_c}$$

$$\exp^{[-E_c+E_F+E_F-E_V]}/_{K_B T} \quad = \quad \frac{N_V}{N_c}$$

$$\exp\left[\frac{2E_F-(E_C+E_V)}{K_B T}\right] \quad = \quad \frac{N_V}{N_c}$$

Taking log on both sides, we have

$$\frac{2E_F-(E_C+E_V)}{K_B T} = \log\left(\frac{N_V}{N_c}\right)$$

$$\mathrm{E_F} - \frac{(E_C+E_V)}{2} = \frac{1}{2}\log\left(\frac{\mathrm{N_V}}{\mathrm{N_c}}\right).\ K_B T$$

$$\mathrm{E_F} - \frac{(E_C+E_V)}{2} = \frac{1}{2}K_B T \log\left(\frac{\mathrm{N_V}}{\mathrm{N_c}}\right)$$

$$E_F = \frac{E_C+E_V}{2} + \frac{1}{2}K_B T \log\left(\frac{N_V}{N_C}\right) \qquad (5)$$

If $N_V = N_C$ then $\log\left(\frac{N_V}{N_C}\right) = 0$

Eq(5) becomes

$$\mathrm{E_F} = \frac{\mathrm{E_C+E_V}}{2}$$

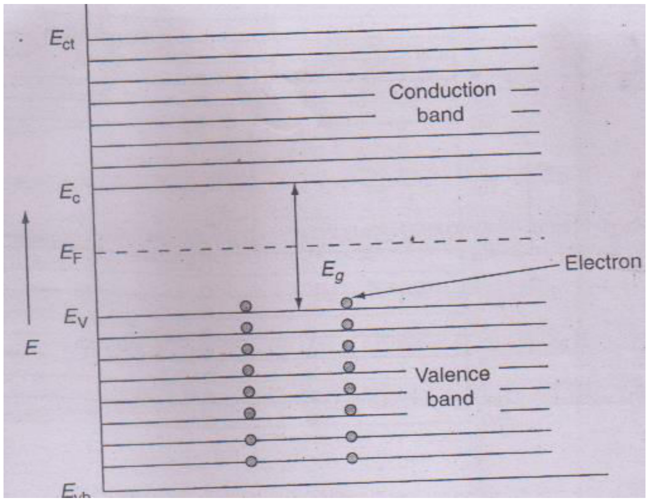
Thus, the Fermi level in an intrinsic semi conductor lies in midway between E_C and E_V.

Dependence of E_F on temperature:

The variation of Fermi level with temperature for intrinsic semiconductor is shown in fig.

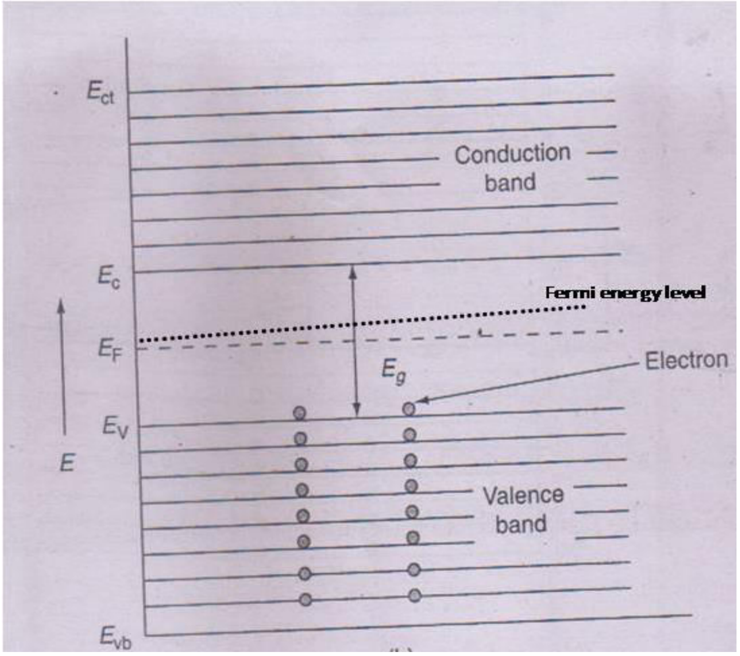
Case (a):

At 0 k, the Fermi level lies exactly in the middle of forbidden gap as shown in fig.



Case(b) :

The Fermi level slightly increases with the increase in temperature as shown in figure.



Electrical conduction in semiconductors

In the semiconductors electrical conduction arises due to two process namely

1. Drift
2. diffusion

Drift:

Definition:-

Under an applied electric field both the charge carriers i.e., electrons and holes acquire an average velocity called the drift velocity (V_d) and this process is called drift.

The drift velocity V_d is small. It is directly proportional to the electrical field E.

i.e., $V_d \propto E$

$V_d = \mu E \longrightarrow (1)$

Where μ is a constant and is called the mobility of charge carriers.

If μ_n and μ_p are the electron mobility and hole mobility respectively, then

$V_n = \mu_n E$ and $(2) \longrightarrow$

$V_p = \mu_p E \quad (3) \longrightarrow$

1. We know that, Current $I = neAV_d$.
But in a semi conductor, the total current is the sum of electrons current and holes current.

