

MODULE-1

MODERN PHYSICS

BLACKBODY RADIATION:

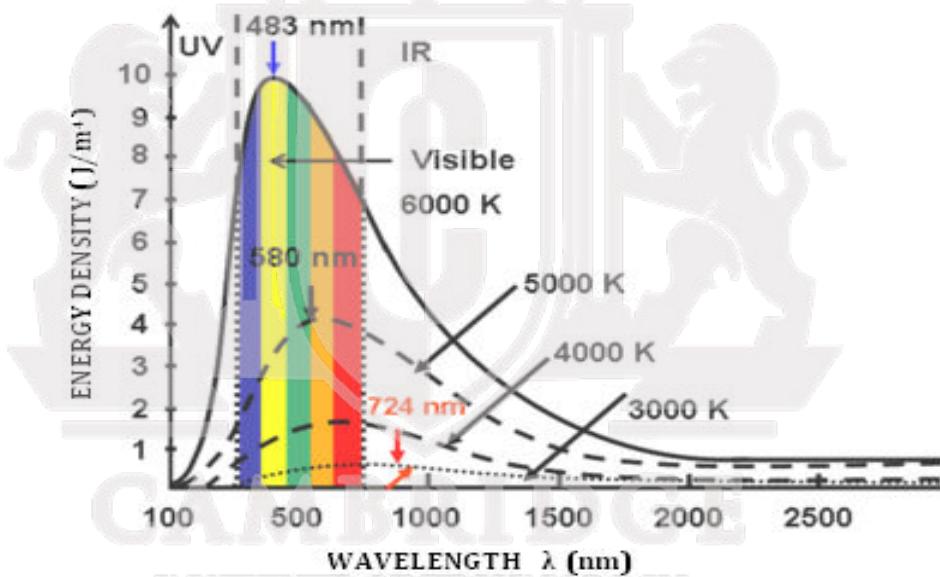
A **black body** in principle absorbs the entire radiations incident on it and also emits all the radiations when it is heated to incandescence. The radiations emitted by such a body are known as **black body radiation**.

1. A black body not only completely absorbs all the radiations falling on it but also behaves as a perfect radiator when heated.

2. The radiation given out by a black body depends only on the temperature and not on the nature of the body.

BLACKBODY RADIATION SPECTRUM AND ITS FEATURES

Following figure illustrates the way in which the energy radiated by a black body is distributed amongst various wavelengths.



The plot had following features:

- There are different curves for different temperatures.
- There is a peak for each curve. This means that the electromagnetic waves of wavelength corresponding to the peak is emitted to the largest extent at that temperature to which the curve corresponds.
- The peak shifts towards the lower wavelength side as higher temperatures are considered.

LAWS GOVERNING THE BLACKBODY RADIATION:

1. Wien's Law
2. Wien's Displacement Law
3. Stefan's Law
4. Rayleigh-Jeans Law
5. Kirchoff's Law
6. Planck's Law

WIEN'S LAW:

Wien's law gives the relation between the wavelength of emitted radiation and the temperature of the source as,

$$E_\lambda d\lambda = C_1 \lambda^{-5} e^{-C_2/\lambda T} d\lambda$$

Where C_1 and C_2 are constants and

$E_\lambda d\lambda$ is the energy emitted per unit volume in the wavelength region λ and $\lambda + d\lambda$.

This law is called **Wien's law of energy distribution** in the blackbody radiation spectrum.

Drawbacks of wien's law:

Wien's law holds good only for **shorter values of wavelength** but fails to explain the region in which wavelengths are longer.

RAYLEIGH-JEANS LAW:

In 1900, Lord Rayleigh applied the principle of equipartition of energy to electromagnetic vibrations and deduced an equation for the black body radiation. This was later modified by Sir James Jeans and came to be called Rayleigh-Jeans law. According to this law the energy density i.e. the amount of energy per unit volume of a blackbody in the wavelength ranging from λ to $\lambda + d\lambda$ is given by

$$E_\lambda d\lambda = 8\pi k T \lambda^{-4} d\lambda$$

Where, k is Boltzmann constant.

Due to the presence of the factor λ^{-4} in the equation, the energy radiated by the blackbody should rapidly decrease with the increase in wavelength.

Drawbacks of Rayleigh-Jeans law (or Ultraviolet catastrophe):

Rayleigh-Jeans law holds good for **longer values of wavelength** but does not fit the experimental curves for shorter values of wavelength.

This discrepancy between the theoretical conclusion and the experimental result is called "**ULTRAVIOLET CATASTROPHE**". As per the equation, black body radiates enormously in the shorter wavelength side, but practically black body chiefly radiates in IR or visible range which is the longer wavelength region of the spectrum.

This wrong prediction in the radiation emitted by the body is called Ultraviolet Catastrophe.

PLANCK'S LAW:

In order to explain the energy distribution in the complete spectrum of a blackbody radiation, Max Ludwig Planck in 1900 put forward the quantum theory of radiation. For deriving the equation Planck made certain assumption based on Quantum mechanical consideration.

Assumptions of Quantum theory of radiations are,

1. The walls of the blackbody consist of a very large number of **electrical oscillators**. Each oscillator vibrates with a frequency of its own.

2 Energy is absorbed or emitted by a blackbody in a discrete manner, in the form of small packets called **quanta**.

3. Each quantum has energy that depends only on the frequency of the radiation and is given by $E = nh\nu$

Where h is a constant known as Plank's constant = 6.625×10^{-34} J-sec and $n=0,1,2, \dots$

4. An oscillator may gain or lose energy when it absorbs or emits radiation of frequency ν given by $\nu = \Delta E/h$

Where, ΔE is the difference in energies of the oscillator before and after emission or absorption.

Based on the above assumptions, Planck derived an equation which successfully explained the entire spectrum of blackbody radiation.

The equation is given by

$$E_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} \left[\frac{1}{e^{h\nu/kT} - 1} \right] d\lambda \quad \dots \dots \dots \quad (1)$$

Planck's law explains the spectrum of blackbody radiation successfully in both the shorter wavelength and longer wavelength regions.

REDUCTION OF PLANCK'S LAW TO WIEN'S LAW AND RAYLEIGH-JEANS LAW:

Derivation of Wien's law from Planck's law

➤ For shorter wavelengths,

When λ is small, $v=c/\lambda$ is large.

When v is large, $e^{hv/kT}$ is very large.

$$\text{i.e., } e^{hv/kT} \gg 1$$

$$e^{hv/kT} - 1 \approx e^{hv/kT} \approx e^{hc/\lambda kT} \quad (\text{Since } v=c/\lambda)$$

Substituting in Equation (1) we get

$$E_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} \frac{1}{e^{hc/\lambda kT}} d\lambda$$
$$\Rightarrow E_\lambda d\lambda = C_1 \lambda^{-5} e^{-C_2/\lambda T} d\lambda \quad \dots \dots \dots \quad (2)$$

where $C_1 = 8\pi hc$ and $C_2 = hc/k$.

This equation is Wien's law of radiation.

Derivation of Rayleigh-Jeans law from Planck's law

➤ For longer wavelengths,

When wavelength λ is large, $v=\frac{c}{\lambda}$ is small.

Since v is very small, $e^{hv/kT}$ will be very small.

Expanding $e^{hv/kT}$ as power series, we have

$$e^{hv/kT} = 1 + hv/kT + (hv/kT)^2 + \dots \dots$$

Neglecting the higher order terms we get,

$$e^{hv/kT} \approx 1 + hv/kT$$

$$\therefore e^{hv/kT} - 1 \approx hv/kT \approx hc/\lambda kT$$

Substituting in equation (1), we get

$$E_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} \times \frac{\lambda kT}{hc} d\lambda$$
$$\Rightarrow E_\lambda d\lambda = \frac{8\pi kT}{\lambda^4} d\lambda \quad \dots \dots \dots \quad (3)$$

This equation is the Rayleigh-Jeans law of radiation.

COMPTON EFFECT:

In 1923, Arthur H Compton discovered the scattering of X -rays by electrons that are weakly bound to atoms in a target material. Compton Effect confirms the existence of photons and hence proves the particle nature of radiation.

When a beam of monochromatic X- rays is incident on a target material of such as graphite sheet, it undergoes scattering in many directions spanning through 0 to 180° leading to the modification in the wavelength. Compton interpreted this interaction as a collision of two particles, a X-ray photon and an electron in the graphite sheet. The scattered X-rays consist of two components. One component called unmodified wavelength denoted by λ (the same wavelength as that of the incident X-rays) and the other component called modified wavelength denoted by λ' (wavelength slightly longer than incident wavelength) . This difference in wavelength $(\lambda - \lambda') = d\lambda$, indicates the enhancement in the wavelength is called **Compton Shift**.

Compton made the measurement by replacing graphite with other materials and found that λ' is independent of the target material, but depends on the angle ' θ ' through which the scattering occurs.

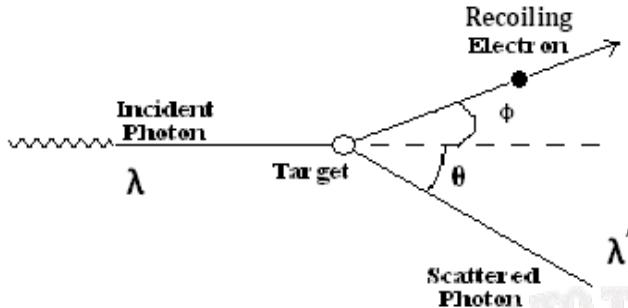
The phenomenon in which there is change in wavelength accompanied by a change in the direction of the scattered X-rays compared to the incident X-rays, consequent to the exchange of energy between the X-ray photons and the electrons in the target material, is called Compton Effect.

Compton used Quantum theory to give a satisfactory explanation for the modified wavelength.

➤ EXPLANATION OF COMPTON EFFECT:

Compton assumed that during the scattering process, the incident photon from X-rays collides with a free electron in the target material (**graphite sheet**). As a result, the photon is scattered at an angle ' θ ' to the incident direction and its energy reduces from E to E' . To account for the change in energy of the photon, the electron is assumed to recoil at an angle

' ϕ ' to the incident direction of the photon and the photon with reduced energy travels in the direction ' θ ' with the original direction.



$$*E = \frac{hc}{\lambda} \text{ (Energy of the photon before the collision)}$$

Where,

h is Planck's constant,

c is the velocity of light and

λ is the wavelength of the incident X-rays.

and

$$*E' = \frac{hc}{\lambda'} \text{ (Energy of the photon after the collision)}$$

By applying the laws of conservation of momentum, Compton derived an equation for the change in wavelength $\Delta\lambda$ of the X-rays. It's given by

$$\Delta\lambda = (\lambda' - \lambda) = \frac{h}{m_0 c} (1 - \cos \theta) \quad \dots \dots \dots (3)$$

where .

m_0 is the rest mass of the electron and c is the velocity of light. This is Compton's equation for Compton shift and the quantity ($\frac{h}{m_0 c}$) has the dimensions of length and is called Compton wavelength whose value is $2.42 \times 10^{-12} \text{ m}$.

PHYSICAL SIGNIFICANCE OF COMPTON EFFECT:

- Proves the particle nature of X-rays
- Energy exchange between X-ray photon and electron during collision occur as though it is particle-particle collision.

WAVE PARTICLE DUALISM:

The nature of light is not unique i.e. it exhibits both particle nature and wave nature.

Some phenomenon like Interference, Diffraction and Polarization can be explained on the basis of Wave nature of light while other phenomenon like Photoelectric effect and Compton Effect can be explained on the basis of particle nature of light. This property where light behaves both as waves and particles is called dual nature of light or wave particle dualism

Example- X-rays assumes the status of the particles in the Compton Effect experiment and the same X-rays get diffracted by a crystal in few other experiments.

De- BROGLIE'S HYPOTHESIS:

Because of the dual nature observed of radiation and light, Louis de Broglie put forward a bold hypothesis. He reasoned out that nature exhibits a great amount of symmetry. "If the radiation behaves as waves sometimes and as particles at other times then it is expected that entities such as electrons which behave as particles should also exhibit wave like behavior under appropriate circumstances". This is known as de Broglie's hypothesis.

According to this Hypothesis, all material particles in motion are associated with a wave. The waves associated with material particles are called **matter waves** or **de Broglie waves**.

De- BROGLIE WAVELENGTH:

According to de Broglie hypothesis, a moving particle is associated with a wave. The waves associated with the particles of matter like electrons are known as matter waves or de Broglie waves.

When a particle has momentum 'p', its motion is associated with λ called **De Broglie wavelength**. It is given by

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

The above equation is known as de Broglie wave equation.

Hence de Broglie wavelength depends upon the mass of the particle and its velocity.

PHASE VELOCITY AND GROUP VELOCITY:

Phase Velocity (v_{phase}):

Phase velocity is the velocity of the individual waves. The velocity with which each phase in a wave moves is called the phase velocity.

If we consider a point to be marked on a travelling wave, then that point represents a particular phase of the wave, and the velocity with which it is transported owing to the motion of the wave is called Phase velocity.



Here, the point on the wave represents the phase $\frac{\pi}{2}$
Phase velocity is given by

$$v_{\text{phase}} = \frac{\omega}{k}$$

Where ω is the angular frequency and k is the wave number.

Group Velocity (v_{group}):

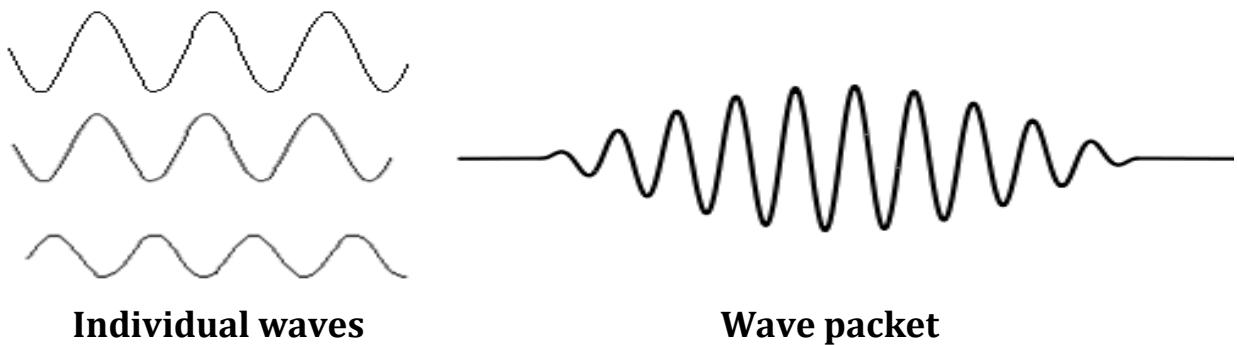
When a group of two or more waves of different wavelengths and different velocities are superimposed on each other, the amplitude of the resultant wave is varied, which forms a wave group or wave packet. The velocity with which the envelope enclosing the wave packet is transported is called the group velocity.

In other words the velocity with which the energy in the wave group is transmitted is called group velocity. Group Velocity is represented by

$$v_{\text{group}} = \frac{d\omega}{dk}$$

where $d\omega$ is the change in angular frequency dk is the change in wave number.

(SOURCE DIGINOTES)



RELATION BETWEEN PHASE VELOCITY AND GROUP VELOCITY:

We know that

$$V_{\text{group}} = \frac{d\omega}{dk} \quad \dots\dots\dots (1)$$

$$V_{\text{phase}} = \frac{\omega}{k} \quad \dots\dots\dots (2)$$

Eq. (2) can be written as

$$\omega = k \cdot V_{\text{phase}}$$

On differentiating,

$$\frac{d\omega}{dk} = V_{\text{phase}} \frac{dk}{dk} + k \cdot \frac{dV_{\text{phase}}}{dk}$$

$$V_{\text{group}} = V_{\text{phase}} + k \cdot \frac{dV_{\text{phase}}}{dk}$$

$$V_{\text{group}} = V_{\text{phase}} + k \cdot \frac{dV_{\text{phase}}}{d\lambda} \times \frac{d\lambda}{dk} \quad \dots\dots\dots (3) \quad (\text{divide and multiply by } d\lambda)$$

We know that,

$$k = \frac{2\pi}{\lambda} \Rightarrow \frac{dk}{d\lambda} = -\frac{2\pi}{\lambda^2} \quad (\text{upon differentiation})$$

$$\Rightarrow \frac{d\lambda}{dk} = -\frac{\lambda^2}{2\pi}$$

Substituting in Eqn (3) we get

$$\therefore V_{\text{group}} = V_{\text{phase}} + \left(\frac{2\pi}{\lambda} \right) \left(\frac{dV_{\text{phase}}}{d\lambda} \right) \left(-\frac{\lambda^2}{2\pi} \right)$$

$$V_{\text{group}} = V_{\text{phase}} - \lambda \frac{dV_{\text{phase}}}{d\lambda}$$

RELATION BETWEEN GROUP VELOCITY AND PARTICLE VELOCITY:

We have the equation for group velocity as

$$v_{\text{group}} = \frac{d\omega}{dk} \quad \dots \dots \dots (1)$$

But, $\omega = 2\pi v = \frac{2\pi E}{h}$ since $E = hv \Rightarrow v = \frac{E}{h}$

Upon differentiation we get,

$$d\omega = \left(\frac{2\pi}{h}\right) dE \quad \dots \dots \dots (2)$$

Also we have $k = \frac{2\pi}{\lambda} \Rightarrow k = \frac{2\pi}{h} p$ since $\lambda = \frac{h}{p}$
 $\Rightarrow dk = \frac{2\pi}{h} dp \quad \dots \dots \dots (3)$

Dividing (2) by (3), we have

$$\frac{d\omega}{dk} = \frac{dE}{dp} \quad \dots \dots \dots (4)$$

We know that $E = \frac{p^2}{2m}$,

Where, p is the momentum of the particle.

Upon differentiation we get,

$$\begin{aligned} \therefore dE &= \frac{2pdः}{2m} = \frac{pdः}{m} \\ \frac{dE}{dp} &= \frac{p}{m} = \frac{mv_{\text{particle}}}{m} \\ \frac{dE}{dp} &= v_{\text{particle}} \quad \dots \dots \dots (5) \end{aligned}$$

From (1), (4) & (5) we have

$$v_{\text{group}} = \frac{d\omega}{dk} = \frac{dE}{dp} = v_{\text{particle}}$$

$\therefore v_{\text{group}} = v_{\text{particle}}$

The velocity of a de Broglie wave group associated with a particle is equal to the velocity of the particle itself.

RELATION BETWEEN PHASE VELOCITY, GROUP VELOCITY AND VELOCITY OF LIGHT:

The equation for phase velocity is

$$v_{\text{phase}} = \frac{\omega}{k} \quad \dots \dots \dots \quad (1)$$

We know that $\omega = 2\pi v = \frac{2\pi E}{h}$ and $k = \frac{2\pi}{h} p$

Substituting for ω and k in equation (1), we get

$$v_{\text{phase}} = \frac{\frac{2\pi E}{h}}{\frac{2\pi}{h} p} = \frac{E}{p}$$
$$v_{\text{phase}} = \frac{mc^2}{mV_{\text{particle}}} = \frac{\eta c^2}{\eta V_{\text{group}}}$$

$$v_{\text{phase}} \cdot v_{\text{group}} = c^2$$

$\Rightarrow v_{\text{phase}}$ is always greater than the velocity of light.

CHARACTERISTICS OF MATTER WAVES:

[1] Matter waves are the waves that are associated with a moving particle.

The wavelength and energy of the matter waves are given by.

$$\lambda = \frac{h}{p} \quad \text{and} \quad E = h v$$

Where, p is the momentum of the particle and v is the frequency of the waves.

- (2) Group velocity of the matter waves is equal to the velocity of the moving particle.
- (3) Phase Velocity of the matter waves is greater than the velocity of the Light (c).

We have $v_{\text{phase}} = \frac{c^2}{V_{\text{group}}} = \frac{c^2}{V} > c$

(4) Phase Velocity of different matter waves may be different.

(5) The amplitude of the matter waves at a particular region and time

depends on the probability density of the particle at that region and time.

END

QUANTUM MECHANICS

Quantum Mechanics is a new branch of study in physics which is indispensable in understanding the mechanics of particles or bodies in the atomic and the subatomic scale. The term quantum mechanics was first introduced by Max Born in 1924. Within the field of engineering, quantum mechanics plays an important role. The study of quantum mechanics has led to many new inventions that include the laser, the diode, the transistor, the electron microscope, and magnetic resonance imaging. Flash memory chips found in USB drives also use quantum ideas to erase their memory cells. The entire science of Nanotechnology is based on the quantum mechanics.

HEISENBERG'S UNCERTAINTY PRINCIPLE:

One of the fundamental principles of quantum mechanics is the “Heisenberg’s uncertainty principle”.

The principle was formulated in 1927 by German physicist Werner Heisenberg. It is also called the indeterminacy principle.

Statement:

“It is impossible to determine precisely and simultaneously both the position and momentum of a particle.”

Further, “in any simultaneous determination of the position and momentum of a particle, the product of the corresponding uncertainties in the measurement is equal to, or greater than $(h/4\pi)$ ”.

$$\Delta x \Delta p \geq h/4\pi$$

Where Δx represents the uncertainty in the measurement of the position of the particle and Δp represents the uncertainty in the measurement of its momentum.

Heisenberg’s uncertainty principle could also be expressed in terms of the uncertainties involved in the measurement of the physical variable-pair, **energy (E) and time (t) and also angular displacement (θ) and angular**

momentum (L).

If ΔE and Δt are the uncertainties involved in determining the energy and time respectively, then

$$\Delta E \Delta t \geq h/4\pi$$

Similarly, if $\Delta\theta$ and ΔL are the uncertainties involved in determining the angular displacement and angular momentum of the particle respectively, then

$$\Delta\theta \Delta L \geq h/4\pi$$

where, the notation Δ associated with the respective variables indicates the minimum uncertainty involved in the measurement of the corresponding variable.

PHYSICAL SIGNIFICANCE OF HEISENBERG'S PRINCIPLE:

- It signifies that one should not think about accurate values for the position and momentum of a particle. Instead one should think about only the probable values for the position and momentum.
- The estimation of such probabilities are made by mathematical functions named probability density functions.

APPLICATION OF HEISENBERG'S UNCERTAINTY PRINCIPLE:

Non-existence of electrons in the nucleus:

As an application of Heisenberg's uncertainty principle, we consider the case of "Non-existence of electrons in the nucleus". This is based on the observations regarding the emission of β -rays during nuclear decay.

Becquerel demonstrated that β -rays are actually streams of **electrons**. During β decay process it was found that the emitted β -rays travelled with different velocities. Becquerel demonstrated that β -rays are actually streams of **electrons**. Their kinetic energy varied from very low values to a maximum value of about 3-4 MeV. Hence the obvious question, "**is it possible that electrons exist inside the nucleus with certain energy, and the same energy appears as their kinetic energy when they are emitted?**"

The proof for this is presented below:

We know by the theory of relativity that, the energy E of a body is expressed as,

$$E = mc^2 = \frac{m_0 c^2}{\sqrt{1 - \frac{v^2}{c^2}}}$$

where 'm₀' is the rest mass of the body and 'm' is the mass while its velocity is v.

Squaring on both sides, we get

$$E^2 = \left\{ \frac{m_0 c^2}{\sqrt{1 - \frac{v^2}{c^2}}} \right\}^2 = \frac{m_0^2 c^4}{1 - \frac{v^2}{c^2}} = \frac{m_0^2 c^6}{c^2 - v^2} \dots\dots\dots (1)$$

Also, we know that, momentum p of the body is given by,

$$p = mv = \frac{m_0 v}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$$\text{or, } p^2 = \frac{m_0^2 v^2}{1 - \frac{v^2}{c^2}} = \frac{m_0^2 v^2 c^2}{c^2 - v^2}$$

Multiplying by c², we have,

$$p^2 c^2 = \frac{m_0^2 v^2 c^4}{c^2 - v^2} \dots\dots\dots (2)$$

Subtracting eq. (3) by (2), we get,

$$\begin{aligned} E^2 - p^2 c^2 &= \frac{m_0^2 c^6 (c^2 - v^2)}{(c^2 - v^2)} \\ E^2 &= p^2 c^2 + m_0^2 c^4 \\ E^2 &= c^2 [p^2 + m_0^2 c^4] \end{aligned} \dots\dots\dots (3)$$

This is Einstein's relativistic energy-momentum equation, where

m₀ = rest mass of electron = 9.1x10⁻³¹kg,

p = momentum and

c = speed of light = 3x10⁸ m/s.

Now, for an electron to exist inside the nucleus, the uncertainty Δx in its position cannot be greater than the nuclear radius. The nuclear radius is in the order of 5 X 10⁻¹⁵ m. We can take this value to be approximately the maximum

space of confinement. Thus the maximum value for uncertainty in position can be taken as

$$(\Delta x)_{\max} \leq 5 \times 10^{-15} \text{ m}$$

By uncertainty principle,

$$\begin{aligned}\Delta x \cdot \Delta p &\geq \frac{h}{4\pi} \\ (\Delta p)_{\min} &\geq \frac{h}{4\pi} \times \frac{1}{\Delta x} \\ \therefore \Delta p &\geq \frac{6.63 \times 10^{-34}}{4 \times 3.14 \times 5 \times 10^{-15}}\end{aligned}$$

$$(\Delta p)_{\min} \geq 1.1 \times 10^{-20} \text{ Ns} \quad \dots \dots \dots (4)$$

This is the uncertainty in the momentum of the electron. But since the momentum of the electron must atleast be equal to the uncertainty in the momentum, we can take

$$(p_x)_{\min} \geq 1.1 \times 10^{-20} \text{ Ns} \quad \dots \dots \dots (5)$$

We know that the rest mass of the electron is $m_0 = 9.11 \times 10^{-31} \text{ kg}$.

Using the inequality (5) in equation (3), we can say that for the electrons to exist inside the nucleus, its energy E must be such that

$$E^2 \geq c^2 [p^2 + m_0^2 c^4]$$

$$(E)_{\min} \geq (3 \times 10^8)^2 [(1.1 \times 10^{-20})^2 + (9.11 \times 10^{-31})^2 (3 \times 10^8)^4]$$

Since the second term inside the bracket is too small, it is neglected.

$$(E)_{\min} \geq 20.6 \text{ MeV}$$

This means to say that, for electrons to exist inside the nucleus, it must have a minimum energy of about 20.6 MeV. But beta-decay studies indicate that the kinetic energy of β -particles is of the order of 3 to 4 MeV. Hence, we can conclude that electrons cannot exist inside the nucleus.

INSTITUTE OF TECHNOLOGY

WAVE FUNCTION:

In quantum mechanics, because of the wave-particle duality, the properties of particles can be described by a wave. Therefore its quantum state can be represented by a wave of any arbitrary shape. This is called a **Wave function**.

The variable quantity characterizing matter waves is known as **wave function**. It gives complete information about the system .It is also called state function as it speaks about the physical state of the system.

Wave function is obtained by solving a fundamental equation called

Schrodinger equation.

- It varies w.r.t position and time.
- It is denoted by a symbol (Ψ)
- Ψ itself cannot be an observable quantity hence, Ψ has no direct physical significance
- Ψ can have real values or imaginary(complex).

Properties of wave function

Property 1: ψ is single valued everywhere.

A function $f(x)$ which is not single valued over a certain interval is shown in Fig. 1. Here $f(x)$ has three values, f_1 , f_2 and f_3 for the same value of P at $x = P$. Since $f_1 \neq f_2 \neq f_3$, it means to say that, if $f(x)$ were to be wave function, then the probability of finding the particle has three different values at the same location P which is absurd. Hence this wave function is not acceptable.

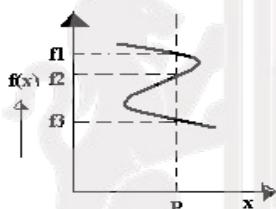


Figure:1

Property 2: ψ is finite everywhere.

A function $f(x)$ which is not finite at $x = R$ is shown in Fig.2. At $x = R$, $f(x) = \infty$. Thus, if $f(x)$ were to be a wave function, it signifies a large probability of finding the particle at a single location ($x = R$), which violates the uncertainty principle. Hence the wave function becomes unacceptable.



Figure: 2

Property 3: ψ and its first derivatives with respect to its variable are continuous everywhere.

A function $f(x)$ which is discontinuous at Q is shown in Fig. 3. At $x = Q$, $f(x)$ is truncated at A , and restarts at B . The function is not defined between A & B . If $f(x)$ is taken to be a wave function, then the state of the system at $x = Q$ cannot be ascertained. Hence the wave function is not acceptable.