Let n be the electron concentration and p be the hole concentration.

Therefore $I = I_n + I_p$

$= neAV_n + pAV_p$

$= eA(nV_n + pV_p)$ [From equations (2) &(3)]

$= eA(n\mu_n E + p\mu_p E)$

$= eA(n\mu_n + p\mu_p)E$

2. Current density $J = \frac{I}{A}$

$J_n = \frac{neA\mu_n E}{A}$ and

$J_p = \frac{peA\mu_p E}{A}$

Therefore, total current density $J = J_n + J_p$

$=\frac{eA(n\mu n+P\ \mu p]E}{A}= e(n\mu_n+P\mu_p)E$

Conductivity $\square = \frac{J}{E}=\frac{e(n\mu n+P\ \mu p]E}{\square} = e(n\mu_n+P\mu_p)$

NOTE:-

1. For an intrinsic semiconductor: $n=p= n_i$

Where n_i is the carrier concentration of the intrinsic semiconductor.

$I_{inc}= eA(n_i\mu_n+n_i\mu_p)E$

$= eAn_i(\mu_n+\mu_p)E$

$\therefore$ Current density $J_{in} = \frac{I_{in}}{A} = \frac{eAn_i(\mu n+\ \mu p]E}{\square} = en_i(\mu n + \mu p)E$

Conductivity $\square_{in} = \frac{J_{in}}{E} = \frac{en_i(\mu n+\ \mu p]E}{\square} = en_i(\mu n + \mu p)$

FOR AN EXTRINSIC SEMICONDUCTOR:-

a)**For n-type semiconductor :-**The hole current is neglected, as the holes are minority carriers and the electrons are the majority carriers.

$n\simeq N_d$ is the donor electron concentration

[$\therefore$ Where N_a can be neglected]

$I = eAV_nN_d$

$= eA\mu_nEN_d$

$J = \frac{\square}{\square} = e\mu_nEN_d$

$\square = \frac{\square}{\square} = e\mu_nEN_d$

b)**For P-type semiconductor :-**The electron current is neglected and $P=N_{ai}$, where N_a is the acceptor hole concentration. [$\therefore$ When N_d can be neglected].

$I = eA\ V_P\ N_a$

$=eA\mu_p\ E\ N_a$

$J =\frac{I}{A} = e\ \mu_p\ E\ N_a$

$\sigma = \frac{J}{E} = e\ \mu_p\ N_a$

DIFFUSION :-

Diffusion takes place due to existence of non-uniform concentration of charge carriers.

Definition:-

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

→ According to Fick's law, the diffusion flux F is directly proportional to concentration gradient <i.e. carrier concentration per unit length >of the particles and is in the opposite direction.i.e;

$$F \propto \frac{-\partial(\Delta N)}{\partial X}$$

$$F = -D\frac{\partial(\Delta N)}{\partial X} \qquad \longrightarrow \qquad (1)$$

Where D is diffusion constant.
And ΔN is the excess carrier concentration.

Let Δn and Δp be the excess concentration in a semiconductor material.
Then Fick's

$$F \propto \frac{-\partial(\Delta N)}{\partial X} \quad \text{(For electrons)}$$

$$F = -D_n\frac{\partial(\Delta N)}{\partial X} \qquad \longrightarrow \qquad (2)$$

$$\text{and} F \propto \frac{-\partial(\Delta P)}{\partial X} \quad \text{(For electrons)}$$

$$F = -D_p\frac{\partial(\Delta P)}{\partial X} \qquad \longrightarrow \qquad (3)$$

→ But the current density due to diffusion depends on charge of particle and rate of diffusion.

$$\therefore \text{Current density (J)} = \text{Charge of particle} \times \text{Rate of diffusion} \qquad \longrightarrow (4)$$

→ The diffusion flux density due to electron is given by

$$J_{n(Diff)} = -\square\left[-Dn\frac{\partial(\Delta N)}{\partial X}\right] \therefore \text{from}(4)$$

$$J_{n(Diff)} = \square D_n \frac{\partial(\Delta N)}{\partial X} \qquad (5) \longrightarrow$$

The diffusion flux density due to hole is given by

$$J_{p(Diff)} = + \square \left[Dp \frac{\partial(\Delta P)}{\partial X} \right] \qquad (6) \longrightarrow$$

Where +e and –e are charge of the hole and electron respectively.

∴ The total current density due to diffusion is given by

$$J_{TOTAL,(DIFF)} = J_{n(diff)} + J_{p(diff)}$$

$$J_{TOTAL(DIFF)} = \square D_n \frac{\partial(\Delta N)}{\partial X} - \square D_P \frac{\partial(\Delta P)}{\partial X} \qquad \longrightarrow \qquad (7)$$

NOTE:- The total current density due to excess electrons is the sum of the current densities due to drift and diffusion of electrons.

$$J_n = J_{n(drift)} + J_{n(diff)}$$

$$= \Delta \square \square_{\square} E + \square D_n \frac{\partial(\Delta N)}{\partial X} \qquad \longrightarrow \qquad (8)$$

Similarly,

The total current density due to excess holes is the sum of the holes densities due to drift and diffusion of holes.

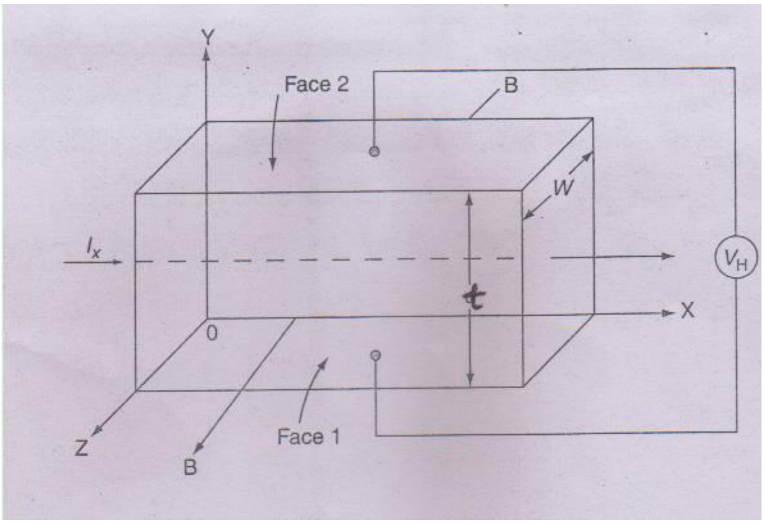
$$J_P = \Delta \square \square \square_{\square} E - \square D_P \frac{\partial(\Delta P)}{\partial X} \qquad \longrightarrow \qquad (9)$$

Hall Effect:

When a current carrying semiconductor is placed in the magnetic field, then a potential difference (voltage) or electric field is developed in the material perpendicular to both the current and the applied magnetic field .this effect is known as Hall Effect and the developed potential difference (voltage) is known as hall voltage.

Explanation:

Consider a semiconductor slab of thickness‘*t*’ and width ‘*w*’ in which current (I) flowing along X-direction and magnetic field is applied along Z- direction as shown in fig.



The charge carriers inside the semiconductor experience a force due to the applied magnetic field called Lorentz force.

As a result, electrons move (drift) towards downward direction with velocity 'V_d' and accumulate at bottom surface (face 1) and the corresponding positive charge on upper surface (face2) of the material as shown in fig.

Thus a potential difference and electric field developed across the surface. This developed electric field along Y-direction exerts a force ($F_e = eE_H$) on the electrons to prevent further accumulation at the bottom surface.

Therefore, the force due to potential difference $F_e = eE_H$

the force due to magnetic field $F_L = BeV_d$

At steady state

$F_e = F_L$

$eE_H = Bev_d$

$E_H = Bv_d \qquad (1) \qquad \longrightarrow$

For n-type:

If 'n' is the electrons carrier concentration in the semiconductor, then current density

$$J = -neV_d$$

$V_d = \frac{J}{-ne} (2) \qquad \longrightarrow$

Substituting eq (2) in eq(1)

$$E_H = \frac{BJ}{-ne}$$

(3) $$\boxed{E_H = R_H BJ} \longrightarrow$$

Where $R_H = \frac{1}{-ne}$ is known as Hall coefficient.

<u>For p-type:</u>

If ‘p’ is the electrons carrier concentration in the semiconductor, then current density

$$J = peV_d$$

$$V_d = \frac{J}{pe}(2) \qquad \longrightarrow$$

Substituting eq (2) in eq(1)

$$E_H = \frac{BJ}{pe}$$

(3) $$\boxed{E_H = R_H BJ} \longrightarrow$$

Where $R_H = \frac{1}{pe}$ is known as Hall coefficient

<u>Hall coefficient in terms of hall voltage:</u>

If the thickness of the sample is‘*t*’ and the developed voltage is V_H, then the Hall voltage

$$V_H = E_H.t \longrightarrow (4)$$

Substituting eq (3) in eq(4);

$$V_H = R_H BJ\, t \longrightarrow (5)$$

If ‘*w*’ is the width of the semiconductor,

then area of the sample $A = w.t$

But current density $J = \frac{I}{A} = \frac{I}{\square\ \square} \longrightarrow (6)$

Substituting eq (8) in eq(7); we get

$$V_H = \frac{R_H IB}{\square}$$

$$R_H = \frac{V_H \square}{IB}$$

$$\boxed{R_H = \frac{V_H w}{IB}}$$

This is the relation between Hall coefficient and hall voltage.

- The electrical conductivity in a semiconductor is given by
  $\square = ne\square$

$$\square = \frac{\square}{\square\square}$$

$$\boxed{\mu = R_H\sigma}$$

APPLICATIONS:

- Knowing R_H and□, the mobility of charge carriers can be measured.
- It is used to fine the carrier concentration

$$\boxed{n= -\frac{1}{\mathbf{eR_H}} \quad \text{and } p= \frac{1}{\mathbf{eR_H}}}$$

- It is used to determine whether the material is p-type or n-type semiconductor.
  i.e.,if R_H is negative then the material is n-type.
  if R_H is positive then the material is p-type.