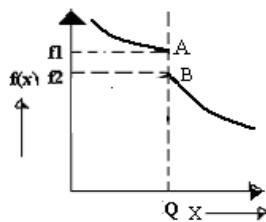


Figure: 3

Also, when ψ is not continuous, its first derivatives will not be finite. The first derivatives should also be continuous, because, if they are not continuous, the second derivatives of ψ will not be finite.

Property 4: For bound states, ψ must vanish at infinity. If ψ is a complex function, then $\psi^* \psi$ must vanish at infinity.

The wave functions that possess all the above properties are called **Eigen functions**.

Physical significance of wave function (ψ):

- It gives the idea about the probability of finding a particle.
- Let us consider a system of electrons. If ψ is the wave function associated with that system, then $|\psi|^2$ gives measure of density of electrons.
- If we consider an electron to be present in the region of volume V then $|\psi|^2 dV$ gives the probability of finding the electron in the region of volume dV
- The certainty of finding the electron in the entire region of volume V is given by

$$\int |\psi|^2 dV = 1.$$

This is known as normalization.

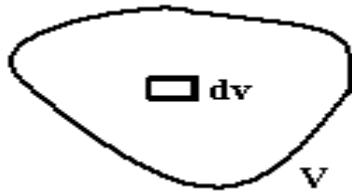
(*SOURCE DIGINOTES*)

Probability density:

According to Max born approximation, probability of locating a particle at a point is directly proportional to $|\psi|^2$. This is called **probability density**.

If $|\psi|^2 = 1$; then we are sure that particle is present .

If $|\psi|^2 = 0$; then the particle is completely absent.



Consider a particle inside the volume V. Let dV be the infinitesimally small element in V. If ψ is the wave function associated with the particle, then $|\psi|^2$ is the probability per unit volume of space, centered at a point where ψ is evaluated at that time

Thus, the probability of finding a particle is

$$P = \int |\psi|^2 dV$$

Here, the product of ψ . ψ^* is real and is written as $|\psi|^2$, where ψ^* is the complex conjugate of ψ .

Probability density is given by

$$|\psi|^2 = \psi \psi^*, \text{ where } \psi^* \text{ is the complex conjugate of } \psi.$$

Normalization condition:

Further, if we are certain that the particle is present in a particular region or space of volume V, then

$$\int_0^V |\psi|^2 \cdot dV = 1$$

This value 1 for probability means, it is clearly a certainty. However, if we are not certain about locating the particle anywhere in the given volume, then it is expected to be present somewhere in space. Then the probability of finding the particle somewhere in the universe must be unity. Thus

$$\int_{-\infty}^{+\infty} |\psi|^2 \cdot dV = 1$$

This condition is known as the normalization condition.

A wave function that satisfies the above condition is said to be normalized.

Eigen function and eigen value

Eigen functions are those functions which possess the properties of that they are single valued & finite everywhere and also their first derivatives with

respect to their variables are continuous everywhere..

To find ψ Schrodinger's wave equation has to be solved. Since it is a second order differential equation, hence it has many numbers of solutions. But all of them may not be the correct solutions in such a case we have to choose only a permitted function. These permitted functions are called Eigen function the corresponding energy values are called **Eigen values**

Operator.

An operator(\hat{A}) is a symbol or a code which directs one to perform an operation on the Eigen function (ψ)to get the information (Eigen value)(λ)

$$\hat{A}\psi = \lambda\psi$$

Schrodinger's Wave Equation:

Schrodinger equation is a fundamental wave equation in quantum mechanics capable of determining the wave function ψ for different physical conditions.

Time independent Schrodinger Wave Equation:

According to de- Broglie theory, for a particle of mass 'm' moving with a velocity 'v', the wave length λ is given by,

$$\lambda = \frac{h}{p} = \frac{h}{mv} \quad \dots \dots \dots (1)$$

where , p is the momentum of the particle.

The de- Broglie wave equation for a particle travelling in positive x-direction can be written in complex form as

$$\Psi = A e^{i(kx - \omega t)} \quad \dots \dots \dots (2)$$

where, A is the amplitude of the wave, ω is angular frequency of the wave, Ψ is the total wave function and k is the wave number.

The space independent part in equation (2) can be represented as a wave function,

$$\Psi = \psi A e^{-i\omega t} \quad \dots \dots \dots (3)$$

Differentiate (3) twice wrt x. Since Ψ depends on x, we get

$$\frac{d^2\Psi}{dx^2} = e^{-i\omega t} \cdot \frac{d^2\psi}{dx^2} \quad \dots \dots \dots (4)$$

Now again differentiate (3) w.r.t. time 't' twice, we get

$$\frac{d\Psi}{dt} = (-i\omega) A e^{i(kx-\omega t)} \Psi$$

$$\frac{d^2\Psi}{dt^2} = (-i\omega)(-i\omega) A e^{i(kx-\omega t)} \Psi$$

$$\frac{d^2\Psi}{dt^2} = -\omega^2 e^{-i\omega t} \Psi \quad \dots\dots\dots (5)$$

The equation for a travelling wave in differential form can be written as,

$$\frac{d^2y}{dx^2} = \frac{1}{v^2} \frac{d^2y}{dt^2}$$

Then by analogy, the wave equation for a de Broglie wave for the motion of a free particle can be written as

$$\frac{d^2\Psi}{dx^2} = \frac{1}{v^2} \frac{d^2\Psi}{dt^2} \quad \dots\dots\dots (6)$$

This equation represents the waves propagating along x-axis with a velocity 'v', and 'x' is the displacement at time 't'.

Substituting equations (4) and (5) in the above equation, we get

$$e^{-i\omega t} \cdot \frac{d^2\Psi}{dx^2} = \frac{1}{v^2} \cdot (-\omega^2 e^{-i\omega t} \Psi)$$

$$\frac{d^2\Psi}{dx^2} = \frac{-\omega^2}{v^2} \Psi$$

But, we know that $\omega = 2\pi\nu$ and $v = \nu\lambda$. Substituting for ω and v , we get

$$\frac{d^2\Psi}{dx^2} = \frac{-4\pi^2 v^2}{\nu^2 \lambda^2} \Psi = \frac{-4\pi^2}{\lambda^2} \Psi \quad \dots\dots\dots (7)$$

But, we have, $\lambda = \frac{h}{p} = \frac{h}{mv}$. Then eq.(7) becomes

$$\frac{d^2\Psi}{dx^2} + \frac{4\pi^2 m^2 v^2}{h^2} \Psi = 0 \quad \dots\dots\dots (8)$$

We know that,

Total Energy = Kinetic Energy + Potential Energy

$$E = KE + PE$$

$$E = \frac{mv^2}{2} + V$$

$$m^2 v^2 = 2m(E - V) \quad \dots\dots\dots(9)$$

Substitute eq. (9) in (8), then

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

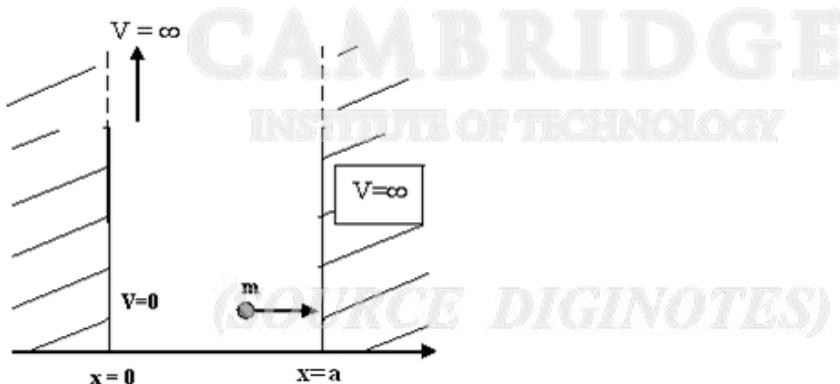
$$\boxed{\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m(E - V)}{\hbar^2} \psi = 0}$$

This is known as time independent Schrodinger wave equation in one dimension.

Applications of Schrodinger's Equation:

(1) Particle in one dimensional potential well of infinite height:

Consider a particle of mass 'm' moving inside a box along the X – direction between two rigid walls A and B. The particle is free to move between the walls of the box at $x = 0$ and $x = a$. The potential energy of the particle is considered to be zero inside the box and infinity at all points outside the box. This means that



1. PE, $V=0$ for $0 < x < a$

2. PE, V=∞ for x ≤ 0 and x ≥ a

The particle is always inside the box and therefore the probability of finding the particle outside the box is zero. Therefore the wave function ψ is zero for $x \leq 0$ and $x \geq a$.

The Schrodinger's equation for a particle is given by

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

Since, $V = 0$ inside the box between the walls, the above equation reduces to

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m E}{\hbar^2} \psi = 0 \quad \dots \dots \dots \quad (1)$$

$$\text{Take, } \frac{8\pi^2 m E}{\hbar^2} = k^2 \quad \dots \dots \dots \quad (1A)$$

Then, equation (1) becomes

$$\frac{d^2\psi}{dx^2} + k^2 \psi = 0 \quad \dots \dots \dots \quad (2)$$

The general solution for equation (2) is of the form

$$\psi = A \sin kx + B \cos kx \quad \dots \dots \dots \quad (3)$$

where A and B are constants. The values of these constants can be evaluated by applying the following boundary conditions.

The particle cannot penetrate the walls. Hence

$$(i) \psi = 0 \text{ at } x = 0$$

$$\therefore (3) \Rightarrow 0 = A \sin 0 + B \cos 0$$

$$\Rightarrow 0 = 0 + B \boxed{\begin{array}{l} B \\ = \\ 0 \end{array}} \Rightarrow$$

$$\therefore \psi = A \boxed{\begin{array}{l} \\ \\ 0 \end{array}} \sin kx \quad \dots \dots \dots \quad (4)$$

Again, (ii) $\psi = 0$ at $x = a$

$$(3) \Rightarrow 0 = A \sin ka$$

But $A \neq 0$; because if $A = 0$, then the entire function will become zero.

Therefore, $\sin ka = 0 = \sin n\pi$

$$ka = n\pi, n = 0, 1, 2, 3, \dots$$

$$\Rightarrow k = \frac{n\pi}{a} \quad \dots \dots \dots \quad (5)$$

Equation (4) becomes

$$\therefore \psi_n = A \sin \left(\frac{n\pi}{a} x \right) \quad \dots \dots \dots \quad (6)$$

Substituting equation (5) in (1A), we get

$$\Rightarrow \frac{n^2 \pi^2}{a^2} = \frac{8\pi^2 m E_n}{h^2}$$

$$\Rightarrow E_n = \frac{n^2 h^2}{8ma^2} \quad \dots \dots \dots \quad (7)$$

$$\text{where } n = 1, 2, 3, \dots$$

When $n = 1$ is the lowest energy level given by

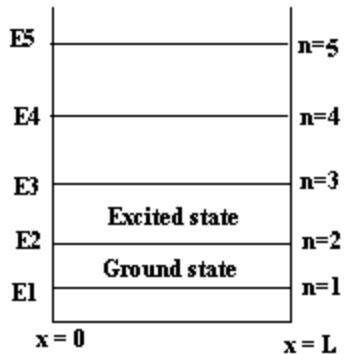
$$E_1 = \frac{h^2}{8ma^2}$$

This energy is called the zero-point energy. Also,

$$E_1 = \frac{h^2}{8ma^2} = E_0, \quad E_2 = \frac{4h^2}{8ma^2}, \quad E_3 = \frac{9h^2}{8ma^2}, \dots$$

For each value of 'n' there is an energy level. The possible allowed values of energy obtained from equation (7) i.e., E_1, E_2, E_3 etc are called **Eigen values** and the corresponding wave function ψ_n is called the Eigen function.

(**SOURCE DIGINOTES**)



The energy corresponding to $n = 1$ is called ground state energy or zero point energy and the energy levels for $n = 2, 3, 4, 5, \dots$, are called excited states.

Inside the well, the particles can have discrete set of values of energy and it is quantized i.e.,

$$E_2 = 4E_0, E_3 = 9E_0, E_4 = 16E_0, \text{ and so on.}$$

Normalization of wave function (evaluation of the value of A):

We have,

$$\psi_n = A \sin\left(\frac{n\pi}{a}\right)x$$

The constant A of this equation can be obtained by applying the normalization condition i.e.,

$$\int_0^a |\psi_n|^2 dx = 1$$

$$\int_0^L A^2 \sin^2 \frac{n\pi x}{a} dx = 1$$

$$\text{We know that } \sin^2 \theta = \frac{1 - \cos 2\theta}{2}.$$

Then

$$\begin{aligned} & \int_0^a \frac{A^2}{2} \left(1 - \frac{\cos 2n\pi x}{a}\right) dx = 1 \\ & \Rightarrow \frac{A^2}{2} \left[\int_0^a (1) dx - \int_0^a \frac{\cos 2n\pi x}{a} dx \right] = 1 \\ & \Rightarrow \frac{A^2}{2} [x]_0^a - \frac{A^2}{2} \frac{a}{2n\pi} \left[\frac{\sin 2n\pi x}{a} \right]_0^a = 0 \end{aligned}$$

$$\Rightarrow \frac{A^2 a}{2} - \frac{A^2 a}{4n\pi} \left[\frac{\sin 2n\pi a}{a} \right]^2 = 0 \Rightarrow \sin(2n\pi) = 0$$

$$\frac{A^2 a}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{a}} \dots\dots\dots (8)$$

$$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

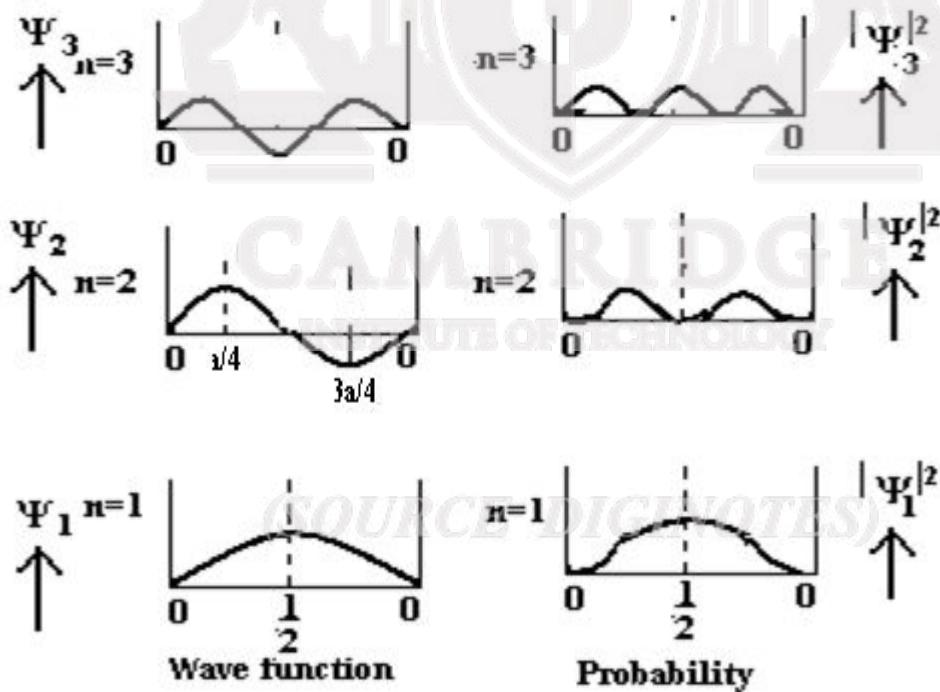
The normalized wave function of the particle is

$$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

Wave functions, probability densities and energy eigen values for a particle in a box:

The first three energy levels (Eigen Values) E_1, E_2, E_3 and their corresponding wave function is ψ_1, ψ_2, ψ_3 and probability densities corresponding to $n = 1, 2, & 3$ respectively.

Figure



Case (1)

For $n = 1$, the eigen function is

$$\psi_1 = A \sin\left(\frac{\pi}{a}x\right)$$

ψ_1 is maximum at $x = a/2$.

Thus a plot of ψ_1 versus x will be as shown in figure and a plot of probability density $|\psi_1|^2$ versus x is as shown in figure. The probability of finding the particle is zero both at $x = 0$ and

$x = a$. It is maximum at $x = a/2$. This means that in the ground state, the probability of finding the particle is maximum at the center of the box.

Also, the ground state energy, $E_1 = \frac{h^2}{8ma^2} = E_0$

Case (2)

At $n=2$, the eigen function for the first excited state is

$$\psi_2 = A \sin\left(\frac{2\pi}{a}x\right)$$

$\psi_2 = 0$ at $x = 0, a/2$ and a .

ψ_2 is maximum at the positions $x = a/4$ and $3a/4$.

The plot of ψ_2 versus x and the probability density $|\psi_2|^2$ versus x is as shown in fig.

Since $|\psi_2|^2 = 0$ at $x = 0, a/2$ and a , this means in the first excited state the particle cannot be observed either at the walls or at the center.

Here, the energy of the first excited state is $E_2 = \frac{4h^2}{8ma^2} = 4E_0$

Case (3)

At $n=3$; the second excited state, the eigen function for the second excited state is given by

$$\psi_3 = A \sin\left(\frac{3\pi}{a}x\right)$$

$\psi_3 = 0$ for $x = 0, a/3, 2a/3$ and a .

ψ_3 has maximum value for $x = a/6, a/2$ and $5a/6$.

A plot of ψ_3 versus x and probability density $|\psi_3|^2$ versus x is as shown in fig.

For each value of n there is an energy level as obtained from equation (1).

Here, $E_3 = \frac{9h^2}{8ma^2} = 9E_0$

Hence, the energy levels are discrete. Each energy value of E_n is called Energy Eigen value. The Eigen value for the corresponding wave function ψ_n is called the Eigen function. The energy values that are permissible in any system are obtained from the solution of the Schrodinger's equation and are called Eigen Values.

2) Energy Eigen value for a free particle

Free particle means a particle that is not under the influence of any electric field or force. For a free particle, $V=0$.

\therefore Schrodinger wave equation becomes

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

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m E}{\hbar^2} \psi = 0 \quad \dots \dots \dots \quad (1)$$

$$\frac{d^2\psi}{dx^2} + k^2 \psi = 0 \quad \dots \dots \dots \quad (2)$$

$$\text{where } \frac{8\pi^2 m E}{\hbar^2} = k^2 \quad \dots \dots \dots \quad (3)$$

The solution for the above equation is of the form

$$\psi = A \sin kx + B \cos kx$$

For a free particle there are no boundary conditions. Therefore there are no values for the constants A, B and K.

Hence Equation (3) becomes $E = \frac{k^2 \hbar^2}{8\pi^2 m}$

Thus for a free particle energy values are not quantized and the problem is dealt in classical mechanics. Thus a free particle is a classical entity.

CAMBRIDGE

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(SOURCE DIGINOTES)

QUESTION BANK

- 1) What are the basic postulates of quantum theory of radiation? Explain how Planck's theory overcomes the drawbacks of Wein's law and Rayleigh-Jeans law.
- 2) What is a blackbody? Draw the blackbody radiation spectrum. Mention its features.
- 3) Show that group velocity is equal to particle velocity.i.e ($V_{\text{group}} = V_{\text{particle}}$)
- 4) State Heisenberg's Uncertainty Principle and P.T non existence of electron in nucleus using Uncertainty principle.
- 5) Find the Eigen values and Eigen functions for an electron in one dimensional potential well of infinite height.
- 6) Set up the time independent Schrodinger wave equation.

MODULE-2**ELECTRICAL CONDUCTIVITY IN MATERIALS****DRUDE-LORENTZ THEORY OF FREE ELECTRON**

Paul Drude, a German Physicist gave a generally accepted theory on electrical conductivity in metals and Lorentz, a Holland Physicst improved it.

Hence this theory is named DRUDE- LORENTZ THEORY. (**Only for information**)

Every metal atom consists of valence electrons and these are responsible for electrical conduction . In a metal, the atoms are tightly packed. Each atom consists of valence electrons. These valence electrons are out of the atom and free to move within the metal. There is continuity in movement of these electrons from atom to atom.

Hence, valence electrons belong to any atom. These electrons are named as free electrons. These are responsible for conduction and hence also called as conduction electrons.

ASSUMPTIONS OF CLASSICAL FREE ELECTRON THEORY

1. In a metal there are freely moving valence electrons called free electrons confined to its body. The electric current in a metal due to an applied field is a consequence of the drift velocity of the free electrons in a direction opposite to the direction of the field.
2. The free electrons are treated equivalent to gas molecules and thus assumed to obey the law of kinetic theory of gases. Given by,

$$^3_2 - KT = ^1_2 - mV_{th}^2$$

Where, K → Boltzmann constant
 V_{th} → Thermal velocity.

3. The electrical potential due to cores (Lattice point) is taken to be throughout the metal.
4. The attraction between the free electrons and the ions and the repulsion between the electrons themselves are considered insignificant (ignored)

MEAN FREE PATH

Mean free path is the average distance travelled by the free electrons two successive collisions. It is denoted by "λ".

MEAN COLLISION TIME

Mean collision time is the average time elapsed between two successive collision. It is denoted by "τ".

RELATION BETWEEN λ AND τ

$$\tau = \lambda$$

$$v$$

V → Total velocity of electrons which is the sum of drift velocity(V_d) and thermal velocity(V_{th}).

RELAXATION TIME

In the absence of electric field, the average velocity of the electrons in any given direction is zero,

i.e., $\mathbf{V}_{\text{average}}$ or $\mathbf{V}_{av} = \mathbf{0}$ (Absence of electric field)

But in the presence of electric field, the average velocity is not zero, i.e.,

$\mathbf{V}_{av} = \mathbf{V}'_{av}$ (Presence of electric field)

Now, once we turn off the field, V_{av} starts reducing exponentially from the value

V'_{av} as shown in the graph below

The decay process is given by

$$V_{av} = e^{-t/\tau} V'_{av}$$

"Relaxation time is the time required for the average velocity of the free electrons to reduce to e^{-1} times its average velocity that existed when the field is just turned off"

LATTICE

The periodic arrangement of fixed ions in 3 dimensions is called lattice.

DRIFT VELOCITY

When an electric field is applied, the free electrons will have net displacement in one single direction and displaces with respect to time in a direction opposite to the direction of the field.

The displacement of free electrons per unit time is called drift velocity. It is called drift velocity. It is denoted by $V_d = \frac{eE}{m\tau}$

Where, $e \rightarrow$ charge of electron $= 1.6 \times 10^{-19} C$

$E \rightarrow$ Electric field τ

\rightarrow mean collision time $m \rightarrow$ mass
of electron $= 9.1 \times 10^{-31} Kg$

EXPRESSION FOR ELECTRICAL CONDUCTIVITY AS PER CLASSICAL FREE ELECTRON THEORY

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

where, $\sigma \rightarrow$ Electrical conductivity

$e \rightarrow$ charge of electron τ

\rightarrow Relaxation time m

\rightarrow mass of electron.

FAILURES OF CLASSICAL FREE ELECTRON THEORY.

1. Specific heat: The theory compares free electron to the gas molecules, same specific heat should be applicable for both. The Specific heat should be applicable for both. The specific heat of a gas at constant volume is given by,

$$C_V = \frac{3}{2} R \quad \dots \dots \dots (1)$$

But experimentally it was found that, $C_V = 10^{-4} RT \quad \dots \dots \dots (2)$

From (1) & (2), we see that, C_V for a metal is not only far smaller than C_V for gas molecule but also its dependent on temperature.

2. Temperature dependence of electrical conductivity (σ)

Experimentally observed value of σ for metals is inversely proportional to temperature T.

$$\text{i.e., } \sigma_{\text{exp}} \propto T^{-1} \quad \dots \dots \dots (1)$$

$$\frac{3}{2} K T = \frac{1}{2} m V_{t2h}$$

Now from classical assumption we have,

$$V_{th} = \frac{\sqrt{3KT}}{m} = \sqrt{T} \dots \quad (2)$$

We know that , $T = \frac{V}{V_{th}}$

$$(\text{or}) \quad T \propto \frac{1}{\sqrt{T}} \quad \dots \dots \quad (3) \quad \text{[from eqn 2]}$$

Also we have,

$$nTe^2 \sigma =$$

$$\overline{\sigma \alpha T}^m \text{ (or) } \sigma \alpha \frac{1}{\sqrt{T}} \dots \dots \dots \quad (4)$$

From (1) & (4) it is clear that the prediction of classical free electron theory is not agreeing with the experimental observation.

3. Dependence of electrical conductivity on electron concentration ‘ n’

Conductivity ‘ σ ’ is given by,

$$\sigma = \frac{n}{m} \tau_{e2} \quad \text{where 'n' is electron concentration .}$$

Metal	Valency	σ (Ωm)	n
Cu	1	5.88×10^7	8.45×10^{28}
Zn	2	1.09×10^7	13.10×10^{28}

According to classical free electron theory, $n \propto \sigma$, which means higher the number of free electrons higher is its conductivity.

From the above table we observe that Zn has more free electrons than Cu, but conductivity of Cu is higher than that of Zn. Hence the prediction, $n \propto \sigma$ does not always hold good.

ASSUMPTIONS MADE IN QUANTUM FREE ELECTRON THEORY.

One of the important realization was, the role played by Pauli's exclusion principle. The assumptions of Quantum free electron theory are,

1. The free electrons possess energy and these energy values are quantised. The allowed energy levels are realized in terms of a set of energy levels.

2. The distribution of electrons in various energy levels occurs as per Pauli's exclusion principle...i.e., single energy level can be occupied by only 2 electrons with opposite spin.
3. The electric potential throughout the lattice is taken to be constant.
4. The attraction and the repulsion between the lattice points and electrons (or) lattice points themselves (or) electrons themselves are ignored.

DENSITY OF STATES

Energy levels of electrons in a solid will look like bands. On a closer look we see that the energy levels in the band are not uniformly distributed. The number of energy levels/unit energy range is explained by density of states.

“Density of states is the number of allowed energy levels in infinitesimally small energy increment dE in the valence band of the material.

$$\text{Given by, } g(E)dE = \frac{8\sqrt{2\pi}m^3}{3} \frac{1}{E^2} dE$$

$$g(E) \propto E^{-2}$$

FERMI ENERGY

Consider a metal of N atoms and hence there will be N allowed energy levels in each band. The electrons will occupy energy levels according to Pauli's exclusion principle. When no external energy is supplied for the electrons, such as thermal energy i.e., at $T=0K$, we see that levels above valence band will be vacant.

“Fermi energy is the energy corresponding to the highest occupied level at zero degree absolute temperature and the energy level is referred to as the **FERMI LEVEL (E_F)**”

At $T=0K$, energy levels lying above the Fermi level are empty and those lying below are completely filled.

FERMI FACTOR AND DEPENDANCE OF FERMI FACTOR ON TEMPERATURE AND ENERGY (PROBABILITY OF OCCUPATION OF VARIOUS ENERGY STATES BY ELECTRONS AT $T=0K$ AND $T>0K$, ON THE BASIS OF FERMI FACTOR)

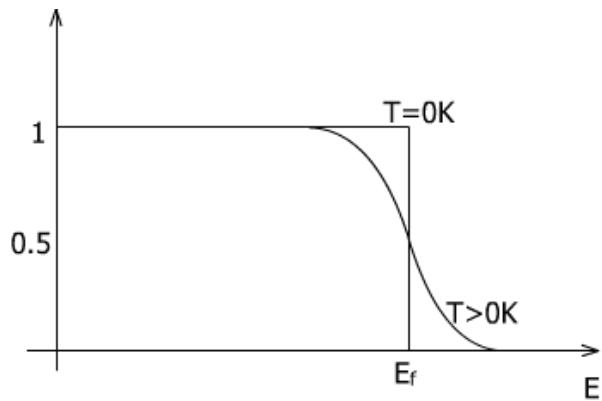
Fermi-Dirac Statistics permits the evaluation of probability of finding electrons occupying energy levels in a certain energy range. This is done through a function called Fermi Factor $f(E)$. It is given by,

$$e^{ET} + 1$$

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

“Fermi factor is the probability of occupation of a given energy state for a material in thermal equilibrium”

Probability of occupation is considered for following cases,



i) Probability of accupation for $E < E_F$ at $T=0K$

$$\text{We have, } F(E) = \frac{1}{e^{\frac{E-E_F}{kT}} + 1}$$

If $E < E_F$, $E - E_F$ will be negative and $T=0$,

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

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

$f(E)=1$

- $f(E)=1$ means, the energy level is certainly occupied.i.e,there is 100% probability that the electrons occupy the energy level below Fermi energy
- All the energy levels below Fermi level are occupied
- $E < E_F$ applies to all the energy levels below E_F

ii) Probability of accupation for $E > E_F$ at $T=0K$

If $E > E_F$, $E - E_F$ will be positive and for $T=0$,

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

$f(E)=0$

- All the energy levels above Fermi level are unoccupied.i.e, 0% probability for the electrons to occupy the energy level above the Fermi level

iii) Probability of occupation at ordinary temperature.

At ordinary temperature, though value of probability remains 1 for $E \ll E_F$, it starts decreasing from 1 as the value of E become closer to E_F . For $E=E_F$,

$$f(E) = \frac{1}{e^0} = \frac{1}{1+1} = \frac{1}{2} = 0.5$$

$$f(E) = \frac{1}{2}$$

There is 50% probability for the electrons to occupy the Fermi energy level

EXPRESSION FOR ELECTRICAL CONDUCTIVITY AS PER QUANTUM FREE ELECTRON THEORY

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

where,

m^* → effective mass of the electron V_F → Fermi velocity
 λ → Mean free path e → charge of the electron
 n → electron concentration

MERITS OF QUANTUM FREE ELECTRON THEORY (SUCCESS OF QUANTUM FREE ELECTRON THEORY IN OVERCOMING THE FAILURES OF CLASSICAL FREE ELECTRON THEORY)

1. Specific heat(C_V)- The small value of specific heat (C_V) for the conduction electrons can be explained as follows.

According to quantum theory, only those electrons that occupy energy levels close to E_F can absorb the energy and move to the higher energy states. Number of such electrons absorbing the energy is small and hence C_V is small, It is given by,

$$C_V = \left(\frac{2K}{E_F} \right)_{RT}$$

Ex., For $E_F=5\text{eV}$

$$\left(\frac{2K}{E_F} \right) \approx 10^{-4}$$

$$C_V = 10^{-4}RT.$$

This confirms with the experimentally observed values.

2. Temperature dependence of electrical conductivity.

The experimental fact that the electrical conductivity σ has a dependence on $\frac{1}{T}$ and not $\frac{1}{\sqrt{T}}$ on T is explained here,

$$ne_2\lambda$$

We have, $\sigma = m \frac{1}{V_F} \cdot \lambda \dots\dots\dots(1)$

The dependence of σ on T is analysed as follows,

The free electrons are subjected to scattering due to vibration of ion in the lattice. If 'r' is the amplitude of vibration, it is same in all the directions then the ions can be considered to be present effectively in a circular cross-section of area πr^2 . The value of mean free path λ decreases when πr^2 increases.i.e,

$$\lambda \propto \frac{1}{\pi r^2} \dots\dots\dots(2)$$

Now consider the facts,

- Energy of ion \propto square of the amplitude
i.e, $E \propto r^2 \dots\dots\dots(3)$
- Energy of ion \propto Temperature
i.e, $E \propto T \dots\dots\dots(4)$ from eqn (3) & (4)
 $\rightarrow r^2 \propto T \dots\dots\dots(5)$

$$(2) \rightarrow \lambda \propto \frac{1}{r^2} \dots\dots\dots(6)$$

$$(5) \& (6) \rightarrow \lambda \propto \frac{1}{T} \dots\dots\dots(7)$$

$$\text{from (1) \& (7)} \rightarrow \sigma \propto \frac{1}{T} \dots\dots\dots$$

3.Electrical conductivity and electron concentration.

It was not possible to understand why metals such as Aluminium and gallium which have 3 free electrons/atom have lower electrical conductivity than metals such as copper and silver which possess only 1 free electron/atom. Quantum free electron theory could explain why,

$$ne^2\lambda$$

We know that, $\sigma = m \frac{1}{V_F} \cdot \lambda \dots\dots\dots(1)$

From(1),it is clear that ' σ ' depends on both ' n ' and also on $\frac{\lambda}{V_F}$ ratio

The value of ' n ' for aluminium is 2.13 times higher than that of copper. But the values of $\frac{\lambda}{V_F}$ for copper is about 3.73 times higher than that of aluminium.

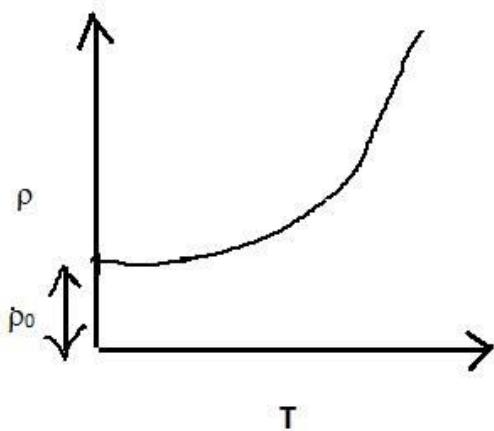
Therefore, conductivity of copper exceeds that of aluminium.

SUPERCONDUCTORS

TEMPERATURE DEPENDENCE OF RESISTIVITY OF A METAL.

Metals have loosely bound electrons in their outermost shell or valence shell which is responsible for conduction. These electrons are called free electrons/conduction electrons.

The dependence of resistivity (ρ) on temperature is as shown below.



The total resistivity of a metal is the sum of the resistivity due to impurities(ρ_0) at $T=0K$ and the resistivity due to phonon scattering which is temperature dependent $\rho(T)$. We can see that the resistance decreases with temperature and reaches minimum at $T=0K$

The Variation is expressed by the **Matthiessen's rule**

$$\rho = \rho_0 + \rho(T)$$

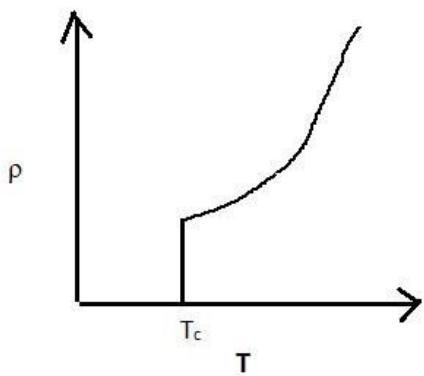
Where, ρ → is the resistivity of the given metal

ρ_0 → is the residual resistivity

$\rho(T)$ → is the temperature dependent of resistivity

(Note: Lattice vibrations are called phonons)

TEMPERATURE DEPENDENCE OF RESISTIVITY OF A SUPERCONDUCTOR:



Resistivity (ρ) is the non superconducting state decreases with decrease in temperature upto a particular temperature T_c . At T_c , ρ abruptly drops to zero. T_c is called the critical temperature and signifies the transition from normal state to the superconducting state of the material under study.

“The resistance offered by certain materials to the flow of electric current abruptly drops to zero below a certain temperature. This phenomenon is called Superconductivity”

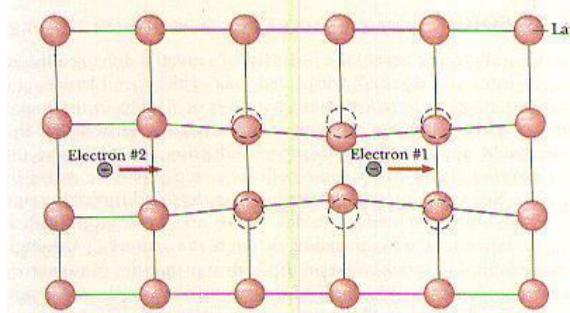
- Materials exhibiting this property are called superconductors.
- The temperature at which the resistance becomes zero is called the critical temperature.
- Critical temperature is different for different materials . The critical temperature is different for different superconductors.

Superconductors elements	symbol	$T_c(K)$
Mercury	Hg	4.2
Gallium	Ga	1.15
Aluminium	Al	1.20
Indium	In	3.40
Tin	Sn	3.72
Tantalum	Ta	4.48
Vanadium	V	5.38
Lead	Pb	7.19
Lanthanum	La	6.00

BCS THEORY

BCS theory-(Bardeen,Cooper and Schrieffer theory)

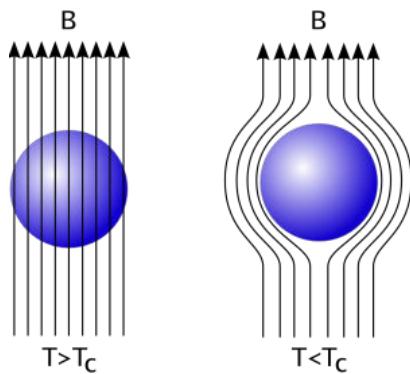
- This theory explains the phenomenon of Superconductivity. This theory is based upon the formation of cooper pairs, which is a quantum mechanical concept.



- When the free electron leaves the atom, the atom becomes positively charged. When electron comes near a positive ion core of the lattice,it experiences an attractive force because of the opposite polarity between electron and ion.
- Due to this attraction ,the ion is displaced from its position, leading to lattice distortion. At the same time,if other electron which comes near that place will also interact with the distorted lattice. This process is looked upon as equivalent to interaction between the two electrons through the lattice .The process is called "electronlattice-electron interaction through the phonon field"
- The attractive force between two electrons will be maximum if they have equal and opposite spin and momenta.This force will even exceed the coulomb repulsive force between electrons. "Hence ,cooper pair is a bound pair of electrons formed by the interaction between the electron with opposite spin and momenta in a phonon field"
- Each cooper pair is associated with a wavefunction. The wavefunction with similar cooper pairs start overlapping which may extend over 10^6 other pairs. This leads to a union of vast number of cooper pairs.
- When the electron flow in the form of cooper pairs,they do not encounter any scattering and the resistance factor vanishes or in other words conductivity becomes infinite hence a material becomes superconductor.

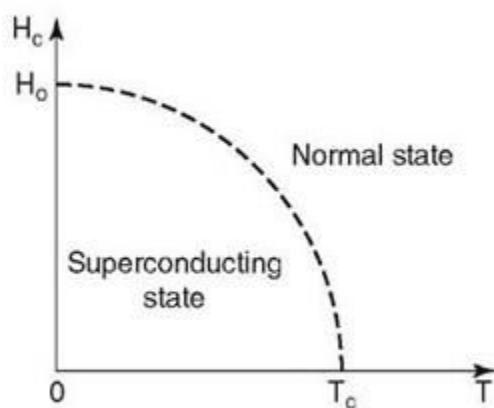
MEISSNER EFFECT.

When a superconducting material is cooled in a magnetic field below the critical temperature, the flux lines are expelled from the body of the material i.e. the material behaves like a perfect Diamagnetic. This effect is known as Meissner effect.



CRITICAL FIELD

The strength of minimum magnetic field required to just switch a material from Superconducting state to normal state is called Critical field.



- If “T” is the temperature of the superconducting material($T < T_c$)
 “ H_c ” is the critical field and
 “ H_0 ” is the field required to turn the superconductor to normal conductor at 0 K.

Then the relation for critical field (H_c) is given by

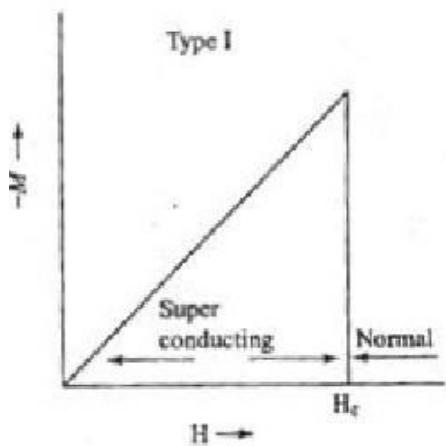
$$H_c = H_0 [1 - T^2/T_c^2]$$

TYPES OF SUPERCONDUCTORS:

Superconductors are classified into two types they are,

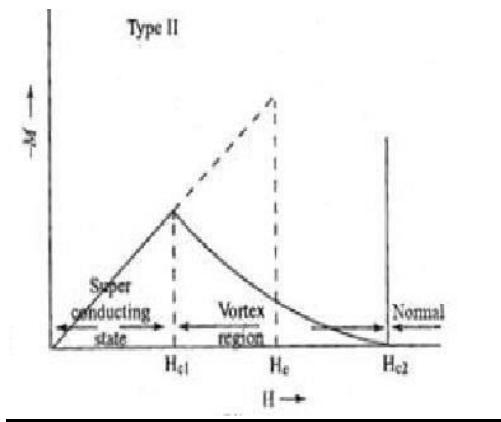
1. Type -I Superconductors(soft)
2. Type-II superconductors(hard)

Type -I Superconductors (soft)



- When magnetic field $H < H_c$, they exhibit complete Meissner effect. In the presence of external magnetic field the material is in the superconducting state and behaves as a perfect diamagnet.
- When $H > H_c$ the magnetic flux enters the material and it loses its diamagnetic property and the material comes to normal state.
- It is found that for type I superconductors the critical field values are low.

Type -II Superconductors (hard)



Where- H is the External magnetic field and M is the -ve magnetic moment.

H_{c1} and H_{c2} are the lower & higher critical fields.

- They are characterized by two critical fields H_{c1} and H_{c2} when $H < H_{c1}$ the Material is in the superconducting state and it behaves as a perfect Diamagnet.
- When $H > H_{c1}$ the flux penetrates the body and fills partially with further increase in H , the flux filling also increases thereby decreasing the diamagnetic part of the material and covers the entire body when H becomes equal or greater than a second critical value H_{c2} .the material then turns into a normal conductor. H_{c1} and H_{c2} are called lower critical field and upper critical field respectively.
- When H lies between H_{c1} and H_{c2} the material loses some of its diamagnetic properties and enters into a mixed state called vortex state.
- When $H > H_{c2}$ the material enters into the normal state .it is found that for type -II superconductor's critical field values are high.

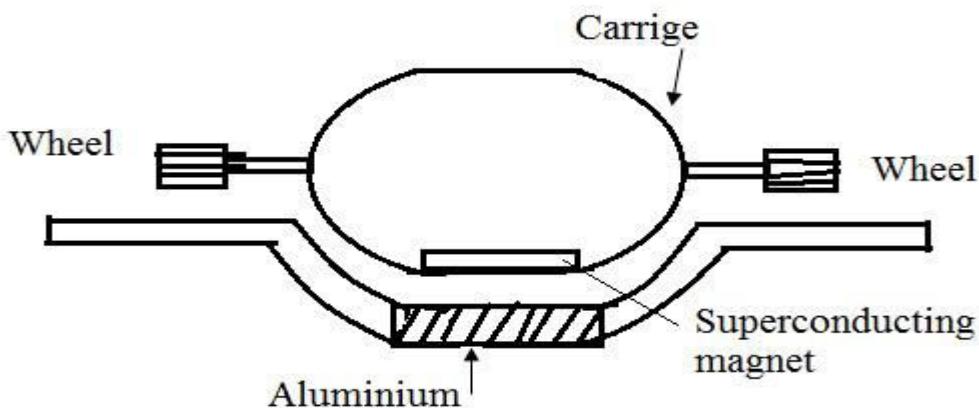
Note: The number of magnetic lines flowing per unit area is called flux. **High temperature superconductivity:**

“Superconductors having higher critical temperatures are called high temperature superconductors”.

All high temperature superconductors are not pure metals, but they are different types of oxides of copper. And bear a particular type of crystal structure called Pervoskite crystal structure. It is found that, the critical temperature is higher for those materials having more number of copper oxygen layers. It is found that the formations of super currents in high temperature superconductors are directional dependent.

The super currents are strong in copper oxygen planes and weak in a direction perpendicular to the copper oxygen planes. **Applications superconductors:**

Maglev vehicles:



Magnetically levitated vehicles are called maglev vehicles. The vehicle is levitated above the tracks hence friction is eliminated.

- Maglev vehicles do not slide over the tracks.
- The maglev vehicles work on the principle of Meissner effect.
- Superconducting magnets are built onto the base of the vehicle, and current is passed through the guideway.
- Magnetic field is produced by the superconducting magnet and current in the guideway.
- Now, enormous repulsion happens between these two magnetic fields as the result vehicle will be set a float.
- The vehicle is levitated to about 10 to 15cm above the guideway.
- When the vehicles runs on the guideway, the wheels are retracted into its body, while stopping the wheels are drawn out and the vehicle slowly settles on the guideway.

SEMICONDUCTORS

Semiconductors have conductivity in the range intermediate between those of conductors and insulators.

The resistivity of semiconductors lie in the range 10^{-6} to $10^{+8} \Omega\text{m}$.

Elements such as Silicon(Si), Germanium (Ge) , Selenium (Se) and compounds such as Gallium Arsenide (GaAs), Gallium Phosphide (GaP) are some examples of semiconductors.

Conductivity of Semiconducting Materials:

Carrier concentration in an intrinsic semiconductor:

The number of electrons in the conduction band per unit volume of the material is called electron concentration (N_e) given as,

$$N_e = \frac{4\sqrt{2}}{h^3} (\pi kT m_e^*)^{3/2} e^{\frac{(E_F - E_g)}{kT}} \dots\dots\dots (1)$$

Where m_e^* is the effective mass of electron E_F is the Fermi Energy and E_g is the energy gap.

Similarly, the number of holes in the valence band per unit volume of the material is called hole concentration. (N_h)

$$= \frac{4\sqrt{2}}{h^3} N_h (\pi kT m_h^*)^{3/2} e^{\frac{(E_F - E_g)}{kT}} \dots\dots\dots (2)$$

Where m_h^* is the effective mass of holes E_F is the Fermi Energy and E_g is the energy gap.

T is the absolute temperature and h is the Planck's constant.

In general, the number of charge carriers per unit volume of the material is called carrier concentration.

The charge carriers, both electrons and holes contribute to the conductivity of the semiconductor.

The conductivity of a semiconductor is given by the expression $\sigma = e [(N_e \mu_e) + (N_h \mu_h)]$ where N_e and N_h are the carrier concentrations of electrons and holes respectively.

μ_e and μ_h are mobility of electrons and holes respectively and 'e' is the magnitude of charge of the electron.

Law of Mass Action for Semiconductors:

Law of mass action says that, for a given semiconductors material either intrinsic or extrinsic, the product of the charge carrier concentration remains a constant at any given temperature, even if the doping is varied. We have the equations for N_e and N_h as

$$N_e = \frac{4\sqrt{2}}{h^3} (\pi K T m_e^*)^{3/2} e^{-\frac{(E_F - E_g)}{kT}} \dots \quad (1) \text{ and}$$

$$N_h = \frac{4\sqrt{2}}{h^3} (\pi K T m_h^*)^{3/2} e^{-\frac{(E_F - E_g)}{kT}} \dots \quad (2)$$

In the above expressions, we see that N_e and N_h depends on E_F .

Consider the product of N_e and N_h ,

$$N_e \cdot N_h = 32 h \cdot (\pi K T)^3 \cdot (m_e m_h)^{3/2} \cdot e^{-\frac{(E_F - E_g)}{K T}}$$

The above equation shows that N_e and N_h do not depend on E_F , but remains a constant.

$N_e \cdot N_h = \text{constant}$	Therefore,
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This condition is applicable to both intrinsic and extrinsic semiconductors.

In the case of an intrinsic semiconductor,

$$N_e = N_h = n_i$$

Where n_i is the intrinsic charge carrier concentration. Therefore,

$$N_e \cdot N_h = n_i^2 = \text{constant.}$$

QUESTION BANK

- 1) Describe Type I and Type II superconductors
- 2) Explain the terms a) relaxation time, b) mean collision time, c) mean free path, and drift velocity
- 3) Discuss in brief BCS theory of superconductivity
- 4) Write a note on maglev vehicles
- 5) Describe how quantum free electron theory has been successful in overcoming the failure of classical free electron theory.

- 6) Define Fermi energy and Fermi factor. Discuss the variation of Fermi factor with temperature and energy

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MODULE-3

LASER

LASER: Light Amplification by Stimulated Emission of Radiation.

- It was invented by American Scientist Maiman in the year 1960.
- Today there are about hundred different kinds of lasers.

Characteristics of Laser beam

The following important properties of laser make it different from other ordinary source of light.

1) Laser is highly monochromatic.

The laser beam is emitted in a very narrow frequency band.

2) Laser light is spatially coherent.

The laser is highly coherent due to stimulated emission of radiation.

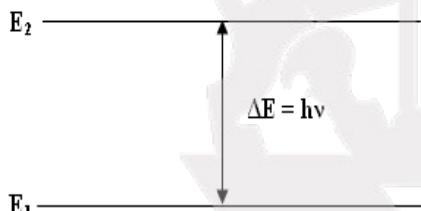
3) Laser light extremely high directionality or unidirectionality.

The laser beam has very small divergence due to the resonant cavity. Hence light intensity does not decrease as fast with distance as it does in ordinary source of light.

4) The laser beam is extremely bright or intense.

Light from laser is much brighter than other ordinary sources of light.

Principle and Production of Laser:



Radiation interacts with matter under appropriate conditions. The interaction leads to an abrupt transition of the Quantum system such as an atom or molecule from one energy state to another. If the transition is from a higher state to a lower one, the system gives out a part of its energy and if the transition is in reverse direction, then it absorbs the incident energy.

In order to understand the manner in which radiation can interact with matter, consider two energy states E_1 and E_2 of a system. If the energy difference between the two energy levels is ΔE ,

Then $\Delta E = E_2 - E_1$

Max planck suggested that if an electromagnetic radiation of frequency 'v' with value

$$v = \frac{\Delta E}{h} = \frac{E_2 - E_1}{h} \quad \text{-----(1)}$$

is incident on the system which is in the energy state E_1 , then the system moves from E_1 to the energy state E_2 (from lower to higher) by absorbing the energy. On the other hand, if the system is in state E_2 , then it emits an electromagnetic radiation of frequency ' ν ' given by eq(1) then energy of the system changes to E_1 .

There are three possible ways through which interaction of radiation and matter can take place:

- Induced Absorption
- Spontaneous Emission
- Stimulated Emission

Induced Absorption:

It is a process in which an atom in the ground state undergoes transition to the higher energy state by absorbing an incident photon.

The process can be represented as

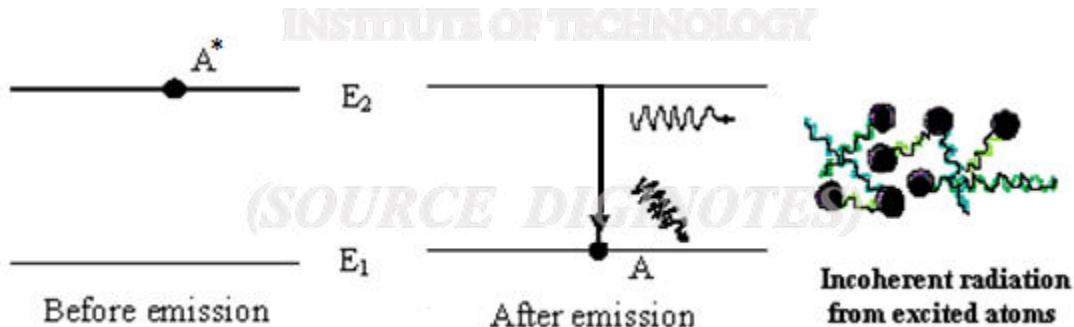


Where Atom* indicates an excited atom



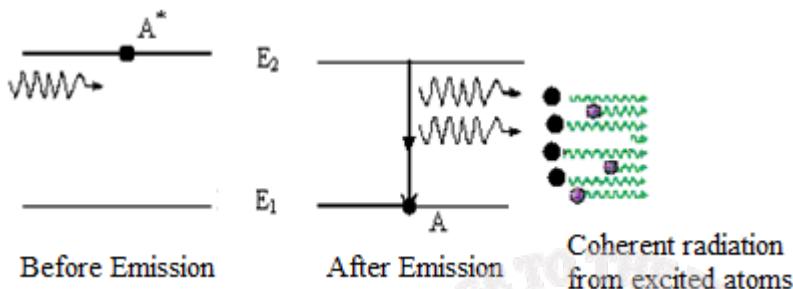
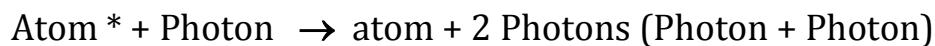
Spontaneous Emission:

It is a process in which an atom in the excited state undergoes transition to the ground state by emitting a photon without any aid of external agency. As shown in the figure, consider an atom in the excited state E_2 . It makes a transition to the ground state E_1 by the emission of a photon of energy $h\nu$. It may be represented as



Stimulated Emission:

It is a process in which an atom in the excited state undergoes transition to the ground state by the influence of a passing photon. During this process a stimulated photon is emitted along with the incident photon and these photons are found to be coherent.



Einstein's Coefficients:

(Expression for energy density of photons in terms of Einstein's Coefficients under thermal equilibrium condition)

- * Consider two energy states E_1 and E_2 .
- * Let E_1 be the lower energy state and E_2 be the higher energy state.
- * Let N_1 be the number of atoms per unit volume in the energy state E_1 and N_2 be the number of atoms per unit volume in the energy state E_2 .
- * Let E_ν be the energy density of radiations.

1. Induced Absorption:

In this case, an atom in the lower energy state E_1 undergoes transition to the higher energy state E_2 by absorbing a photon.

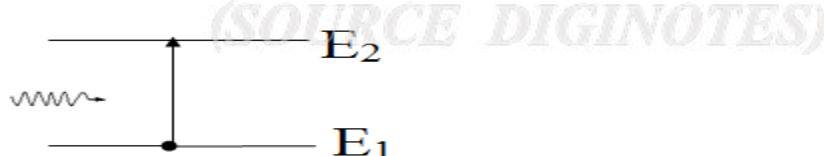
The number of such absorptions per unit time per unit volume is called Rate of induced absorption.

Rate of induced absorption $\propto N_1 E_\nu$

$$= B_{12} N_1 E_\nu \dots \dots \dots (1)$$

Where N_1 is number of atoms in the state E_1 ,

E_ν is the energy density in frequency range ν and $\nu + d\nu$ and B_{12} is called Einstein coefficient of induced absorption.

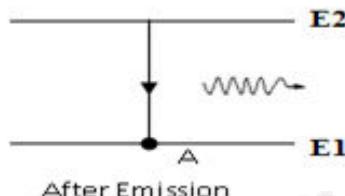


2. Spontaneous Emission:

In this case, an atom in the higher energy state E_2 undergoes transition to the lower energy state E_1 by emitting a photon without any aid of external agency. The number of such spontaneous emissions per unit volume per unit time is called Rate of spontaneous emission.

Rate of spontaneous emission $\propto N_2$

$$= A_{21} N_2 \dots\dots (2)$$

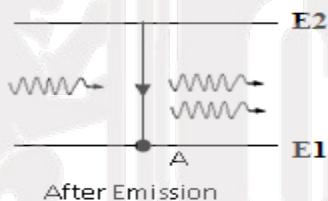


Where, A_{21} is called Einstein's coefficient of spontaneous emission.

3. Stimulated Emission:

In this case, an atom in the higher energy state E_2 undergoes transition to the lower energy state E_1 under the influence of passing photon.

During this process a stimulated photon is emitted along with the incident photon.



The number of such stimulated emissions per unit time per unit volume is called the Rate of stimulated emission.

Rate of stimulated emission $\propto N_2 E_\nu$

$$= B_{21} N_2 E_\nu \dots\dots (3)$$

Where, B_{21} is called the Einstein coefficient of stimulated emission

At thermal equilibrium, the number of upward transitions must be equal to the number of downward transitions.

Rate of absorption = Rate of spontaneous emission + Rate of stimulated emission

$$B_{12} N_1 E_\nu = A_{21} N_2 + B_{21} N_2 E_\nu$$

$$E_\nu (B_{12} N_1 - B_{21} N_2) = A_{21} N_2$$

$$E_\nu = \frac{A_{21} N_2}{B_{12} N_1 - B_{21} N_2}$$

$$E_v = \frac{A_{21}N_2}{B_{21}N_2 \left[\frac{B_{12}N_1}{B_{21}N_2} - 1 \right]} \quad \dots \dots \dots (4)$$

By Boltzmann law, we have

$$\frac{N_1}{N_2} = e^{\left(\frac{E_2 - E_1}{KT}\right)} = e^{\left(\frac{h\nu}{KT}\right)}$$

\therefore (4) becomes,

$$E_v = \frac{A_{21}}{B_{21}} \left| \frac{1}{\frac{B_{12}}{B_{21}} \frac{hv}{kT} - 1} \right| \quad \dots \quad (5)$$

According to Planck's law, the equation for energy density of radiation at given temperature, E_ν is

$$E_V = \frac{8\pi h\nu^3}{C^3} \left[\frac{1}{e^{\frac{h\nu}{kT}} - 1} \right] \quad \dots \dots \dots (6)$$

Comparing equation (5) and (6), we get

$$\frac{A_{21}}{B_{21}} = \frac{8\pi h v^3}{c^3} \text{ and } \frac{B_{12}}{B_{21}} = 1 \text{ or } B_{12} = B_{21}$$

This means that the probability of induced absorption is equal to the probability of stimulated emission. By neglecting the subscripts, A_{21} and B_{21} can be represented as A and B respectively i.e., $A_{21} = A$ and $B_{21} = B$.

Then at thermal equilibrium, the equation for energy density is

$$E_v = \frac{A}{B \left[e^{\frac{hv}{kT}} - 1 \right]}$$

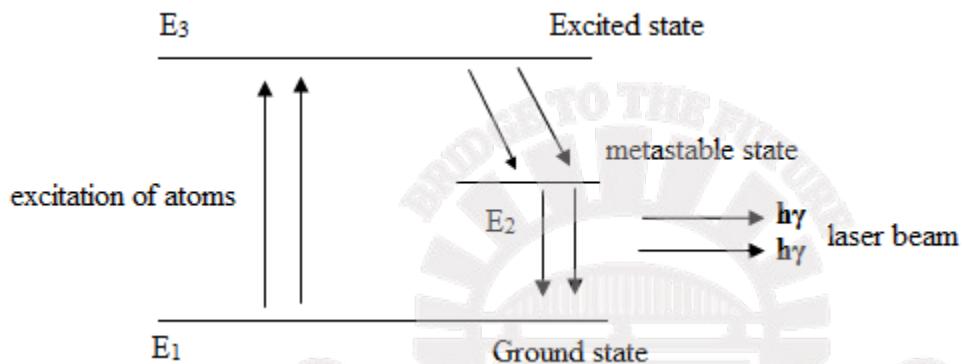
Energy states of atoms:

Ground state: It is the lowest possible energy state of an atom which is the most stable state. Atoms can remain in this state for unlimited time.

Excited state: These are the possible energy states of an atom which are higher than the ground state. Atoms remain in these energy states for a very short time called the lifetime typically of the order of 10^{-8} s to 10^{-9} s.

Metastable State: These are excited states of an atom with relatively large lifetime of the order of 10^{-3} s.

CONDITION FOR LASER ACTION: *(Population inversion and metastable state)*



"Population inversion is the state of a system at which the population of a particular higher energy state is more than that of a lower energy state". To achieve population inversion a special kind of excited state called **metastable state** are used and it can be explained as follows.

Atoms in the ground state undergo transition to the higher energy state E₃ by absorbing incident photons. Since E₃ state is ordinary excited state, atoms in the E₃ state don't stay over a long time, as a result the atoms immediately undergoes spontaneous downward transitions to the E₂ state. Since E₂ is metastable state, atoms in the E₂ state stay over a long duration of about 10^{-2} to 10^{-3} seconds. Under these conditions a stage will br reached where the population in E₂ overtakes that of E₁. This condition is called population inversion.

REQUISITES OF A LASER SYSTEM:

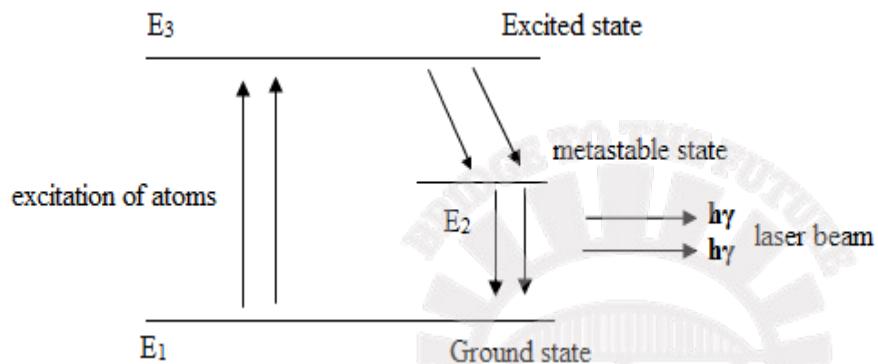
There are three requisites of laser systems.

1. An excitation source for pumping action
2. An Active medium to achieve population Inversion
3. An Optical resonant cavity or laser cavity

1. An Excitation source for pumping action: The process of supplying energy to the medium to excite an atom from lower energy state to a higher energy state is called pumping.

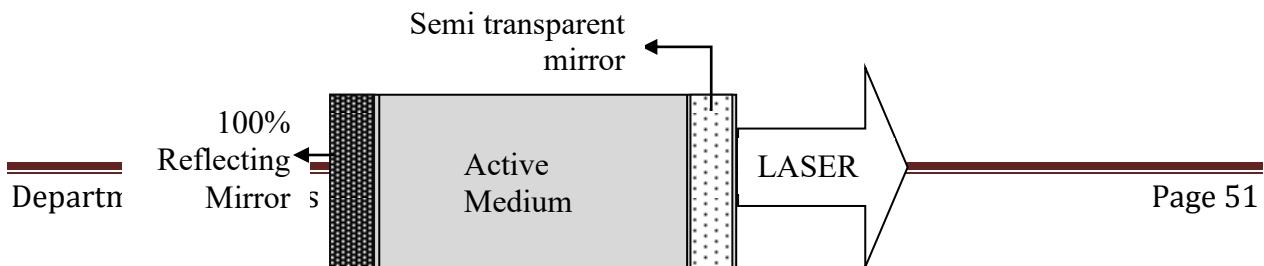
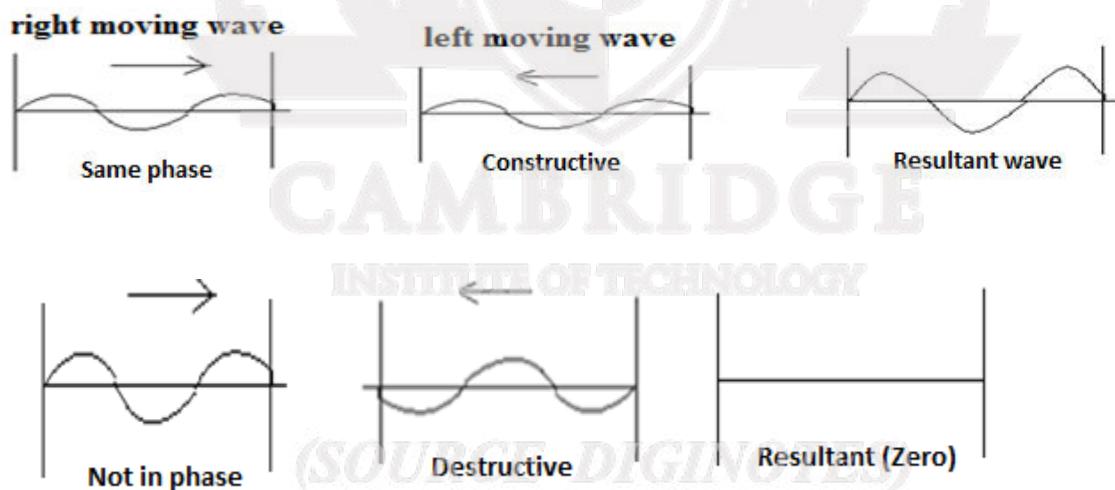
Energy can be supplied to atoms in different forms like Optical pumping, Electrical pumping and Chemical Pumping

2. An active medium to achieve Population Inversion:



Active medium refers to the medium in which the laser action takes place. The energy levels of the atoms or molecules which are involved in laser action are identified. Accurate information about the energy levels and their lifetimes helps in identifying the level between which the population inversion can be achieved.

3. An Optical resonant cavity or laser cavity:



A laser device consists of an active medium bound between two mirrors. The mirrors reflect the photons to and fro through the active medium. A photon moving in a particular direction represents a light wave moving in the same direction. Thus, the two mirrors along with the active medium form a laser cavity.

CARBON DIOXIDE LASER [CO₂ LASER]:

Construction and working with the help of energy level diagram:

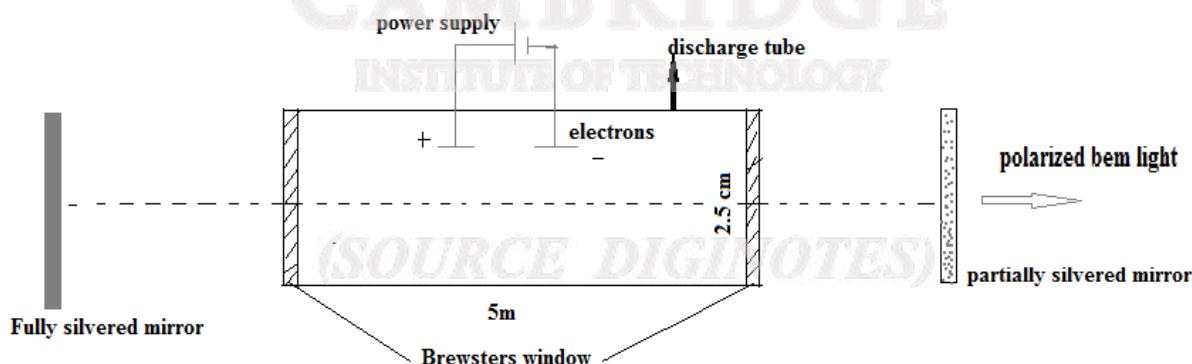
Introduction:

CO₂ Lasers belong to the class of molecular gas laser. This operates in the far IR region involving a set of **rotational vibrational transitions**.

CO₂ laser was developed by C.K.N. Patel in the year 1963.

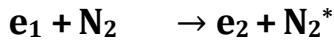
Construction:

- 1) A CO₂ laser consists of a discharge tube of length 5m and diameter nearly 2.5cm.
- 2) The tube is filled with a mixture of CO₂, N₂ and He gases in the ratio of 1:2:3
- 3) The pressure inside the tube is 6-17 torr.
- 4) Also water vapour is added to the discharge tube. Water vapour additives help to deoxidize CO to CO₂ in case CO₂ molecules break into CO and O during discharge.
- 5) The two ends of the tube are sealed with flat Quartz plate which functions as Brewster window(to get the linearly plane polarized light)
- 6) Two optically plane mirrors are fixed on either sides of the tube, one of the mirrors is fully silvered and can reflect the light 100% and other is partially silvered helps to transmission of laser beam.



Working:

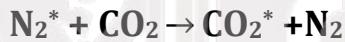
When the suitable voltage is applied across the two electrodes, a glow discharge of the gases is initiated in the tube. During discharge, electrons get free from the gas atoms and starts moving towards the positive electrode and begin colliding with N_2 molecule in their path. The collision belongs to collision of 1st kind. N_2 molecules are raised to the 1st vibrational level $v = 1$ which is a metastable state. The process is represented as



Where, e_1 and e_2 are energy values of the electrons before and after collision.

N_2 and N_2^* are energy of N_2 molecules in ground state $v = 0$ and $v = 1$ state respectively. Hence population inversion is achieved in $v = 1$ of N_2 and molecules stay for about 10^{-3} to 10^{-2} seconds.

There is a close coincidence in energy of 001 state of CO_2 and $v = 1$ state of N_2 . Therefore, N_2^* collides with CO_2 at ground state. This leads to the transition of CO_2 to 001 state and de-excitation of N_2 to ground state. This type of collision belongs to collision of 2nd kind. 001 state is metastable state for CO_2 molecule. Hence population inversion is achieved in CO_2 molecule in 001 state. This process can be represented by



Where,

N_2^* and N_2 are energies of N_2 molecule in $v = 1$ state and ground state respectively.

CO_2 and CO_2^* are energies of CO_2 molecule in ground state and 001 state respectively

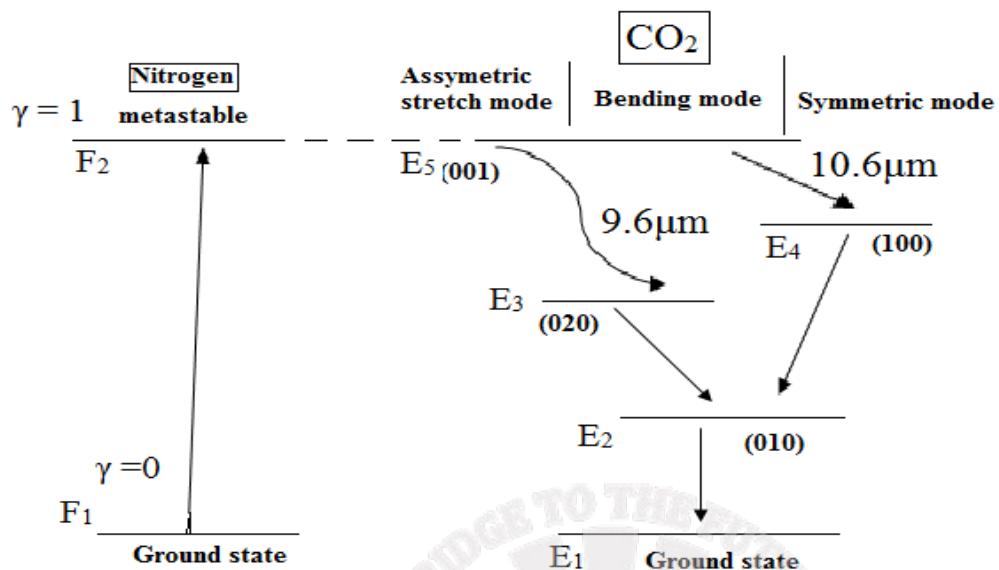
Let us designate the (010) state, (020) state, (100) state and (001) state as E_2 , E_3 , E_4 , E_5 levels respectively as shown in the figure.

Once population inversion is established in E_5 level the CO_2 molecule undergoes stimulated emission to E_3 and E_4 levels:

- (a) Transition from E_5 level to E_4 with a wavelength of $10.6 \mu m$ which is in far IR region.
- (b) From E_5 level to E_3 level with a wavelength of $9.6 \mu m$ which is also in far IR region.

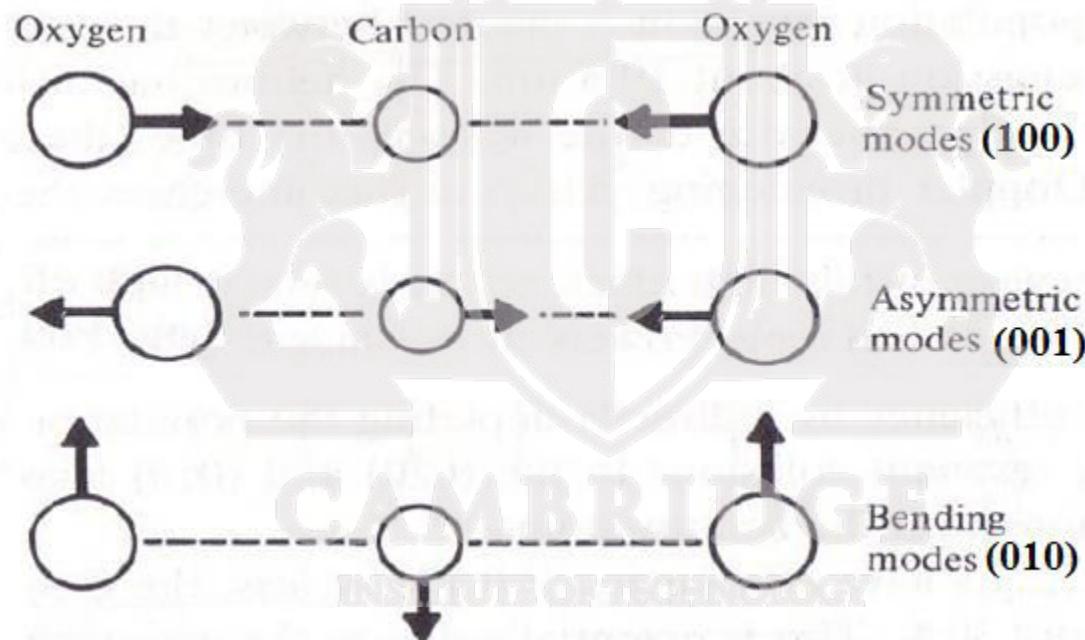
Molecule (CO_2) from E_4 level and E_3 level undergoes inelastic collision with unexcited CO_2 molecules and de-excite to E_2 level. Later CO_2 molecule in E_2 level undergoes collision with He and water vapour molecules and came down to the ground state E_1 .

CO_2 laser has an efficiency of up to 30%.



VIBRATIONAL ENERGY LEVELS OF A CO_2 MOLECULE:

A carbon dioxide molecule has two oxygen atoms between which there is a carbon atom. It has 3 different modes of vibration.



- 1) **Symmetric stretching mode:** In this mode, oxygen atoms vibrate along the molecular axis, either approaching towards or departing from the carbon atom . The carbon atoms remains stationary.
The vibration state is given by (100)
- 2) **Asymmetric stretching mode:** During the vibration in this mode, all the 3 atoms oscillate along the molecular axis. But, the two oxygen atoms move in one direction while the carbon atom moves in the opposite direction.

This vibrational state represented as (001).

- 3) **Bending mode:** In bending mode, all the 3 atoms oscillate normal to the molecular axis. While vibrating, the two oxygen atoms pull together in one direction as the carbon atom is displaced in the opposite direction. The state is (010)

SEMICONDUCTOR LASER (GALLIUM ARSENIDE LASER):

Principle: A Semiconductor diode laser is a specially fabricated p-n junction diode which emits light when it is forward biased. The 'n' junction is the active medium.

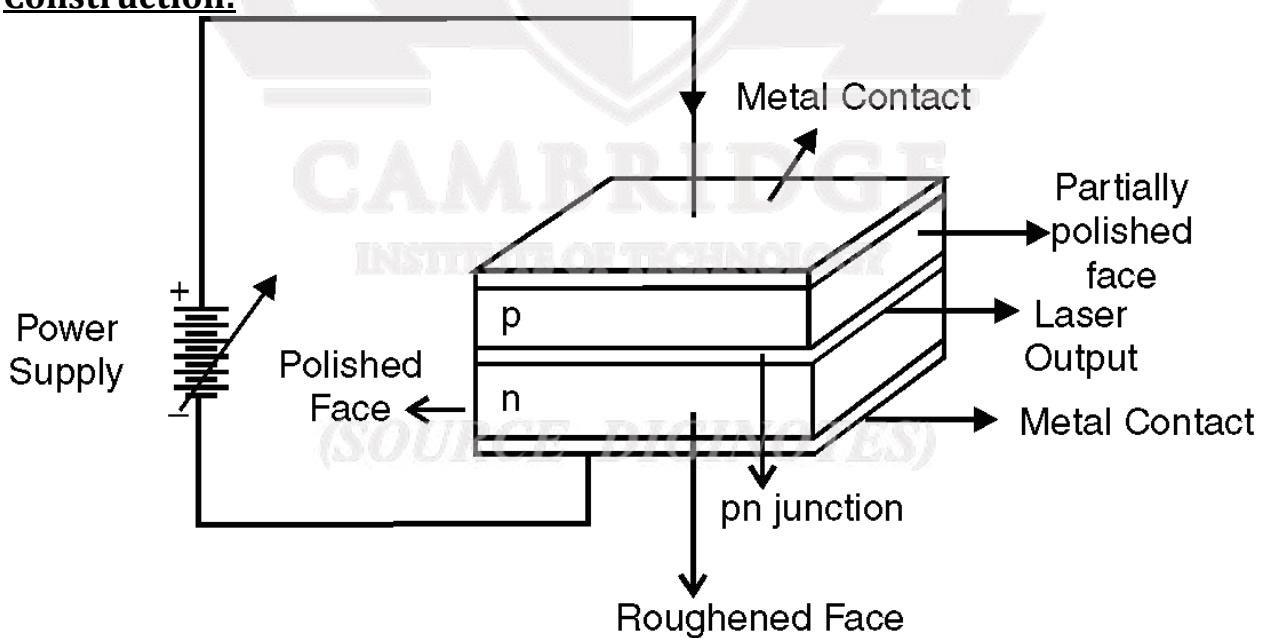
Recombination is the main principle: Recombination is the process wherein electrons and holes meet each and result in the release of heat energy. It's actually the transition of an electron from conduction band to valence band.

Recombination occurs due to forward biasing the system and occurs in the p-n junction (depletion region). Hence it is called as **Active medium**.

We make use of **Direct Band gap and degenerate semiconducting** materials. Direct band gap semiconductors are the materials where, there is no loss of energy and the released energy will be in visible region. Semiconductors that are highly doped are called degenerate semiconductors. The p-region is degenerate in holes and the n-region in electrons.

Example GaAs (Gallium Arsenide), CdSe (Cadmium Selenide).

Construction:



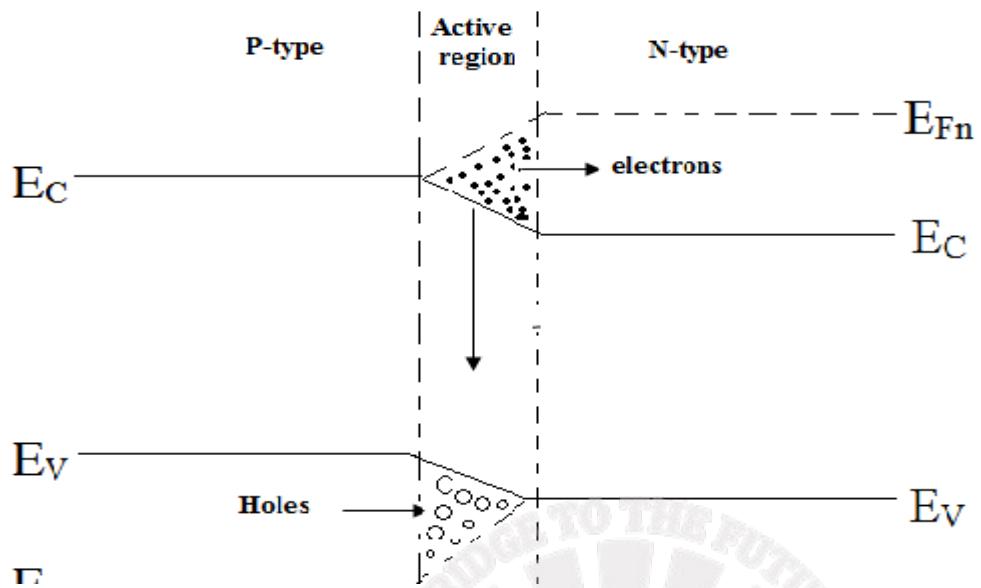
- GaAs diode is a single crystal of Ga and As.
- Consists of heavily doped n and p sections.
- N-section is formed by doping with Tellurium and p-section with Zinc.
- Doping concentration is 10^{17} to 10^{19} dopant atoms/cm³
- Size of the diode is very small. Sides are 1mm and junction width is 1μm to 100μm.
- A pair of parallel planes is polished and these play the role of reflecting mirrors. They provide sufficient reflection to sustain the lasing action.
- Other two sides are roughed surface to suppress the reflections of the photons.
- End surfaces of p-n sections parallel to the plane of junction are provided with the electrodes in order to facilitate application of a forward bias voltage with the help of voltage source.

Working:

- Suitable forward bias voltage is applied to the diode to overcome the potential barrier. Due to forward biasing, more and more electrons are injected into the n-region. This leads to the increase in population of electrons in n-region and population of holes in the p-region. When the current crosses certain value called threshold current, electrons from n-type come to higher energy level of the depletion region and population inversion is attained.
- Once the populations of charge carriers in the depletion region increases, the electrons are made to recombine with the holes in the lower energy level of depletion region.
- At this stage, a photon released by spontaneous emission may trigger stimulated emissions over a large no of recombinations leading to the buildup of laser radiation of high power.
Thus, the current flow provides pumping in semiconductor laser.
- The wavelength of emitted light is

$$\lambda = \frac{hc}{E_g} = \frac{6.626 \times 10^{-34} \times 3 \times 10^8}{1.4 \times 1.6 \times 10^{-19}} = 8874 \text{ Å}^\circ$$

The energy gap of Ga As is 1.4 eV.

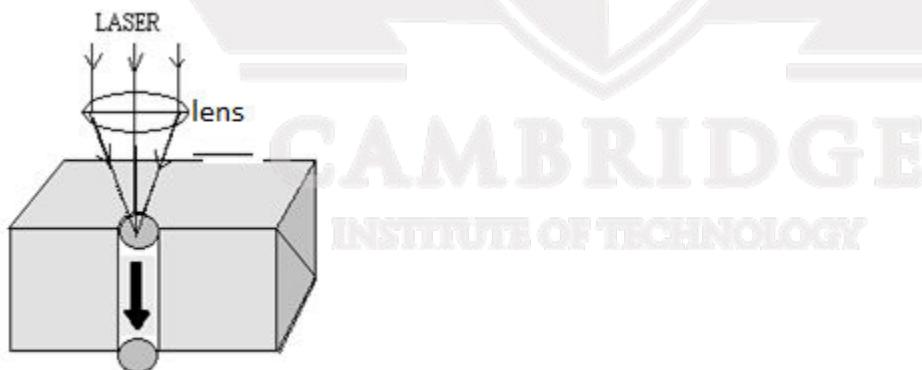


Applications of semiconductor laser:

- 1) Used in optical communication
- 2) Used as reading devices for compact disc players.
- 3) Semiconductor lasers are used in laser printers.
- 4) Semiconductor lasers are used in medicine, interferometry and barcode scanners.

APPLICATIONS OF LASERS:

1) Laser drilling:



(SOURCE DIGINOTES)

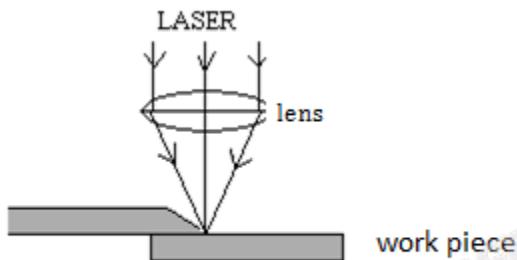
Drilling of holes is achieved by subjecting the material to powerful light pulses. The pulses will be of 10^{-4} to 10^{-3} second duration. The heat generated by the pulse evaporates the material locally and thus makes a hole.

Nd-YAG (Neodymium Yttrium Aluminium Garnet) laser is used to drill

holes in metals whereas Co₂ laser is used in both metallic and Non-metallic materials.

This process has high accuracy, ability to produce holes of small diameter (0.5 to 0.5mm) , wear out of tools is avoided.

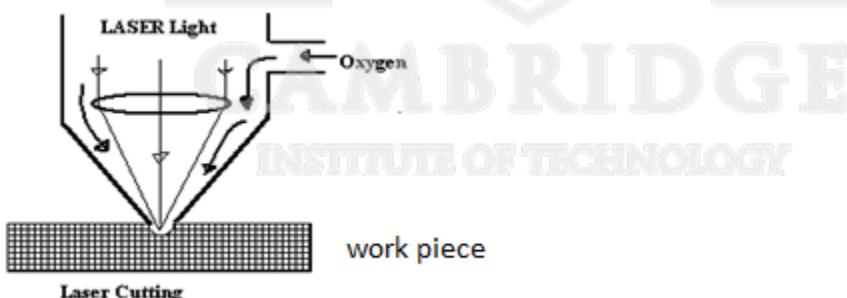
2) Laser welding:



In laser welding, the laser beam is focused on the spot which is to be welded. Due to the heat generated, the material melts. The heat produced by the beam is so intense that impurities in the material float up on the surface. On cooling, the material becomes a homogenous solid structure. This makes stronger joint. Co₂ laser is used for laser welding.

Using this technique, spots can be located precisely and no foreign material has chance to get into the welded joint.

3) Laser cutting:



Laser cutting of metals is generally done by blowing oxygen gas along with the laser beam. The laser focusing part is surrounded by nozzle into which oxygen gas is fed. The combustion of gas burns the metal and the tiny splinters along with the molten part of the metal will be blown away by the oxygen jet. The blowing action increases the depth and also speed of cutting. In laser cutting, the cut edges will be of very high quality. Usually

CO_2 laser is used for laser cutting.

- a) The cutting process could be programmed which results in high production rates.
- b) The quality of cutting is very high.
- c) There will be no thermal damage and chemical change when the cutting is done in inert atmosphere.
- d) Cutting a complicated profile even in 3-dimension is possible.

MEASUREMENT OF POLLUTANTS IN THE ATMOSPHERE:

Various pollutants present in the atmosphere include oxides of nitrogen, carbon dioxide, carbon monoxide, sulphur dioxide, Dust, smoke, etc. Using LASER one can study and measure the pollutant concentration and other aspects in atmosphere. The data obtained by conventional method is not the real time data because the atmosphere is subjected to slow and continuous variation. This limitation is overcome when measurements are done using laser.

In the application of laser for measurement of pollutants, laser is made use the way a RADAR system is used hence it is often referred as LIDAR (LIGHT DETECTION AND RANGING).

LIDAR operates on the same principle as RADAR except that it uses light rather than radio waves to collect information.

There are 3 types of LIDAR

- 1) Range finders: used to determine the distance of a solid or hard target
- 2) Differential absorption LIDAR (DIAL): used to measure chemical concentrations in the atmosphere.
- 3) Doppler LIDAR: used to measure the velocity of a moving target.

LIDAR (light detection and ranging) is used in the measurement of atmospheric pollutants

LIDAR can give information about the distance and velocity of the pollutant object.

A LIDAR system contains transmitting part and receiving part.

The transmitting part consists of pulsed laser and receiving part consists of the following:

- a) A concave mirror which receives the reflected light pulses.
- b) A photo detector which converts optical energy to electrical energy.
- c) A narrow band filter which cuts off the background noise and extraneous light.
- d) A data processor which gives information about the dimensions of the object.

While measurements are carried out, the laser beam undergoes scattering at places where pollutants are to be measured. A back scattered light is received

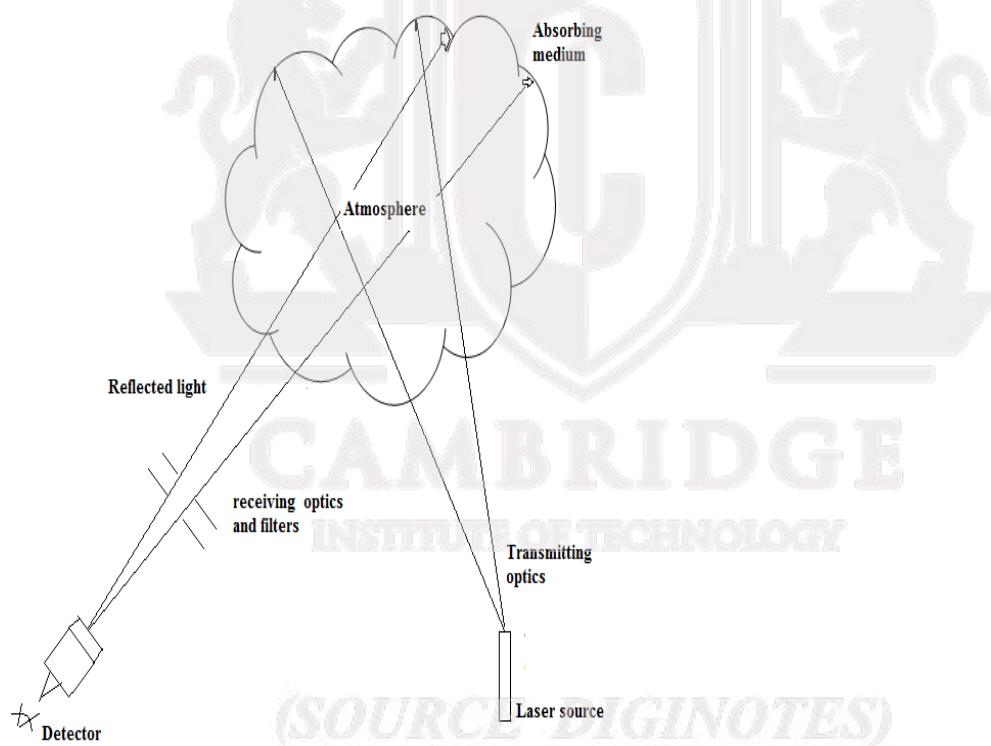
by the concave mirror and finally the compositions of the pollutants of the sample can be measured by the following method.

1) Absorption technique:

The laser beam is passed through the sample collected from the atmosphere. When the beam passes through the sample, it undergoes absorption. Depending upon the absorption pattern, composition of the pollutants can be determined.

2) Raman Back Scattering:

In this method also laser beam is passed through the sample and spectrum of the transmitted light is obtained. Due to the Raman scattering, in the spectrum, we will see not only one but several lines; one line of high intensity corresponding to the incident light's wavelength. The other lines of low intensity lie symmetrically to this line. These additional spectral lines are called side bands. This depends on the oscillating frequencies of different types of molecules. Thus by observing Raman spectra of the back scattered light in the sample, the composition of pollutants can be measured.



HOLOGRAPHY:

Holography was discovered by Dennis Gabor in 1948.

Holography is a process of capturing pictorial details of 3-dimensions on a 2-dimensional recording aid by using the phenomenon of interference".

The technique amounts for complete recording and hence it is called Holography after the Greek words 'Holos' and 'Graphos' which means 'complete' and 'writing' respectively. The recording aid is called a hologram.

PRINCIPLE: The principles underlying holography are interference and diffraction. Therefore, to produce hologram highly coherent beams are required and laser serves the purpose.

Holography can be explained in two steps

- 1) Recording of a Hologram
- 2) Reconstruction of the Hologram.

Recording of a Hologram:

*A broadened laser beam from a laser source is obtained. The object whose hologram is to be recorded and a mirror are placed one next to the other as shown in fig.

*The expanded laser beam is then directed on this arrangement in which a part of the beam is incident on the mirror and the rest of the beam is incident on the object.

* A photographic plate is placed in such a position that it receives the light reflected from the mirror and the object.

* The reflected light from the mirror is incident on the photographic plate and will be in the form of plane wavefronts. This is called **reference beam**.

* The reflected light from the object gives rise to spherical wavefronts as every point on the object scatters the incident light. This is called **object beam**.

* The surface of the photographic plate is photo sensitive and responds to the resultant effect of interference between the spherical wavefronts of the object beam and the plane wavefronts of the reference beam.

* The superposition of these two beams (Reference beam + Object beam) produces an interference which is recorded on the plate. The pattern consists of concentric circular rings called **GABOR ZONE PLATE**. The recording consists of countless number of zone plates.

* The photographic plate carrying interference pattern is called a **hologram**.

Reconstruction of the image:

*The original laser beam is directed at the hologram in the same direction as the reference beam was incident on it at the stage of recording.

* This beam undergoes diffraction in the hologram. Because of diffraction, secondary wavelets originate from each zone plate which interferes constructively in certain directions and generates both real and virtual image.

* Each and every zone plate participates in this process to generate the image of the object as the beam is incident on the entire hologram.

Applications of Holography:

- 1) Holographic interferometry
- 2) Holographic Diffraction Gratings
- 3) Information coding
- 4) Thick holograms
- 5) Acoustical Holography
- 6) It finds application in microscopy called holographic microscopy
- 7) It is used to produce three dimensional images in cinematography

NOTE:

1. The ratio of populating two energy states is given by the Boltzmann factor,

$$\frac{N_1}{N_2} = e^{-\frac{hv}{kT}} = e^{-\frac{\Delta E}{kT}}$$

2. Let the energy difference between two states is ΔE which is equal to the energy of each of the emitted photon. If M is the no of photons emitted per second. And P is the power generated in each pulse then.

$$\text{Power (P)} = N \times \Delta E$$

Energy of each pulse can be written as.

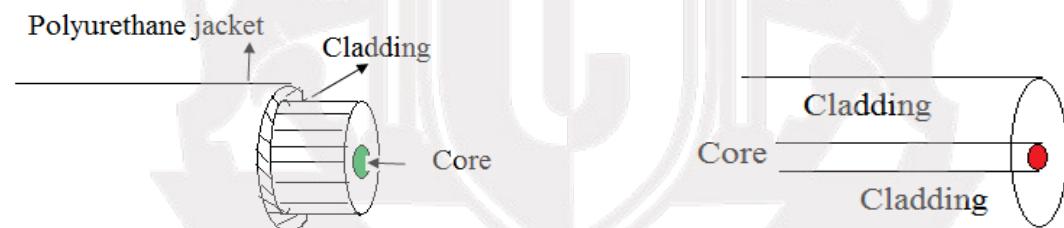
$E = \text{Power} \times \text{duration of the pulse.}$

$$E = P \times t$$

OPTICAL FIBERS

- Fiber optics is an overlap of science and technology which deals with transmission of light waves into optical fibers, their emission and detection.
- It is a waveguide through which light can be transmitted with very little leakage through the sidewalls.
- These are essentially light guides used in optical communications as waveguides.
- ***The principle behind the transmission of light waves an optical fiber is TIR(Total internal Reflection)***
- They are transparent dielectrics and able to guide visible and infrared light over long distances.

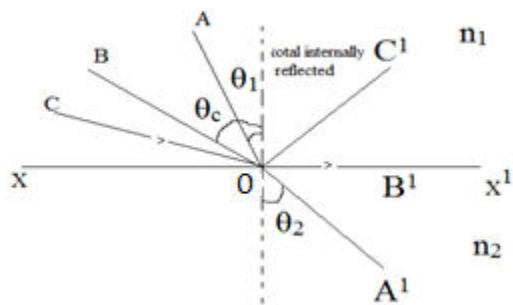
CONSTRUCTION OF OPTICAL FIBER:



- An optical fiber is cylindrical in shape
- It has two parts **a)** inner part and **b)** outer part.
- The inner part is made of glass or plastic and its cylindrical in shape, it is called **core**. Core is having high refractive index.
- Outer part is a concentric cylinder surrounding the core, and is called **cladding**. Cladding is also made of same material with little lesser refractive index.
- The polyurethane jacket is used to enclose cladding which safeguards the fiber against chemical reaction with surroundings and also crushing.
- Many fibers which are protected by individual jackets are grouped to form a cable. A cable may consist of one to several hundred such fibers.

TIR (TOTAL INTERNAL REFLECTION):

It is the principle behind the transmission of light waves in an optical fiber which is a well known optical phenomenon in physics.



A ray **AO**, travelling in a medium of refractive index n_1 is separated by the boundary XX' , from another medium of lower refractive index n_2 . So $n_1 > n_2$. The incident ray **AO** makes an angle θ_1 with the normal in the medium of refractive index n_1 . The same **AO** undergoes **refraction** into the medium of refractive index n_2 and it bends away from the normal, since $n_1 > n_2$. θ_2 is the angle made by the refracted ray with the normal.

If we increase θ_1 for certain value of $\theta_1 = \theta_c$ called critical angle, $\theta_2 = 90^\circ$, for such a case, the refracted ray grazes along the boundary of separation along **OB'** while incident ray is along **BO**.

If $\theta_1 > \theta_c$, incident ray **CO** always gets reflected back into the same medium in which it is incident on the boundary. This takes place as per the law of reflection.

For refraction, we have the Snell's law

$$n_1 \sin \theta_1 = n_2 \sin \theta_2$$

For $\theta_1 = \theta_c$ and $\theta_2 = 90^\circ$

$$n_1 \sin \theta_c = n_2 \sin 90^\circ = n_2 \quad (\sin 90^\circ = 1)$$

$$\theta_c = \sin^{-1} \left[\frac{n_2}{n_1} \right]$$

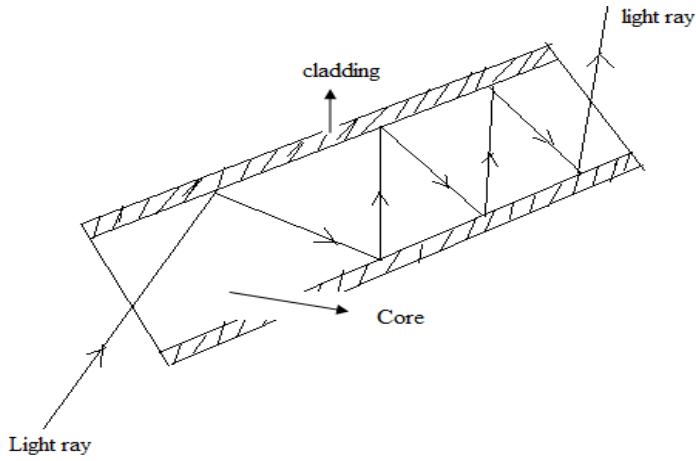
PROPAGATION MECHANISM:

Explain mechanism of light propagation in optical fibers.

(Or)

Explain how optical fibers work as waveguides.

"Optical fibers are the devices used to transmit light effectively along any desired path."

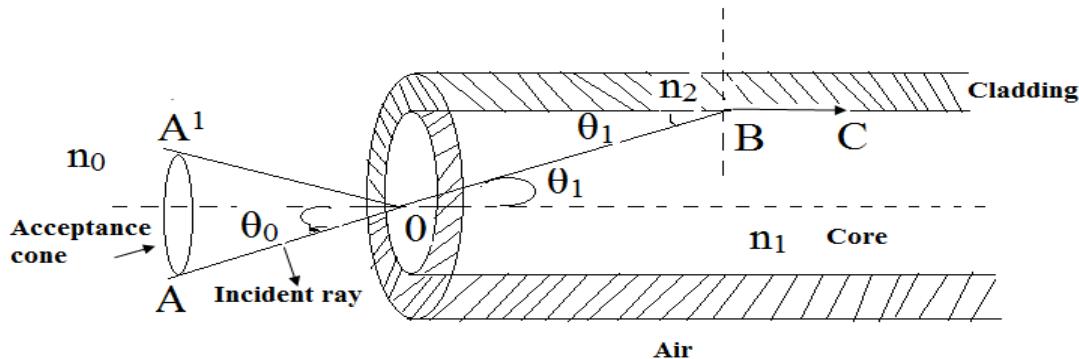


- Optical fibers work on the principle of total internal reflection (TIR)
- For total internal reflection there are two essential conditions, they are
 - 1) The light ray must pass from denser to rarer medium.
 - 2) The angle of incidence must be greater than the critical angle $i > c$
- A waveguide is a tubular structure through which energy of some sort could be guided in the form of waves.
- The waveguide as a light guide. also called fiber waveguide or fiber light guide
- An optical fiber consists of a core and cladding.
- In any optical fiber the refractive index of cladding is always lesser than that of its core to achieve TIR, i.e. R.I cladding $<$ R.I of core
- When a light is incident at one end of the fiber, it undergoes total internal reflection and finally emerges at the other end of the fiber. It is found that intensity of emergent light is almost same as that of incident light. In this way optical fibers transmit light effectively along any desired path.

RAY PROPAGATION IN THE FIBER. ANGLE OF ACCEPTANCE AND NUMERICAL APERTURE.

Q: Explain with a neat diagram Acceptance angle and numerical Aperture of an optical fiber. Hence derives an expression for numerical aperture.

(SOURCE DIGINOTES)



- Consider a ray **AO** entering into the core at an angle θ_0 to the fiber axis. Then it is **refracted along OB** at an angle θ_1 in the core and further falls at critical angle of incidence (equal to $90^\circ - \theta_1$) at **B** on the interface between core and cladding. Since the incidence is critical angle of incidence, the ray is refracted at 90° to the normal drawn to the interface i.e. **grazes along BC**.
- Any ray that enters into the core at an angle of incidence less than θ_0 will have refractive angle less than θ_1 because of which its angle of incidence $90^\circ - \theta_1$ at the interface will become greater than the critical angle of incidence and hence undergoes **total internal reflection**.
- On the other hand any ray that enters at an angle of incidence greater than θ_0 , will have to be incident at the interface at an angle less than the critical angle, it get **refracted** into the cladding region. Then it travels across the cladding and emerges into the surroundings and will be lost.
- If now **OA** is rotated around the fiber axis keeping θ_0 same, it describes a conical surface.
- Therefore if a beam converges at a wide angle into the core, then those rays which are funneled into the fiber with in this cone will only be totally internally reflected, and thus confined within for propagation..

θ_0 is called waveguide acceptance angle or the acceptance cone half angle.

$\sin\theta_0$ is called Numerical aperture (N.A) of the fiber.

The light gathering capacity of an optical fiber is known as Numerical aperture.

Condition for propagation:

Let n_0 , n_1 , n_2 be the refractive indices of surrounding medium, core and cladding respectively.

For refraction at the point of entry of the ray “AO” into the core, we can apply Snell’s law, i.e., at point A

$$n_0 \sin \theta_0 = n_1 \sin \theta_1 \quad \text{----- (1)}$$

At the point B

The angle of incidence = $90^0 - \theta_1$

Apply Snell's Law

$$n_1 \sin (90^0 - \theta_1) = n_2 \sin 90^0$$

$$n_1 \cos \theta_1 = n_2 \quad (\sin 90^0 = 1)$$

$$\cos \theta_1 = \frac{n_2}{n_1} \quad \dots \dots \quad (2)$$

Equation (1) can be written as

$$\begin{aligned} \sin \theta_0 &= \frac{n_1}{n_0} \sin \theta_1 \\ &= \frac{n_1}{n_0} \sqrt{(1 - \cos^2 \theta_1)} \\ &= \frac{n_1}{n_0} \sqrt{1 - \left(\frac{n_2}{n_1}\right)^2} \\ &= \frac{n_1}{n_0} \sqrt{\frac{n_1^2 - n_2^2}{n_1^2}} \\ &= \frac{n_1}{n_0} \frac{\sqrt{n_1^2 - n_2^2}}{n_1} \\ \boxed{\sin \theta_0 = \sqrt{\frac{n_1^2 - n_2^2}{n_0}}} \end{aligned}$$

If the medium surrounding the fiber is air then $n_0 = 1$

$$\text{Therefore, } \sin \theta_0 = \sqrt{n_1^2 - n_2^2}$$

i.e.

$$\boxed{\text{N.A} = \sqrt{n_1^2 - n_2^2}}$$

If θ_i is the angle of incidence, then the ray will propagate if $\theta_i < \theta_0$

(Or) $\sin \theta_i < \sin \theta_0$

(Or) $\sin \theta_i < \sqrt{n_1^2 - n_2^2}$

$$\boxed{\sin \theta_i < \text{N.A}}$$

→ Condition for propagation

Note: for light propagation, angle of incidence is less than θ_0

FRACTIONAL INDEX CHANGE (Δ):

The fractional index change Δ is the ratio of the refractive index difference between the core and cladding to the refractive index of core of an optical fiber.

$$\boxed{\Delta = \frac{n_1 - n_2}{n_1} \dots \dots (3)}$$

RELATION BETWEEN N.A. AND Δ :

From equation (3) $(n_1 - n_2) = n_1 \Delta \quad \dots \dots \quad (4)$

$$\begin{aligned}
 N.A &= \sqrt{n_1^2 - n_2^2} \\
 &= \sqrt{(n_1 + n_2)(n_1 - n_2)} \\
 &= \sqrt{(n_1 + n_2) n_1 \Delta} \quad \text{from eq(4)}
 \end{aligned}$$

Since, $n_1 \approx n_2$, $(n_1 + n_2) = 2n_1$

$$\text{i.e } N.A = \sqrt{2n_1^2 \Delta}$$

$$N.A = n_1 \sqrt{2\Delta}$$

MODES OF PROPAGATION:

MODE is,

- The pattern of motion in a vibrating body.
- The light ray paths along which the waves are in phase inside the fiber.
- In simple terms these modes can be visualized as the possible number of allowed paths of light in an optical fiber.

Through it is expected that all the rays which enter into the core at an angle less than the acceptance should travel in the core, it is not even theoretical. By the application of Maxwell's equation, we can get to know that, out of the light that enters into the core within the waveguide acceptance angle, only the light waves in terms of certain number of modes will be sustained for propagation in the fiber.

V-NUMBER:

"The number of modes supported for the light propagation in the optical fiber is known as V- number."

V – Number is given by

$$V = \frac{\pi d}{\lambda} \sqrt{n_1^2 - n_2^2}$$

Where, d is the diameter of the core, λ is the wavelength of light

n_1 is the R.I of the core

n_2 is the R.I of the cladding

$$(\text{Or}) \quad V = \frac{\pi d}{\lambda} N.A$$

If the fiber is surrounded by a medium of R.I n_0 , then the expression is

$$V = \frac{\pi d}{\lambda} \sqrt{\frac{n_1^2 - n_2^2}{n_0}}$$

For $V \gg 1$

$$\boxed{\text{Number of modes} = \frac{V^2}{2}}$$

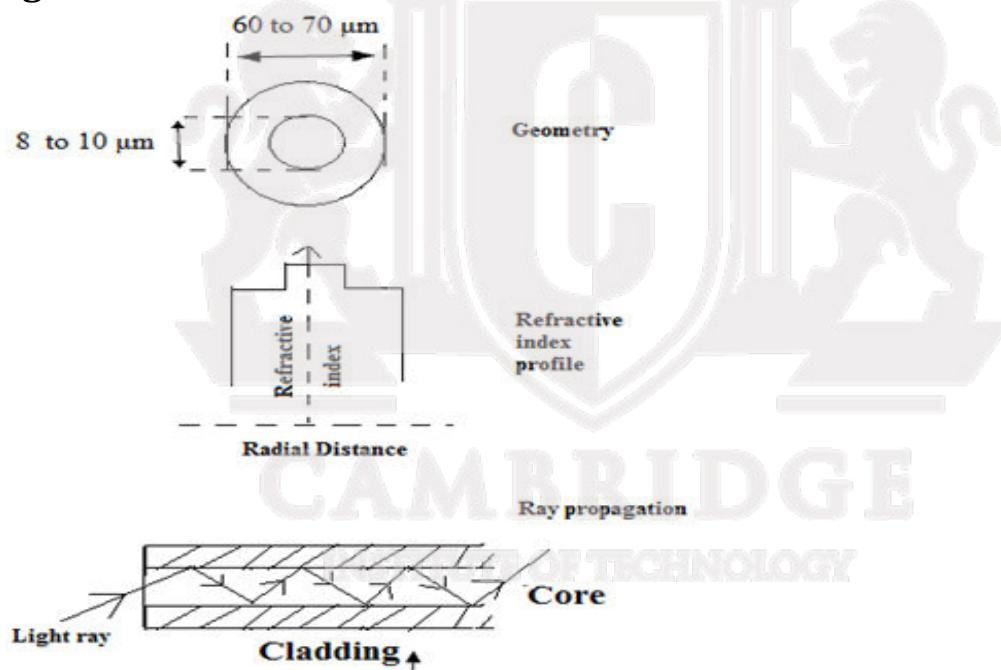
TYPES OF OPTICAL FIBERS:

- Optical fibers are classified into 3 major categories based on the materials used for making optical fibers, number of modes transmitted and the R.I profile of the fibers.
- In any optical fiber, the whole material of the cladding has a uniform refractive index value but the refractive index of core material may either remain constant or subjected to variation in a particular way. (R.I. of the core changes in graded index multimode fiber)
- The curve which represents the variation of refractive index with respect to the radial distance from the axis of the fiber is called the **Refractive Index Profile**.

Optical fibers are classified into 3 categories namely:

- a) Single mode fiber
- b) Step index multimode fiber
- c) Graded index multimode fiber

Single mode fiber:



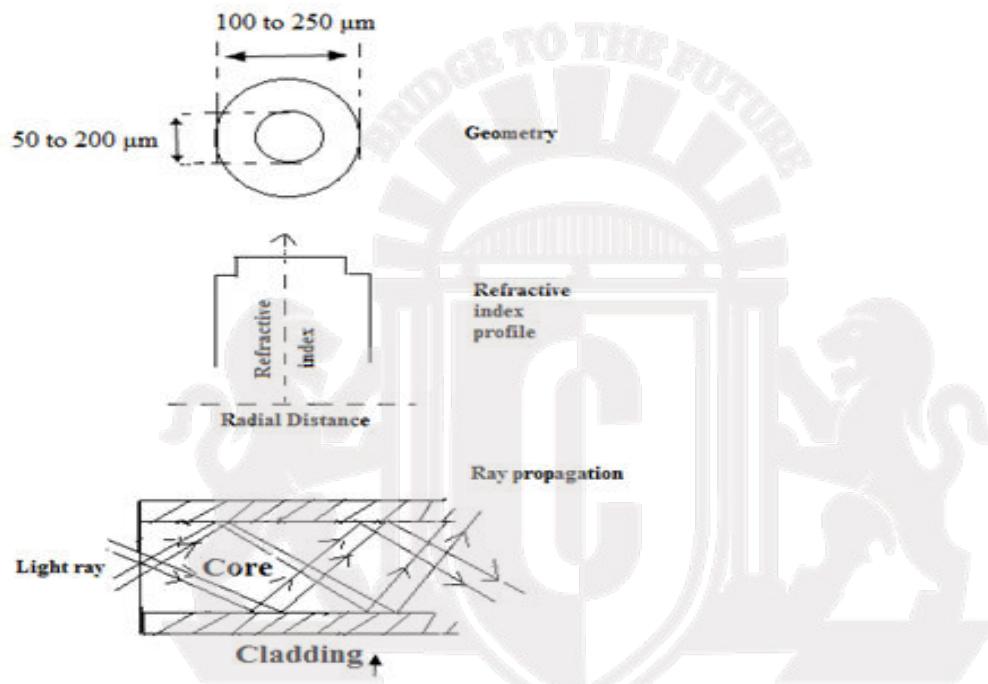
-
- Here core material has uniform refractive index value.
 - Cladding also has uniform refractive index but of little lesser value than that of core. This results in a sudden increase in the value of R.I from cladding to core.
 - R.I profile takes the shape of a step.
 - Diameter of the core is 8 to 10 μm.

Diameter of the cladding is 60- 70 μm

Since the core is very narrow, it can guide just a single mode. Hence it is called single mode fiber.

- These are the most extensively used ones and constitute 80% of all the fibers that are manufactured.
- They need lasers as the source of light
- It is less expensive, but very difficult to splice.
- Used in submarine cable system.

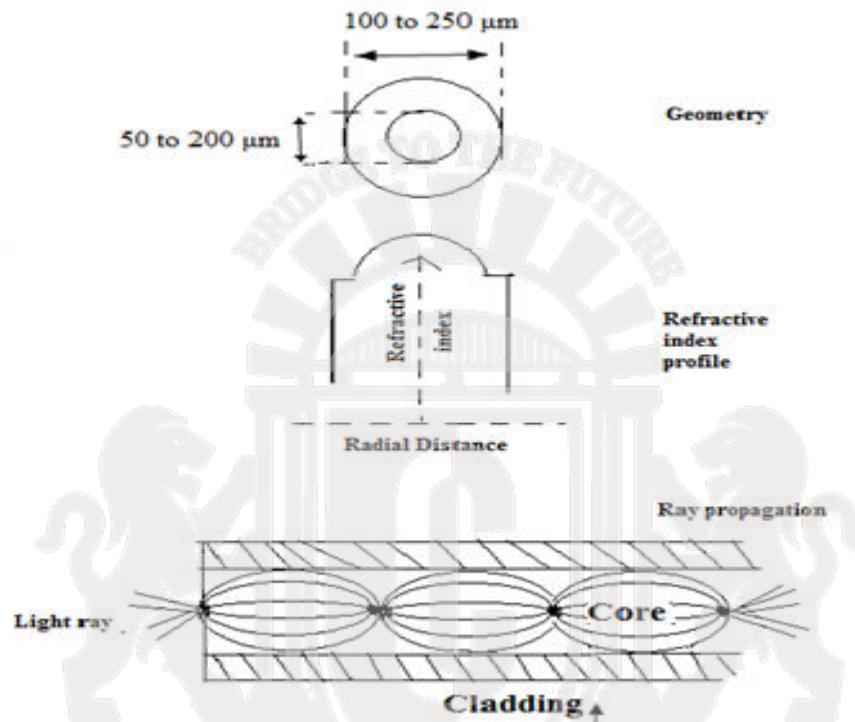
Step index multimode fiber:



- Here, the core material has uniform refractive index value.
- Cladding also has uniform refractive index but of little lesser value than that of the core. This results in a sudden increase in the value of R.I from cladding to core.
- R.I profile takes the shape of a step.
- Diameter of the core is 50 to 200 μm .
- Diameter of cladding is 100- 250 μm
- Here the core material has a much larger diameter, which supports propagation of large number of modes.
- R.I profile is also similar to single mode optical fiber.
- Uses LED or laser as source of light.

- It is least expensive all and is used in data links which has lower band width requirements

Graded index multimode optical fiber:



- It is also denoted as GRIN.
- The geometry of GRIN is same as that of step index multimode fiber.
- The special feature of the core is that its R.I value decreases in the radially outward direction from the axis, and becomes equal to that of the cladding at the interface. But the R. I of the cladding remains uniform.
- Diameter of the core 50 to 200 μm .
- Diameter of cladding 100- 250 μm
- Uses LED or laser as source of light
- Application is in the telephone trunk between central offices.

ATTENUATION (POWER LOSS OR FIBER LOSS):

The power loss suffered by the signal when it propagates through the fiber is called **Attenuation**. It is also known as fiber loss.

Types of losses in fiber are:

- i) Absorption
- ii) Scattering
- iii) Radiation loss

i) Absorption loss:

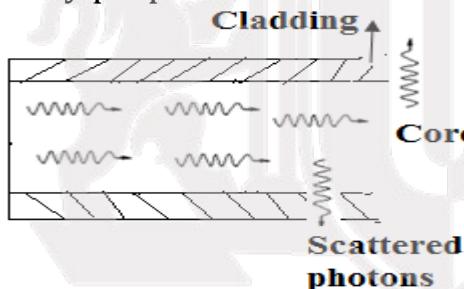
a. Absorption by impurities: Iron, Chromium, Cobalt and Copper are some of the impurities generally present in the glass fiber. When signal propagates through the fiber, a few photons associated with the signal are absorbed by the impurities present in the fiber. This results in power loss.

b. Intrinsic absorption: The absorption that takes place in the fiber material assuming that there are no impurities in it.

ii) Scattering loss:

a. Rayleigh scattering:

When a signal propagates through the fiber, a few photons associated with the signal are scattered by the scattering objects such as impurities present in the fiber. The dimensions of the scattering objects are very small compared to the wavelength of light. This type of scattering is similar to Rayleigh scattering. It is found that the co-efficient of scattering is inversely proportional to the wavelength of the object.

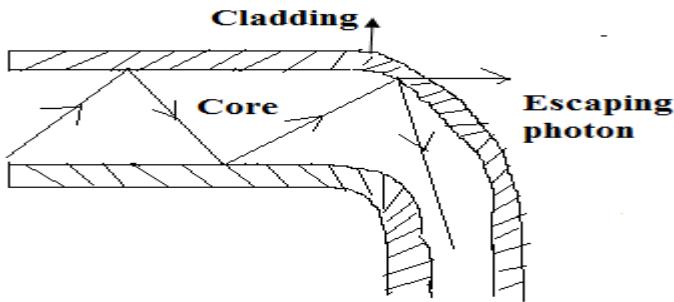


b. Others: Scattering also occurs due to trapped gas bubbles, unreacted starting materials and some crystallized region in the glass.

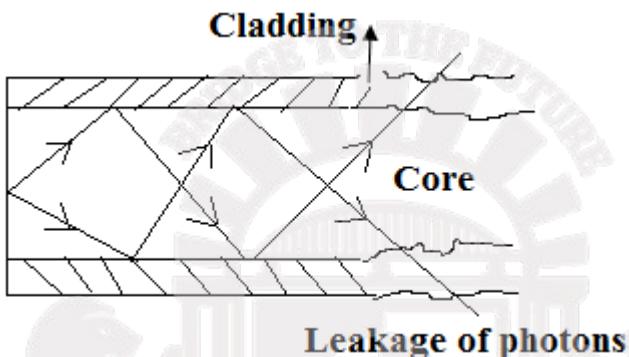
iii) Radiation loss:

It is due to the bending of fibers and it can be explained as follows:

a) Macroscopic bending: They are the bends with radii much larger compared to fiber diameter. It occurs while wrapping the fiber on a spool or turning it around a corner. If the bending is too sharp then the power loss becomes very high.



b) Microscopic bending: It occurs due to the non uniformity in the fibers while manufacturing. Because of this a few modes undergo leakage which results in power loss.



EXPRESSION FOR ATTENUATION CO-EFFICIENT (α):

By lamberts law "The rate of decrease of intensity with distance $(\frac{dP}{dL})$ is directly proportional to the initial intensity P".

$$\text{i.e. } -\frac{dP}{dL} \propto P \quad \dots \dots (1)$$

(-ve sign indicates that it is a decrement)

$$-\frac{dP}{dL} = \alpha P$$

Where α is a constant called Attenuation co-efficient.

$$\frac{dP}{P} = -\alpha dL$$

By integrating both sides we have

$$\int \frac{dP}{P} = -\alpha \int dL \quad \dots \dots (2)$$

An optical fiber of length L

If P_{in} is the initial intensity with which the light is launched into the fiber. and P_{out} is the intensity of the light received as output end of the fiber.

$$\text{Equation (2)} \quad \int_{P_{in}}^{P_{out}} \frac{dp}{p} = -\alpha \int_0^L dL$$

$$[\log p] = -\alpha L \quad (\text{Apply the lower limit and upper limit})$$

$$\log_e P_{out} - \log_e P_{in} = -\alpha L$$

$$\alpha = -\frac{1}{L} \log_e \left[\frac{P_{out}}{P_{in}} \right]$$

$$\alpha = -\frac{1}{L} \log_{10} \left[\frac{P_{out}}{P_{in}} \right] \quad \text{--- Bel /unit length}$$

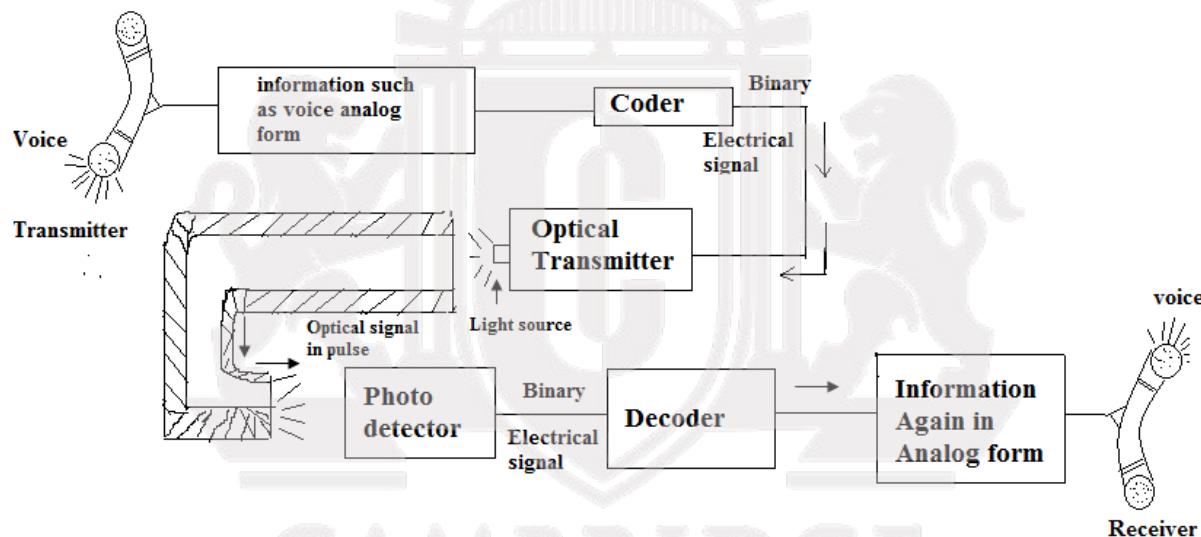
An optical fiber technology it is expressed α in terms of decibel / Kilometer (dB/Km). hence it follows that

- 1) The length of the fiber is expressed in Km.
- 2) The unit of Bel is 10 dB (1 Bel=10 Decibel)

$$\alpha = -\frac{1}{L} \log_{10} \left[\frac{P_{out}}{P_{in}} \right] \times 10 \text{dB/Km}$$

DISCUSS THE POINT TO POINT COMMUNICATION SYSTEM USING OPTICAL FIBERS:

Optical fiber communication is the transmission of information by propagation of optical signal through optical fibers over the required distance which involves driving optical signal from electrical signal at the transmitting end and conversion of optical signal back to electrical signal at the receiving end.



- Firstly we have analog information such as voice of a telephone user. The voice gives rise to electrical signals in analog form coming out of the transmitter section of the telephone.
- The analog signal is converted to binary data (digital) with the help of an electronic system called **Coder**.
- These electrical pulses are converted into optical pulses by modulating the light emitted by an optical source, in the binary form. This unit is called **optical transmitter**(converts electrical signals into light signals)
- This optical Signal is fed into the fiber.

- Out of the incident light which is funneled into the core within the half angle acceptance cone, only certain modes will be sustained for propagation within the fiber by means of total internal reflection. While propagating signal undergoes attenuation and delay distortion. Delay distortion is the reduction in the quality of signal with time. These effects cause degradation of the signal as the light propagates and may reach a limiting stage beyond which it may not be possible to retrieve the information from the light signal.
- The receiver section uses **Photo detector** which converts the optical signal into corresponding electrical signal then electrical signal is amplified and recast in the original form by means of an electrical regenerator, which is part of receivers section.
- Lastly using the **Decoder**, the binary electrical signal is converted back to analog electrical signal, which will be same information such as voice, which was there at the transmitting end.

QUESTION BANK

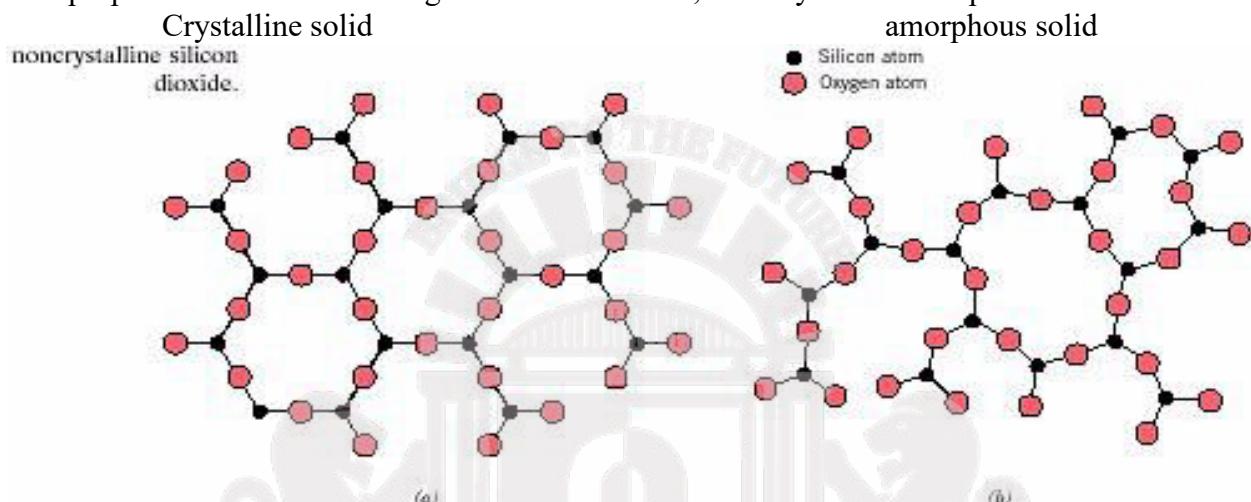
- 1) Obtain an expression for energy density of radiation under equilibrium condition in terms of Einstein co-efficients.
- 2) Describe briefly the application of laser in welding, cutting and Drilling
- 3) Describe the recording and reconstruction process in HOLOGRAPHY with the help of suitable diagrams.
- 4) Describe the construction and working of semiconductor laser.
- 5) Describe the construction and working of carbon dioxide laser .with the help of energy level diagram.
- 6) What is numerical aperture? Obtain an expression for numerical aperture in terms of refractive indices of core and cladding, and then arrive at the condition for propagation
- 7) Discuss the point to point communication system using optical fibers with the help of a block diagram.
- 8) Explain the types of optical fibers.
- 9) Write a note on measurement of pollutants in atmosphere using laser.

MODULE-4

CRYSTAL STRUCTURE

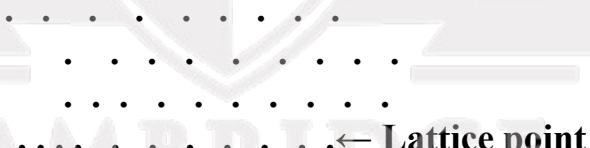
INTRODUCTION:

Matter is normally divided into three states namely solids, liquids and gases. Solids could be either amorphous or crystalline. In amorphous solids, only short range order could be found in the arrangement of the constituent atoms or molecules and hence no definite structure could be assigned to them. And they do not have a sharply defined melting point and are isotropic. In Crystalline solid is characterized by a high degree of symmetry and structural regularity in the arrangement of constituent atoms or molecules. They have a sharply defined melting point and their properties are different along different directions, i.e. they are anisotropic.



Crystal: A crystal is a solid composed of atoms molecules or ions arranged in a regular periodic array.

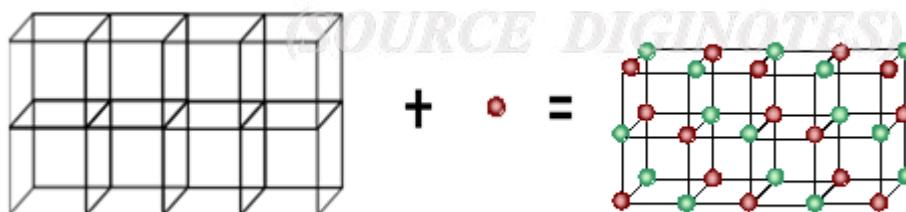
Lattice: The imaginary points in space about which the atoms are located are called lattice points



Basis: A group of atoms attached to every lattice point is known as basis.

$$\begin{pmatrix} o & o & o \\ o & o & o \end{pmatrix} \leftarrow \text{atoms}$$

Crystal structure: A crystal structure is formed when the basis is substituted in the space lattice

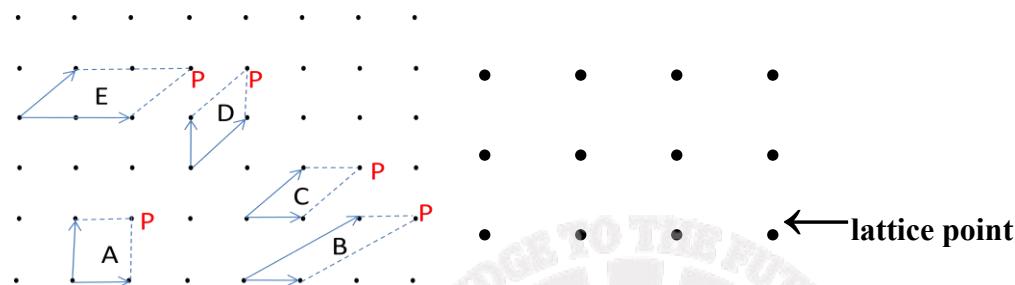


Lattice + Basis = Crystal Structure

Space lattice: A crystal consists of a three-dimensional periodic array of atoms or molecules. In order to study the crystal geometry, it is necessary to mark the intervals at which periodically. “A space lattice is a regular periodic array of points in space.”

Or

“A geometrical representation of the crystal structure in terms of lattice points is called space lattice.”



Bravais lattice: A space lattice is a regular periodic array of points in space, a particular type of space lattice is known as Bravais lattice.

Or

if each lattice point in the crystal lattice substitutes an identical set of one or more atoms then the lattice points becomes equivalent then the lattice is called **Bravais Lattice**

In two dimensions with no restriction on the length ‘a’ and ‘b’ or on the angle γ between two lines.

On the other hand, the lattice points are non-equivalent then it is called non-Bravais lattice.

Non Bravais Lattice :



NON - BRAVIA'S LATTICE

On the other hand if some of the lattice points are non-equivalent then it is said to be **Non-Bravais lattice**.

Consider the crystal lattice. The lattice points ABC etc are equivalent. Similarly another set of lattice points A^1, B^1 and C^1 etc are equivalent which constitutes another Bravais Lattice. But the lattice prompts $A & A^1, B & B^1$ etc are not equivalent. Therefore the lattice is called non Bravais Lattice. Thus a non Bravais lattice is a superposed pattern of two or more different Bravais Lattices.

Unit cell and lattice parameters:

“A parallelepiped formed by fundamental vectors a, b and c of space lattice is called **unit cell**”.

or

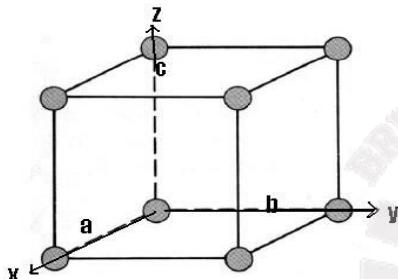
“The unit cell is defined as the smallest portion of the space lattice which can generate the complete crystal by repetition in three dimensions.”

**"The lengths of the primitive lattice translation vectors in a unit cell and the three interfacial angles in a unit cell are known as lattice parameters".
i.e. a , b , c . and α , β , and γ .**

Each crystal is built up of a repetitive stacking of unit cells each identical in size shape and orientation the unit cell with basis is thus the fundamental building block of the crystal.

A unit cell is always drawn with lattice points at each corner, but there may also be lattice points at the center of some of the faces or at the body center of the cell. Although there are infinite number of ways of choosing the unit cell, but the simplest one is conventionally accepted.

$$\vec{R} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$$



Where \vec{a} , \vec{b} , \vec{c} are the three vectors joining the origin to the nearest non-coplanar points and n_1, n_2 , and n_3 are integers.

\vec{a} , \vec{b} , \vec{c} are the basis vectors set

The angle between \vec{a} & \vec{b} is α

The angle between \vec{b} & \vec{c} is β

The angle between \vec{c} & \vec{a} is γ

Primitive cell: Primitive cell is a unit cell which contains atoms only at the corners.

Or

"The unit cell that contains one lattice point only at the corners is known as primitive cell"

A non primitive cell is a unit which incorporates an integral multiple of primitive cells. And it is imagined only for the sake of easy visualization of the symmetry in arrangement of points.

a and c are primitive cells

b is non primitive cell

In the non primitive cell of b in addition to the corner points there is one more point at the center which is not at the corner.

Direction and Planes in a crystal lattice

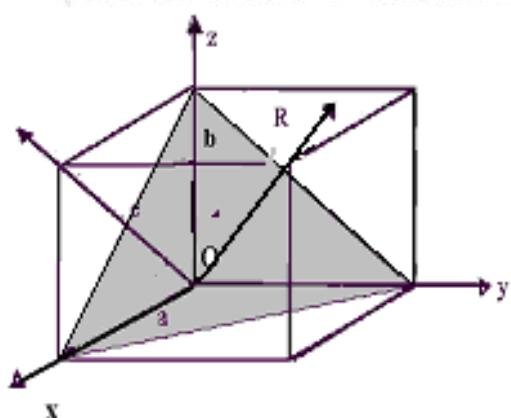
In a crystal system it is necessary to refer to planes comprising of lattice points and also to directions of straight lines on which the lattice points lie in a space lattice.

In a crystal there exist directions and planes which contain a large concentration of atoms. The crystal direction is a line joining any two points of the lattice or it is an imaginary line passing through the origin and a given lattice point in the

through the origin and a given lattice point in the



e is one more lattice point



crystal lattice.

Let us consider a simple cubic lattice. In order to specify the directions in a lattice we make use of lattice vectors. For example if we want to indicate the direction in the fig., the point can be generated starting from the origin 'O' and move n_1 steps in the direction of \vec{a} , n_2 steps in the direction of \vec{b} and n_3 steps in the direction of \vec{c} . The position vector \vec{OR} can be represented as

$$\vec{R} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$$

Where, n_1 , n_2 , & n_3 are integers and \vec{a} , \vec{b} , \vec{c} are constants called basis vectors.

As per this vector equation, the direction vector \vec{R} depends purely on the Integers n_1 , n_2 and n_3 . since \vec{a} , \vec{b} , \vec{c} are constants we can remove. Then the directions are specified as $\vec{R} = [n_1 n_2 n_3]$.

In a Cubic unit cell, the direction [111] is resultant vector, X –axis is [100] direction Y axis [010] direction and Z axis is [001] direction.

Crystal planes and Miller indices:

"The crystal lattice to be made up of a parallel set of equidistant planes known as crystal planes or lattice planes."

"The reciprocal of the intercepts made by the plane on the crystallographic axes when reduced to smallest numbers."

Or

The position of a crystal plane can be specified in terms of three integers called miller indices.

Procedure for finding Miller Indices:

1. Find the intercepts of the plane with the crystal axis along the axes x, y and z in terms of the lattice constants a, b and c respectively.

2. Express x, y, and z as fractional multiplier of respective basic vectors, then we obtain the fraction

$$= \frac{x}{a} = \frac{y}{b} = \frac{z}{c}$$

Department of Physics

3. Take the reciprocal of the fractions to obtain

$$\frac{a}{x}, \frac{b}{y}, \frac{c}{z}$$

4. Find the least common multiple [LCM] of the denominator by which multiply the above three ratios.

This operation reduces them to a set of 3 integers h, k, l called miller indices for the crystal plane.

The position of the plane in the space lattice is denoted as (hkl).

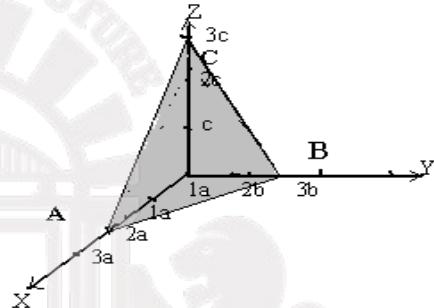
Example: Consider a parallel plane ABC with intercepts $2a$ along X – axis, $2b$ on Y axis and $3c$ on Z axis, where $a, b & c$ are lattice constants respectively.

The intercepts of $x, y, z = 2; 2; 3$

Reciprocals of integers = $1/2; 1/2; 1/3$

LCM is 6; we get $3; 3; 2$

The Miller indices of the Plane ABC,
 $(h K l) = (3 3 2)$.



Example.

1) The intercepts of the plane is

$$X = \frac{4}{5}a, Y = \frac{2}{3}b, Z = \frac{1}{2}c$$

2) Taking the ratio of intercepts with the basis vectors.

$$\left[\frac{x}{a}, \frac{y}{b}, \frac{z}{c} \right] = \left[\frac{4}{5}, \frac{2}{3}, \frac{1}{2} \right]$$

3) Taking the reciprocals of the 3 fractions.

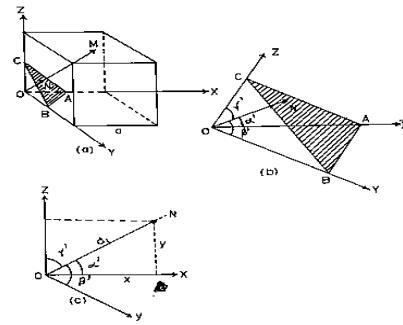
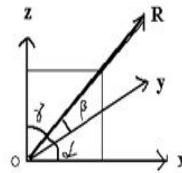
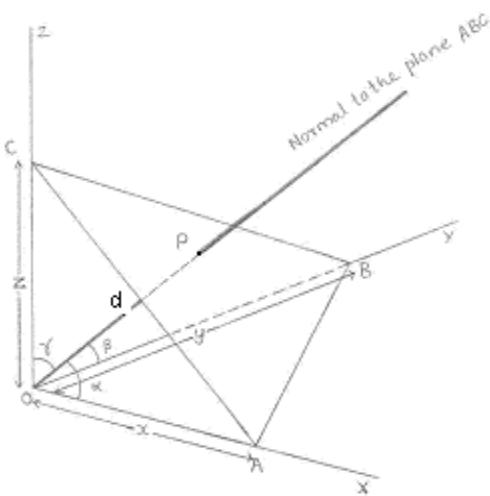
$$\left[\frac{5}{4}, \frac{3}{2}, \frac{2}{1} \right]$$

4) Throughout by the least common multiple by 4

$$\left[\frac{5}{4} \times 4, \frac{3}{2} \times 4, \frac{2}{1} \times 4 \right]$$

$(5 6 8)$ which is read as five six eight.

Expression for interplanar spacing in terms of miller indices:



Interplanar distance is defined as the distance between two adjacent lattice planes is known as the interplanar distance.

Let ABC be one of the parallel planes represented by the miller indices (hkl). Its intercepts on the crystal axes are x, y and z.

Another plane parallel to this plane, passes through the origin O. if OP is drawn perpendicular from O to the plane ABC, then OP is equal to the interplanar distance denoted by d_{hkl} . Let angle made by OP with respect to the co-ordinate axes x, y and the z, be α, β, γ .let us consider the space lattice in which x, y, z are orthogonal.

Then since OP is normal to the plane x, y, z will be the hypotenuses to the 3 right angled triangles all of which have a common adjacent side OP

$$d_{hkl} = X \cos \alpha = y \cos \beta = z \cos \gamma \quad \dots \dots \dots (1)$$

If a, b, c is the lengths of the basis vectors then as per our convention in designating the miller indices.

$$(h k l) = \left(\frac{a}{x}, \frac{b}{y}, \frac{c}{z} \right)$$

$$(X y z) = \left(\frac{a}{h}, \frac{b}{k}, \frac{c}{l} \right)$$

Using the above equation (1) we have

$$d_{hkl} = \frac{a}{h} \cos \alpha = \frac{b}{k} \cos \beta = \frac{c}{l} \cos \gamma \quad \dots \dots \dots (2)$$

$$\text{From equation (2)} \quad d_{hkl} = \frac{a}{h} \cos \alpha \\ \cos \alpha = h d_{hkl} / a$$

Squaring both the sides

$$\cos^2 \alpha = h^2 d_{hkl}^2 / a^2 \text{ similarly for } \cos^2 \beta = \cos^2 \gamma$$

But for orthogonal co-ordinates we know that

$$\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = 1 \dots \dots \dots (3)$$

From equation (2) and (3) we have

$$d_{hkl}^2 \left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right] = 1$$

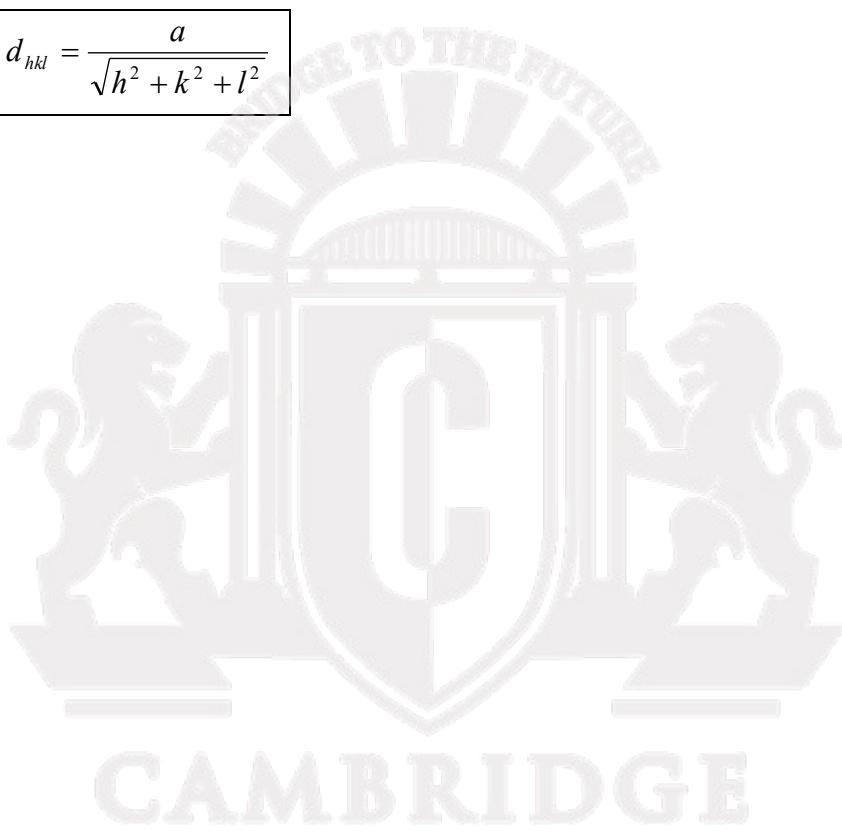
Then, the interplanar distance 'd' is given by

$$d_{hkl} = \frac{1}{\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right]^{1/2}}$$

Where, d_{hkl} is the interplanar distance.

For cubic lattice $a=b=c$ then, $d_{hkl} = \frac{1}{\left[\frac{h^2}{a^2} + \frac{k^2}{a^2} + \frac{l^2}{a^2} \right]^{1/2}}$

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



Crystal systems:

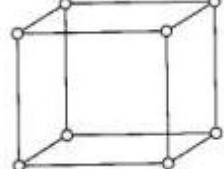
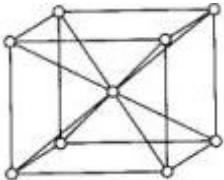
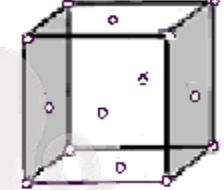
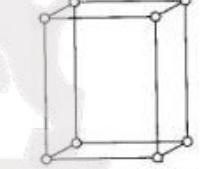
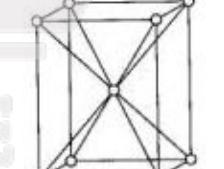
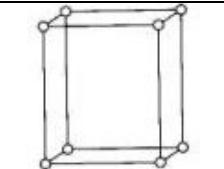
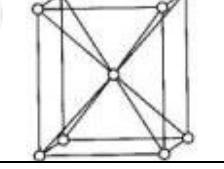
Different crystals have different arrangements of lattice points which give rise to different types of space lattices. For representing the type of distribution of lattice points in space, a coordinate system is needed. To serve this purpose, it requires seven different co-ordinate systems, the co-ordinate systems are called crystal systems. They are named on the basis of geometrical shape and symmetry as follows.

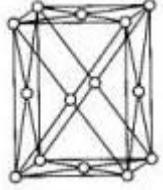
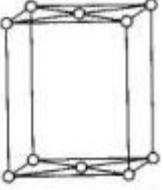
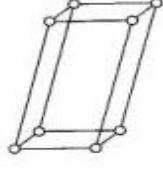
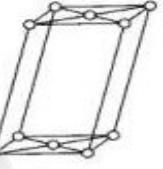
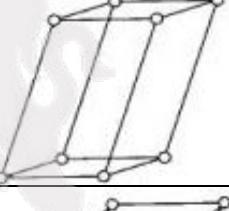
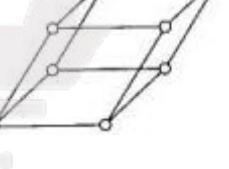
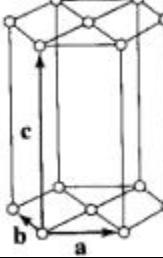
Based on the geometrical considerations these are divided into 7 groups distinguished from one another by their angles between them and intercepts of the faces along them in these basic systems further divided into 14 special systems(Bravais lattice)

Crystal is broadly classified into seven types they are also called seven ***crystal systems***.

- (1) Cubic
- (2) Tetragonal

- (3) Orthorhombic
- (4) Mono clinic
- (5) Triclinic
- (6) Trigonal (Rhombohedral)
- (7) Hexagonal

S.No	Crystal System	No of space lattice points	Unit cell characteristic s	Bravais lattice and symbol	Unit cell geometry	Example
I	Cubic	3 $a=b=c$ (lengths) $\alpha=\beta=\gamma=90$ (Angles)		Simple cube (P) (SC)		Au, Cu, Ag NaCl,
				Body Centered (I) (bcc)		
				Face Centered (F) (fcc)		
II	Tetragonal	2 $a=b\neq c$ $\alpha=\beta=\gamma=90$. Simple		SnO ₂ , TiO ₂ ,
				Body Centered		
III	Orthorhombic	4 $a\neq b\neq c$ $\alpha=\beta=\gamma=90$		6. Simple (P)		KNO ₃ , K ₂ SO ₄ , PbCo ₃
				7. Body Centered (I)		

				Face Centered(F) (Fcc)		
				Base Centered (C)		
IV	Monoclinic	2	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ$, $\beta \neq 90^\circ$	Simple (P)		Borax $2\text{H}_2\text{O}$,
				Base Centered (C)		
V	Triclinic	1	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$	Simple(P)		$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$
VI	Trigonal, Rhombohedral	1	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$ $< 120^\circ$	Simple (P)		Calcite As, sb, Quartz
VII	Hexagonal	1	$a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	Simple (P)		$\text{Zn}, \text{Mg},$ Cd, SiO_2

1. Cubic: In this crystal all the three lengths of the primitives are equal and are at right angles to each other i.e., $a = b = c$, and $\alpha = \beta = \gamma = 90^\circ$

2. Tetragonal: In this crystal, the two lengths of the primitives are equal and one is different but all the interfacial angles are equal to 90° , i.e., $a=b \neq c$ and $\alpha=\beta=\gamma=90^\circ$.

3. Orthorhombic: In this unit cell the lengths of the primitives' one different but all the interfacial angles are equal to 90^0 , i.e., $a \neq b \neq c$ and $\alpha = \beta = \gamma = 90$

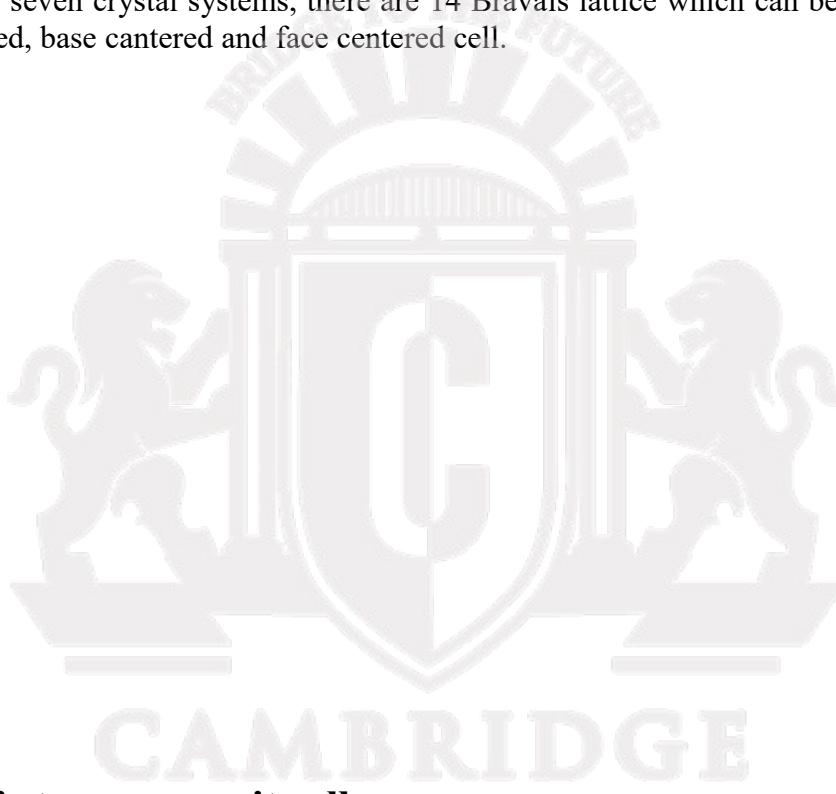
4. Monoclinic: In this unit cell the length of the primitives are different. Two interfacial angles equal to 90 and one not equal to 90 , i.e., $a \neq b \neq c$ and $\alpha = \gamma = 90$, $\beta \neq 90$.

5. Triclinic: In this Crystal all the three primitives and all the three angles are not equal, i.e. $a \neq b \neq c$ and $\alpha \neq \beta \neq \gamma \neq 90$ Ex: $K_2Cr_2O_7$

6. Trigonal (Rhombohedral): In this crystal three lengths of the primitives are equal and all the interfacial angles are equal but not equal to 90 , i.e., $a = b = c$ and $\alpha = \beta = \gamma \neq 90$. <120

7. Hexagonal: In this crystal two lengths of the primitives are equal and one is different and two interfacial angles equals 90 and one equals 120 , i.e. $a = b \neq c$ $\alpha = \beta = 90$. $\gamma = 120$.

The modified corners (cells), along with the primitive / unit cell are said to be Bravais lattice. If we consider all seven crystal systems, there are 14 Bravais lattice which can be classified based on body centered, base centered and face centered cell.

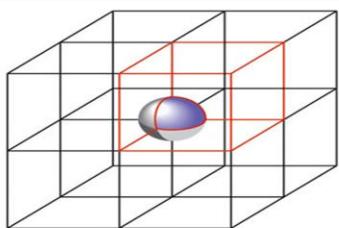


Number of atoms per unit cell:

The atoms in a crystal may be shared by more than one unit cell. Ex: an atom in a simple cubic structure is shared by eight unit cells. An atom at the face centered in a cubic cell shared only two unit cells. In body centered unit cell, the atoms at the centre of the cell is not shared by the cell with other cells.

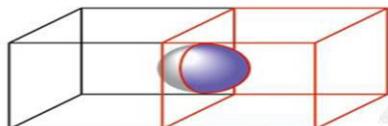
(*SOURCE DIGINOTES*)

of Atoms/Unit Cell



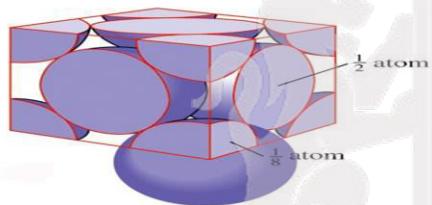
For atoms in a cubic unit cell:

- Atoms in corners are $\frac{1}{8}$ within the cell



For atoms in a cubic unit cell:

- Atoms on faces are $\frac{1}{2}$ within the cell



A face-centered cubic unit cell contains a total of 4 atoms: 1 from the corners, and 3 from the faces.

- 1) **Simple cubic (SC):** A simple cubic cell has eight atoms at each of its eight corners. As each atom at the corner is shared by eight unit cells. Only $1/8^{\text{th}}$ of each atom belongs one cell.

$$\text{Number of atoms per unit cell} = \frac{1}{8} \times 8 = 1$$

- 2) **Body centered cubic(BCC) :** As there are 8 corners atoms ,the no of corner atoms belonging to the unit cell $\frac{1}{8} \times 8 = 1$ also, there is an atom at the centre of the unit cell which is not shared with other cell

$$\text{Number of atoms per unit cell} = 1 + 1 = 2$$

- 3) **Face centered cubic (FCC):** The number of corner atoms belonging to a unit cell is $\frac{1}{8} \times 8 = 1$. Also, there is an atom at the centre of each of the six faces. Each atom at the face centered is shared by two unit cells. Hence $\frac{1}{2}$ of each face centered atom belonging to the unit cell. As there are 6 faces, the no of face centered atoms belonging to the unit cell is $\frac{1}{2} \times 6 = 3$

$$\text{Number of atoms per unit cell} = 1 + 3 = 4$$

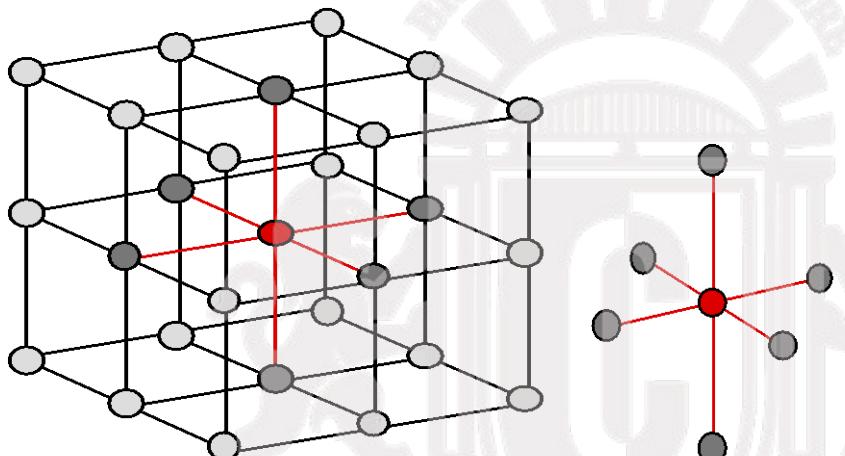
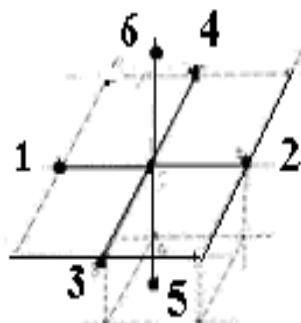
Co-ordination number: In a crystal, each atom is surrounded by a definite number of nearest equidistant neighbors.

"Co-ordination number is the number of nearest neighbors directly surrounding a given atom within a crystal".

1) **Simple cubic (SC) structure.**

In a simple cubic structure, there will be one atom at each corner of the unit cell. Let us consider one corner atom at of a unit cell in the crystal lattice, and then it will have 4 nearest atoms (1, 2, 3 & 4) in the horizontal plane. There are 2 more atoms nearest one is directly above (5) and the directly below (6). Except these 6 atoms, all other atoms lie at greater distance.

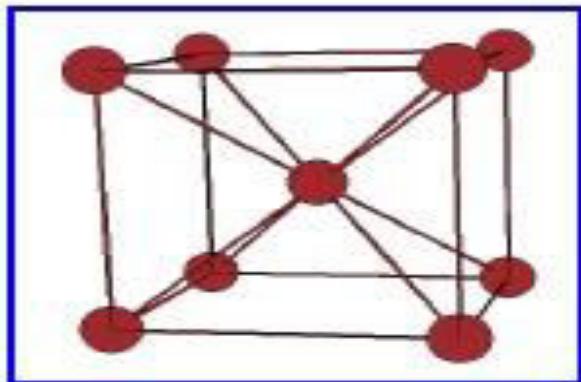
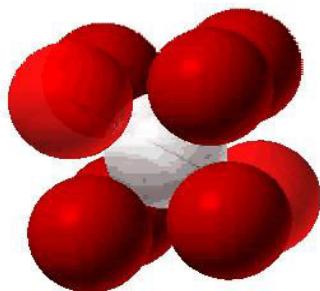
Thus the co-ordination number for an atom in the simple cubic is =6



2) **Body centered cubic(BCC) structure:**

In this structure, there will be one atom at the body center and eight atoms at the corners of the unit cell.

Thus for an atom at the body centre, obviously there are eight (8) nearest neighbors.
Hence the co-ordination number of an atom in bcc structure =8



Body Centered Cubic
and related structures

3) Face centered cubic(FCC) structure:

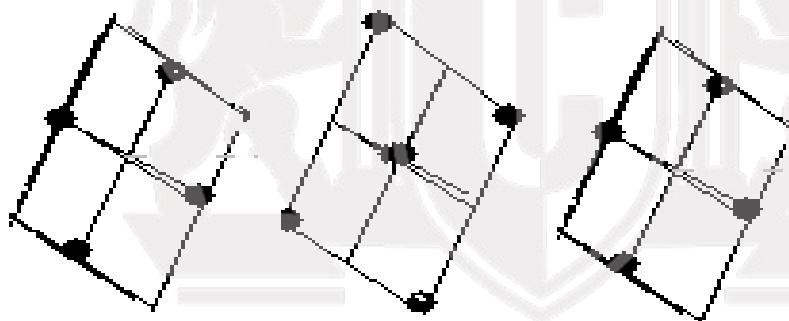
For a lattice of FCC structure, 3 consecutive planes can be taken.

It can be recognized that each atom irrespective of the 3 planes to which it belongs to lie, there are 4 such atoms in each plane.

Thus the number of nearest atoms to $3 \times 4 = 12$

Hence the co-ordination number for the FCC structure =12.

It is seen that in the 3-d lattice for FCC structure, each atom possesses the same surroundings as that shown



Relation between Atomic radius and lattice constant for cubic lattices:

1. Simple Cell Structure:

Let consider one face of the unit cell of a sc structure. We can see from the figure that there are 4 atoms at each corner of the cube. Due to symmetry, the distributions of atoms at their corners lie at the center of the square with spherical bodies touching each other.

From figure, it is seen that

$$a = 2r \quad \text{lattice Constant}$$

$$R=a/2 \text{ (Atomic radius)}$$

2. Bcc Structure:

In bcc cell atoms are in contact diagonally along the body which is as shown in the figure. There are two atomic radii from the center atom and one from atomic radius from each of the corner atom to the body diagonal and its length are equal to $4r$. From figure, we get

$$\text{Triangle, ABC, } AC^2 = AB^2 + BC^2$$

$$AC^2 = a^2 + a^2 = 2a^2 \text{ and}$$

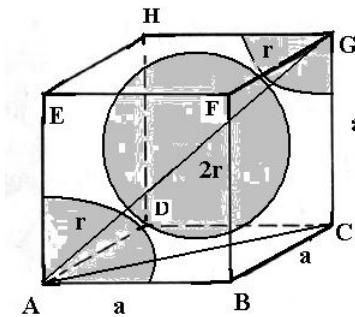
$$AG = r + 2r + r = 4r$$

$$\text{Along diagonal, } AG^2 = AC^2 + CG^2$$

$$(4r)^2 = 2a^2 + a^2 = 3a^2$$

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

$$4r = a\sqrt{3} \quad r = a\sqrt{3}/4 \text{ (atomic radius)}$$



3. Fcc structure:

In an FCC cell, atoms are in contact diagonally along the face of the cube which is as shown in the figure. There are four atomic radii along the face diagonal. From the geometry of the figure,

$$\text{Triangle ABC,}$$

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

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

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

or

$$Ac = \sqrt{4r^2}$$

$$\text{Also } Ac = \sqrt{a^2 + a^2}$$

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

$$= a\sqrt{2}$$

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

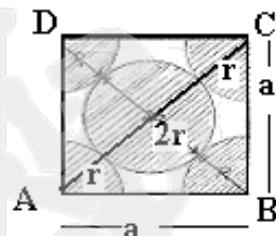
$$a\sqrt{2} = 4r$$

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

$$r = a\sqrt{2}/2\cdot 2 = a\sqrt{2}/2\cdot \sqrt{2}\cdot \sqrt{2}$$

$$r = a/2\cdot \sqrt{2} \text{ (Atomic radius)}$$

$$a = 2\sqrt{2}r \text{ (lattice constant)}$$



Atomic packing factor (APF):

We have seen different kinds of crystal structure and each structure (unit cell) have different amount of matter contents. For a given space, some structures shall have more voids and some have more matter contents.

The fraction of space occupied by atoms in a unit cell is known as atomic packing factor.

Packing factor is concerned to density of packing and can be evaluated by considering the actual type of crystal structure. But the atoms are perfectly spherical in shape then “**packing factor is**

the ratio of the volume occupied by the atoms in the unit cell to the total volume of the unit cell."

i.e. APF = $\frac{\text{volume occupied by the atoms in the unit cell}}{\text{Total volume of the unit cell}}$

We are considering here unit cells of cubic type the lattice parameter for them is "a". it implies the edge length of the cube is a.

Total Volume of the unit cell = a^3

As the atoms are assumed to be spherical in shape,

Volume of the each atom = $4/3 \pi R^3$

There are n atoms in a unit cell, the volume occupied by all the atoms in the unit Cell= $n \times 4/3 \pi R^3$

Where, R is the radius of an atom.

According to definition

$$\boxed{\text{APF} = \frac{n}{a^3} \times \frac{4}{3} \pi R^3}$$

1. Simple Cubic Cube (Sc) lattice:

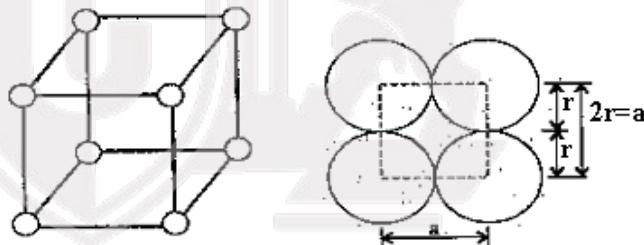
In simple cubic lattice number of atoms per unit cell, n = 1.

The corner atoms touch each other and lattice constant and radius of the atom can be related as, $a = 2R$.

The volume of the atom, $v = \frac{4}{3} \pi R^3$ and volume of the unit cell,

$$\begin{aligned} \text{APF} &= \frac{n}{a^3} \times \frac{4}{3} \pi R^3 \\ &= \frac{1}{2R^3} \times \frac{4}{3} \pi R^3 \\ &= \frac{1}{8R^3} \times \frac{4}{3} \pi R^3 \\ &= \frac{4\pi}{24} = \frac{\pi}{6} = 0.166 \times 3.142 \\ &= 0.52 \end{aligned}$$

$\therefore \text{APF} = 52\%$

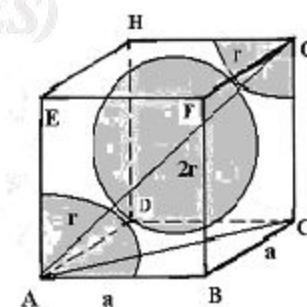
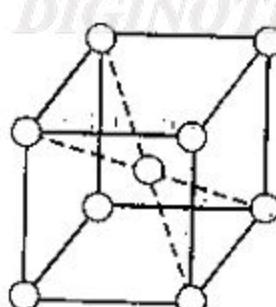


This means that, in a sc lattice, 52 % of the unit cell volume is occupied by atoms.

2. Body Centered Cube (Bcc) Lattice:- In a bcc lattice each corner atom touches the body centered atom and no of atoms per unit cell = n = 2.

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

$$\text{APF} = \frac{n}{a^3} \times \frac{4}{3} \pi R^3$$



$$\begin{aligned}
 &= \frac{2 \times \frac{4}{3} \pi R^3}{a^3} = \frac{2 \times \frac{4}{3} \pi R^3}{\left(\frac{4R}{\sqrt{3}}\right)^3} \\
 &= \frac{2}{\frac{64R^3}{3\sqrt{3}}} \times \frac{4}{3} \pi R^3 = \frac{\frac{8\pi}{64}}{\frac{\sqrt{3}}{8}} = \frac{\sqrt{3}\pi}{8}
 \end{aligned}$$

$$= 0.21 \times 3.14$$

$$\text{APF} = 0.68.$$

$$\text{APF} = 68 \text{ \%}.$$

This means that, in a bcc lattice, 68 % of the unit cell volume is occupied with atoms.

3. Face Centered Cube (FCC) Lattice:

In a FCC lattice each corner atom touches the face centered atom and the no. of atoms per unit cell n = 4

$$\begin{aligned}
 &\therefore a = 2\sqrt{2} R \\
 \text{APF} &= \frac{n}{a^3} \times \frac{4}{3} \pi R^3
 \end{aligned}$$

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

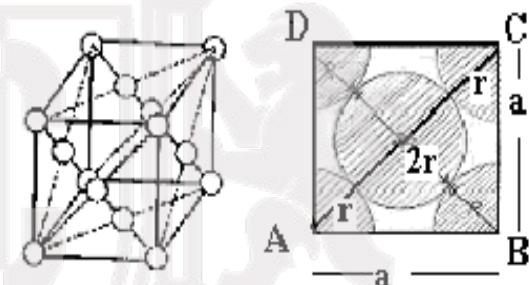
$$= \frac{4}{16\sqrt{2}R^3} \times \frac{4}{3} \pi R^3$$

$$= \frac{16\pi}{48\sqrt{2}} = \frac{\pi}{3\sqrt{2}}$$

$$= 0.23 \times 3.142 = 0.74$$

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

This means in an FCC unit cell, 74 % of the unit cell volume is occupied by atoms. Thus the FCC unit cell is the most densely packed than bcc and SC.



DATA ON CUBIC LATTICE					
Sl. No.	Type of lattice	Coordination Number	No. of atoms/unit cell	Relation B/W. a and r	APF %
1	SC	6	1	a = 2R	52.4
2	Bcc	8	2	a = 4R/\sqrt{3}	68
3	Fcc	12	4	a = 2\sqrt{2} R	74

Structure of Diamond:

- 1) In diamond structure each carbon atom linked to four other by covalent bond.
- 2) Diamond exhibits FCC crystal structure which is a combination of two inter-penetrating FCC sub lattices, one of which is displaced from the other by one fourth of the length of the unit cell.
- 3) Hence a unit cell of diamond contains 18 carbon atoms.
- 4) one each at the eight corners,(C) (00000000)
- 5) one each at the face centers(F) (1/2,1/2,1/2,1/21/2,1/2)
- 6) And four atoms in the interior tetrahedral positions(D)(3/4,1/4,3/4,1/4)

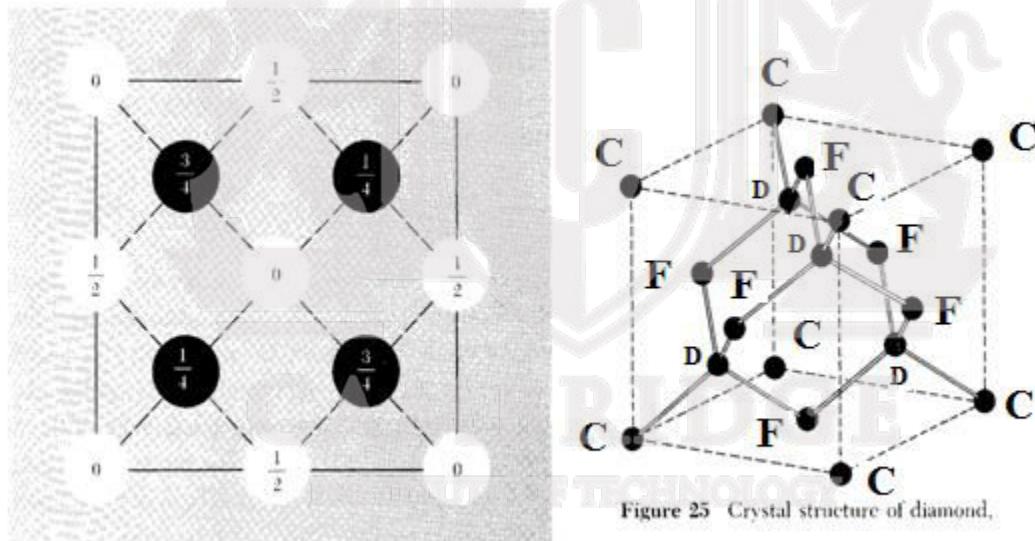
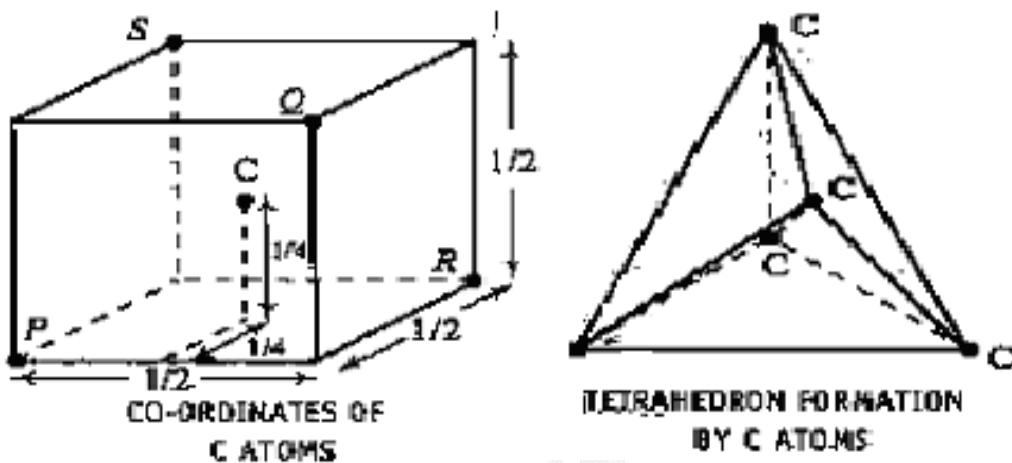


Figure 25 Crystal structure of diamond.

Figure 04 Atom positions in the cubic cell of the diamond

(*SOURCE DIGINOTES*)



8). Consider a part of the unit cell. Then the coordination of the carbon atoms at the positions PQR and S can be expressed inter length of the cube edge given as 000, $\frac{1}{2}0\frac{1}{2}$, $\frac{1}{2}\frac{1}{2}0$, $0\frac{1}{2}\frac{1}{2}$ respectively. The coordinates of the central carbon atom are $[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$.

9) The number of atoms per unit cell $n = 8$.

10) Each atom has **four** nearest neighbors .Therefore the coordination number is 4.

11) The nearest neighboring distances $2R = \frac{a\sqrt{3}}{4}$

12) The lattice parameter $a = \frac{8R}{\sqrt{3}}$

13) The distance between two carbon atoms or lattice constant is $a = 3.5 \text{ \AA}^0$.

14) The length of each bond is 0.154nm and the angle between the bonds is 109.5° .

15) Atomic packing factor= APF = $\frac{n}{a^3} \times \frac{4}{3} \pi R^3$

$$\begin{aligned}
 &= \frac{8}{8R^3} \times \frac{4}{3} \pi R^3 \\
 &= \frac{\sqrt{3}\pi}{16} = 0.34 \text{ or } 34\%.
 \end{aligned}$$

16) The importance of this structure will become evident when we study semiconductors, carbon, silicon, germanium all crystals lie in diamond structure.

17) Density of Diamond is $\rho = \frac{nA}{N_A V} = \frac{8(12.01 \times 10^{-3})}{(6.023 \times 10^{23})(3.567 \times 10^{-10})^3} = (3.514 \times 10^3) \text{ kg/m}^3$

Atomic weight of carbon is $A = 12.01 \text{ amu}$. & Lattice constant $a = 3.567 \text{ \AA}$

Volume of the unit cell $V = a^3 = (3.567 \times 10^{-10})^3$ & the Avogadro number is $N_A = (6.023 \times 10^{23})$

Pervoskites:

Pervoskites as class of compounds came into prominence in the year 1986. A type of oxide compounds were found to exhibit superconductivity, that too at temperature higher than the metallic superconductor.

Pervoskites crystal structure:

Pervoskites is the common name for all oxides with the formula ABO_3 where A & B are two different kinds of metals.

Ex:

CaTiO_3 (calcium Titanate)

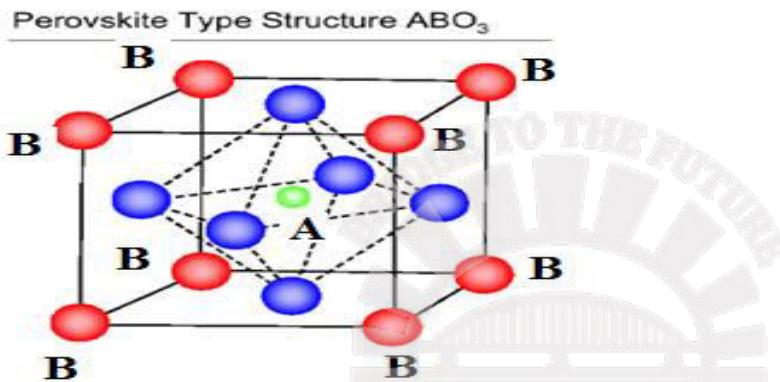
BaTiO_3 (Barium Titanate)

$\text{YBa}_2\text{Cu}_3\text{O}_7$ (yttrium Barium copper oxygen)

One type of metal atoms B, are at the eight corners of the unit cell and

One atom of other type of metal A at the center.

The oxygen atoms lie at the centre of the six square faces as shown in the fig.



In this fig there is one "A" type atom at the centre. Hence the no of atoms /unit cell =1 There are 8 corner atoms of "B" type. Therefore total share of all the corner atoms/unit cell = $8 \times \frac{1}{8} = 1$

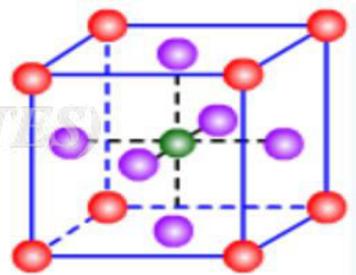
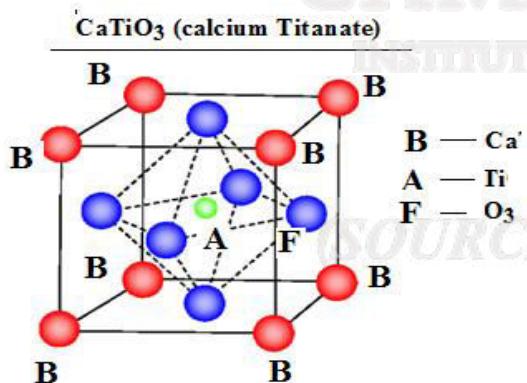
There are 6 face centered atoms of oxygen, therefore total share of all the oxygen atoms/unit cell = $6 \times \frac{1}{2} = 3$

Hence the no of oxygen atoms /unit cell =3

All together per unit cell, the combination results in ABO_3

Ex: **CaTiO_3 (calcium Titanate)**

BaTiO_3



There are 8 corner atoms of Ca^{2+} (**RED COLOUR**)

Therefore, Total share of all the corner atoms/unit cell= $8 \times \frac{1}{8} = 1$

Hence, the number of Ca^{2+} atoms/ unit cell=1

In this fig, there is one Ti atom at the centre, (**GREEN COLOUR**) hence the Number of atoms/unit cell=1

There are 6 face centered atoms of oxygen. (**BLUE COLOUR**)

Therefore,

Total share of cell of the oxygen atoms/unit cell= $6 \times \frac{1}{2} = 3$

Hence,

The Number of oxygen atom/unit cell=3

All together atoms per unit is the combination results in CaTiO_3

Polymorphism and Allotropy:

When a material has more than one crystal structure it is known as Polymorphism. Or the phenomenon in which a solid chemical compound exists in more than one crystalline form is known as polymorphism.

When an elemental solid exists in more than one crystalline form, the phenomenon is known as allotropy and different crystalline forms are known as allotropes. For ex: diamond and graphite are the allotropic forms of carbon.

X-RAYS

X – Rays are electromagnetic radiations of wave lengths between 1 \AA^0 to 100 \AA^0 . X-rays were first discovered by Roentgen in 1895. X-rays are produced when high speed electrons strikes a target material. X-ray carries very high photon energy and hence they have high penetration power than ordinary light. It has many more applications in medical and research field.

Bragg's Law:

A simplified way of looking at the process by a crystal was proposed by W.L. Bragg. He suggested that through the crystal a set of equidistant parallel crystal planes in which the atoms are arranged in regular interval, a parallel plane is represented.

Suppose a parallel beam of X-rays is incident in a direction of making a glancing angle θ with the surface of the plane. Each atom acts as a scattering centre of X-rays & sends out spherical wave fronts. Since the X-rays are highly penetrating radiations. It is necessary to consider the rays scattered not only from a single layer but from several layer.

Let us consider two parallel rays PQR and ABC which are scattered or reflected by two atoms at Q and B. in adjacent layers. The path difference between PQR and ABC is $(BM + BN)$. The condition that the scattered wave fronts be in the same phase is that the path difference between scattered wave from one layer and that from the next be an integral multiple of wavelength (λ).

From figure, angle $BQM = \theta$, $BQN = \theta$ and $BQ = d$

\therefore In the ΔBQM and BQN

$$\sin\theta = MB/BQ$$

$$\therefore MB = d \sin\theta$$

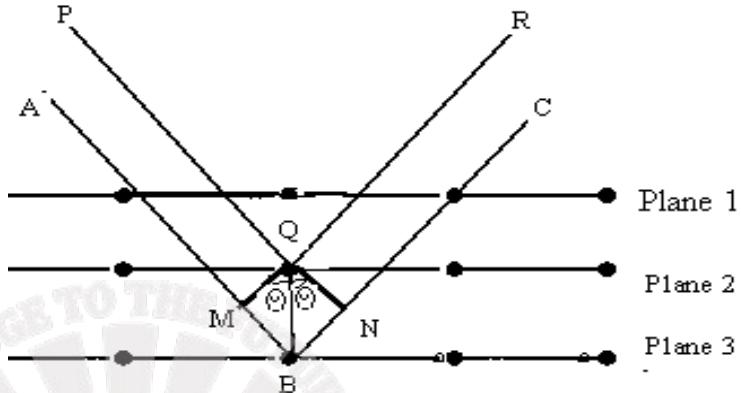
$$\text{Similarly, } BN = d \sin\theta$$

$$\therefore \text{Path difference} = BM + BN$$

$$= d \sin\theta + d \sin\theta \\ = 2d \sin\theta$$

Therefore two rays will reinforce with each other and produce maximum intensity. i.e.
Path difference = $n\lambda$,

$i.e. = 2d \sin\theta = n\lambda$



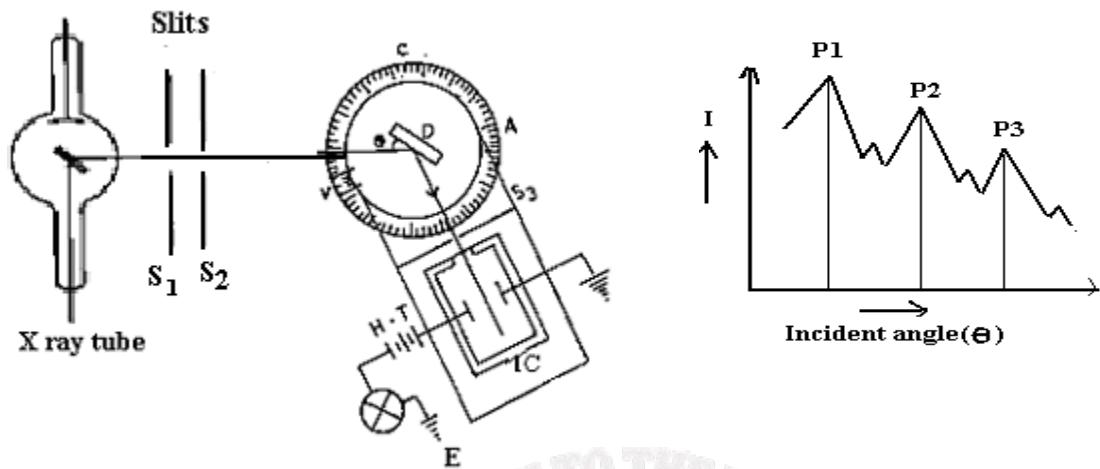
Where n is an integer ($n = 1, 2, 3, \dots$), d is the interplanar spacing distance & θ is the angle of incident radiation.

Bragg's X ray Spectrometer:

Bragg's X-ray spectrometer consists of a X-ray tube which produces x-rays. Electrons produced by a filament F as shown in fig. The accelerated through large potential difference of the order of several kilovolts and made incident on a tungsten or molybdenum target. The X-rays are collimated by two slits S₁ and S₂ the collimated X-rays are made incident on a crystal D mounted on a rotating turn table which is provided with a graduated circular scale to measure the angular displacement of the crystal.

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If the turn table is rotated by an angle θ , the diffracted beam rotates by an angle 2θ , the intensity of diffracted beam is recorded by an ionization chamber connected to an electrometer E.

When the crystal is rotated, peaks of ionization current are observed when Bragg's condition is satisfied at that particular angle.

By Bragg's Law, we have $2d \sin \theta = n\lambda$.

The peaks P₁, P₂ & P₃ correspond to first, second and third order reflections. If θ_1 , θ_2 and θ_3 are the angles of incidence for the different orders of reflection with $n = 1, 2$ and 3 respectively for a given wavelength λ then we can write.

$$2d \sin \theta_1 = \lambda$$

$$2d \sin \theta_2 = 2\lambda \quad \&$$

$$2d \sin \theta_3 = 3\lambda$$

$$\Rightarrow 2d \sin \theta_1 : 2d \sin \theta_2 : 2d \sin \theta_3 = \lambda : 2\lambda : 3\lambda$$

$$\Rightarrow \sin \theta_1 : \sin \theta_2 : \sin \theta_3 = 1 : 2 : 3$$

The above equation can be used to verify the accuracy of the measurements.

Using Bragg's equation, if the distance 'd' between the successive planes in the crystal is known then the wavelength of X rays can be determined and if λ is known then d can be determined.

The value of interplanar spacing's calculated from this experiment is used to determine the crystal structure.

Determination of crystal structure:

One gets different values of d depending upon the particular set of parallel planes that satisfy Bragg reflection as θ is changed .by taking the ratios of the different values of d obtained. It is possible to decide the particular crystal system to which the experiment crystal belongs.

Let us consider the case of a cubic crystal the interplanar spacing for (100) planes for d_1 , and that for (110) & (111) planes are d_2 & d_3 .the geometry of the planes in a cubic crystal

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

$$d_1 : d_2 : d_3 = 1 : \frac{1}{\sqrt{2}}$$

$\therefore \frac{1}{\sqrt{3}}$ it indicates that the crystal structure of the cubic.

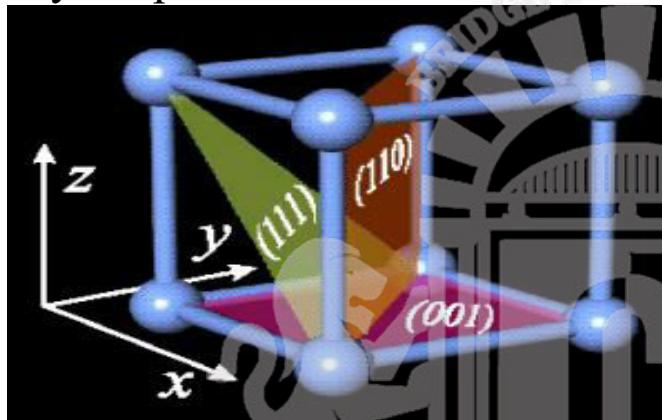
Knowing λ and a , the values of Θ can be compared. These values of Θ are compared with those obtained values from the Bragg's spectrometer reading. A perfect match between computed and observed value establishes the validity of Bragg's law.

Similarly for FCC , $d_1 : d_2 : d_3 = 1 : \frac{1}{\sqrt{2}} : \frac{2}{\sqrt{3}}$ and
 BCC, $d_1 : d_2 : d_3 = 1 : \frac{2}{\sqrt{2}} : \frac{1}{\sqrt{3}}$

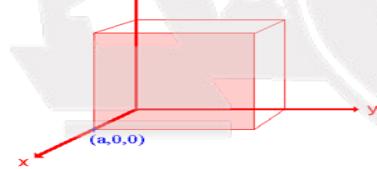
Applications of X-rays:

1. Scientific research
2. Industrial and Engineering
3. Medical uses

Crystal planes



An example:

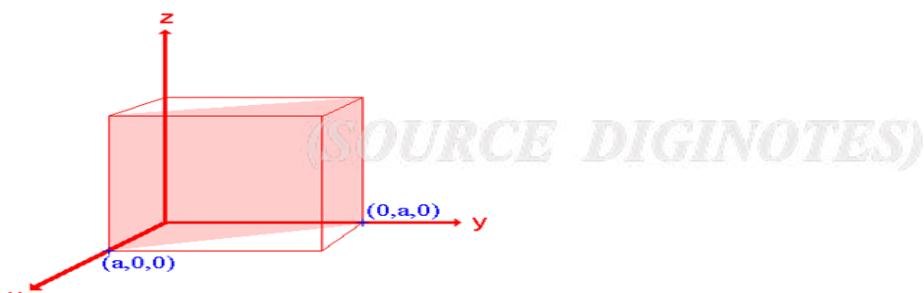


Intercepts: a, ∞, ∞

Reciprocals: $a/a, a/\infty, a/\infty$
 $= 1, 0, 0$

Miller index for this plane : $(1\ 0\ 0)$

(note: this is the normal vector for this plane)



Intercepts: a, a, ∞

Reciprocals: $a/a, a/a, a/\infty$
 $= 1, 1, 0$

Miller index for this plane : $(1\ 1\ 0)$

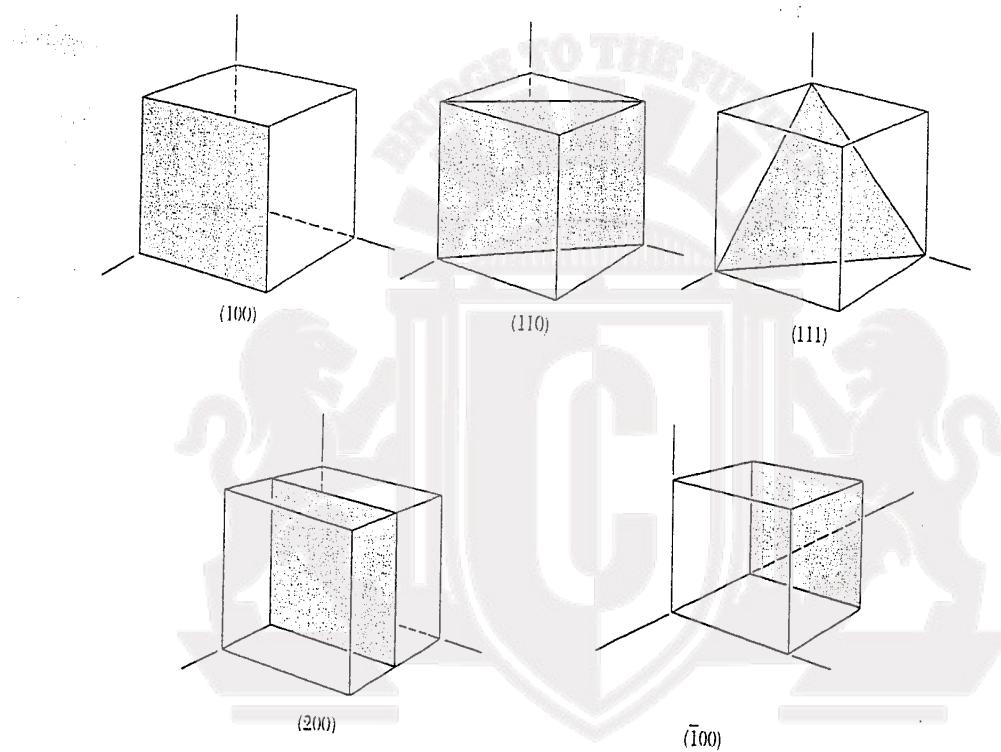
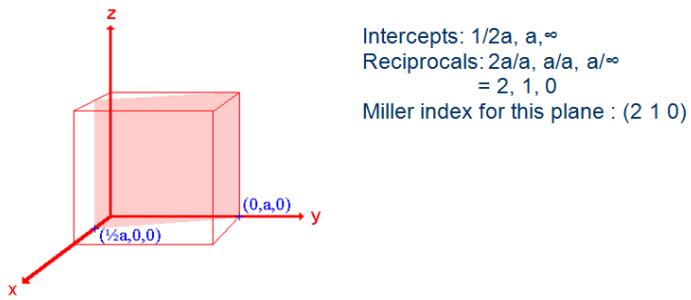


Figure 16 Indices of important planes in a cubic crystal. The plane (200) is parallel to (100) and to (100).

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QUESTION BANK

- 1) Derive an expression an Interplanar spacing in a cubic system by using Miller indices
- 2) Describe the seven crystal systems
- 3) Define coordination number and packing factor. Calculate the coordination number and packing factor for SC and BCC structures
- 4) With a neat figure, explain the structure of diamond and show that atomic packing factor of diamond is 0.34.
- 5) Define lattice points, primitive cell, Bravais lattice, and space lattice 6)
Explain the procedure to find miller indices with an example.
- 7) Explain how Bragg's spectrometer is used for determination of interplanar spacing in a crystal.

MODULE: 5 **Nanomaterials**

Introduction;

- Materials with a characteristic length scale (diameter and size) less than 100nm are called Nanomaterials.
- The prefix 'nano' means a billionth 10^{-9}
- The field of nanotechnology deals with various structures of matter having dimensions of The order of a billionth of a meter these particles is called nano particles.
- Nanoscale materials are materials where at least one dimension is less than approximately 100nm.
- A nanometer is one millionth of a millimeter approximately 10^5 times smaller than the diameter of a human hair.
- Nanotechnology is based on the fact that particles which are smaller than about 100nm gives rise to new properties of nanostructures built from them. Particles which are smaller than the characteristic length for a particular phenomenon show different physical and chemical properties than the particles of larger sizes.
- Ex: mechanical properties, optical properties, conductivity, melting point and reactivity have all been observed to change when particles become smaller than the characteristic length., gold and silver nanoparticle were used in window glass planes to obtain a variety of beautiful colours.Nanotechnology has wide range of applications like producing lighter but stronger materials, constructing switches for computers, improving drug delivery to specific organs of the body etc.

Quantum structures:

*When the reduction from the bulk material is in one direction, it results in a structure called film. (I.e. from 3-D to 2D)

* If the reduction in two directions, obviously the resultant will be in 1-D which is called quantum wire (i.e. From 2-D to 1-D)

- * If the reduction in all the three directions, the material reduces to a point which is known as quantum dot. it is also called as a nanoparticles or cluster.

Density of states:

Density of states is the possible electron quantum energy states between energies E and E+dE per unit volume, the density of states for metals in three dimensions in a bulk material is given by,

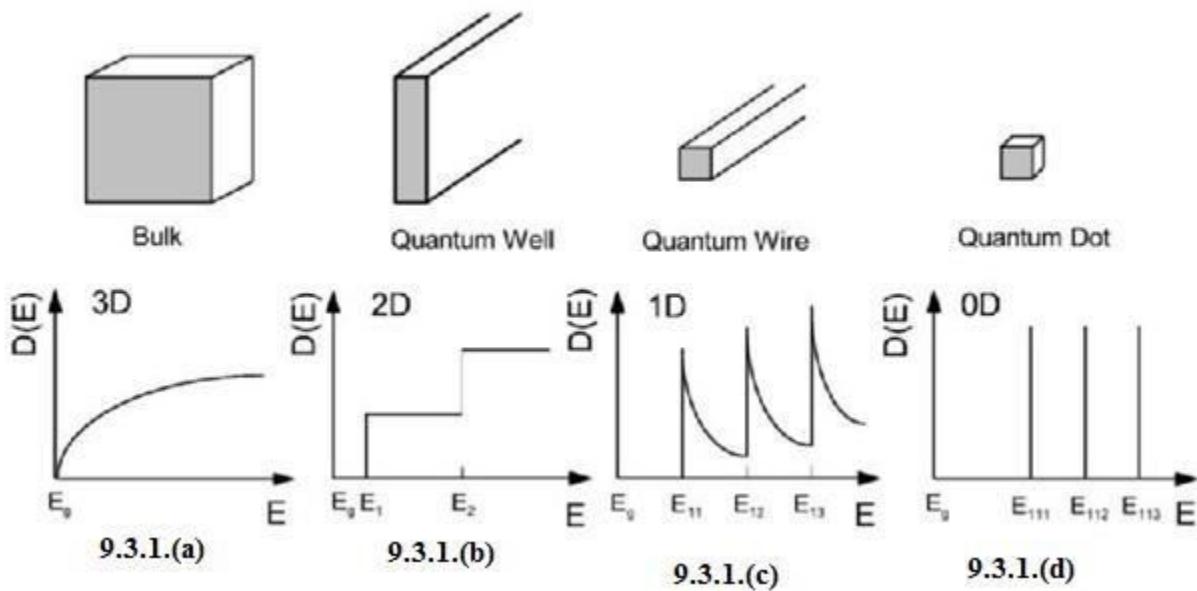
$$D(E) = \frac{8\sqrt{2} \pi m^{3/2}}{h^3} E^{1/2} dE$$

Hence the density of states with energy as shown in the fig 9.3.1.(a)

From the above equation we can conclude that the density of states in a bulk material is proportional to $E^{1/2}$ and hence increases with energy.

If the electrons are confined in one or more directions by reducing the dimensions of the material in those directions, the density of states changes due to quantization of energy.

- For a quantum well, which is a material reduced in one dimension to nano-scale there is quantization of energy due to confinement of electrons in one direction. The density of states for a quantum well is constant as shown in fig 9.3.1. (b).for different quantum states it has different constant values.
 - For a quantum wire which is a material reduced in two dimension to nano-scale there is quantization of energy due to confinement of electrons in 2-D the density of states for a quantum wire.
- The density of state for a given quantum state will decrease with increasing energy as shown in fig 9.3.1.(c) , for the different quantum states , it has variation as shown in fig 9.3.1.(c).
- For a quantum dot, which is a material reduced in all three directions to nano scale, there is quantization of energy due to confinement of electrons in all the directions. Hence, for a quantum dot only some discrete energy states are allowed for the electrons. As only certain energy states are allowed. The density of states has a discrete structure as shown in fig 9.3.1.(d).



SYNTHESIS OF NANOMATERIALS

There are two methods followed in preparing nanomaterials.

*Top-down approach and *Bottom-up approach.

In the top-down approach, the material is reduced from bulk size to nano-scale.

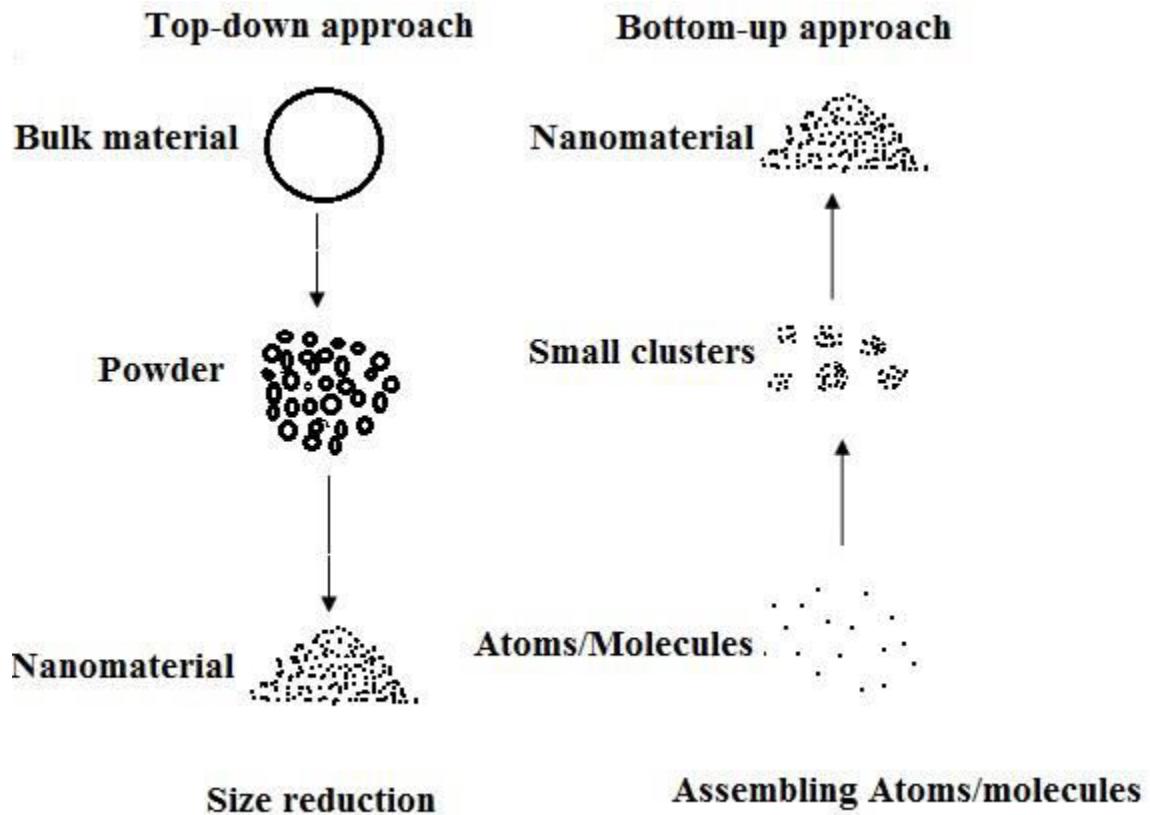
There are many methods which follow this approach .the examples

are, 1) Ball milling method and 2) Nanolithography.

- In ball milling method, the bulk material which is taken in powdered form is reduced further by grinding technic until nano –scale size is reached.
- Lithography is a process which involves forming a thin film of material on substrate, (substrate: is a material on the surface of which an adhesive substance is spread as a coating) where in a precise control over its thickness and area is exercised. it is basically employed in semiconductor technology in the manufacture of integrated circuits & VLSI

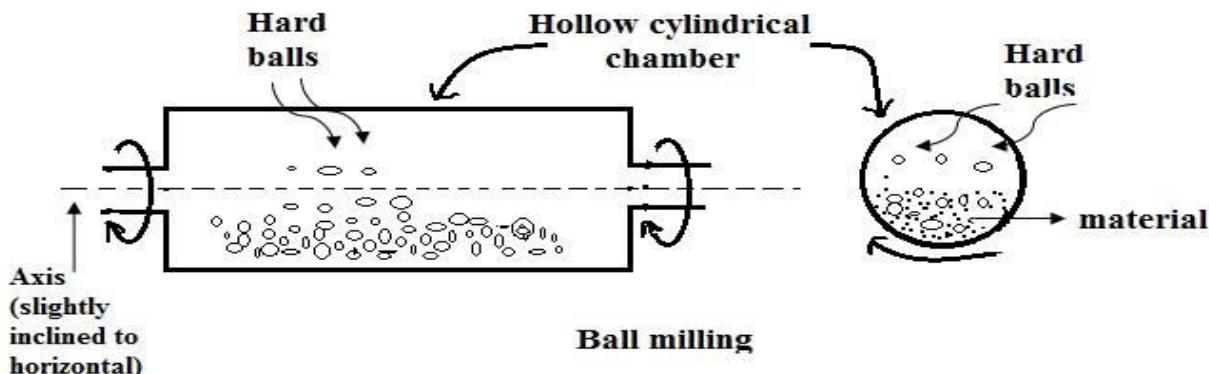
In the bottom-up approach, matter in atomic or molecular level gets assembled to form tiny clusters which grow to reach nano-size.

Few examples for this approach are Arc discharge, chemical vapour deposition, physical vapour deposition, sol-gel method.



Ball milling method:

This is a method used for top down approach i.e., bulk material is broken down into nanosize particles.



Construction:

- The ball milling consists of a hollow cylindrical chamber that can rotate about its own axis.
- It consists of a hard and heavy balls made of tungsten carbide or steel inside the chamber.
- Larger balls are used for milling to produce smaller particle size.
- The chamber is mounted such that, its axis is slightly inclined to the horizontal to enable the material inside to slide, and accumulate around in one region.

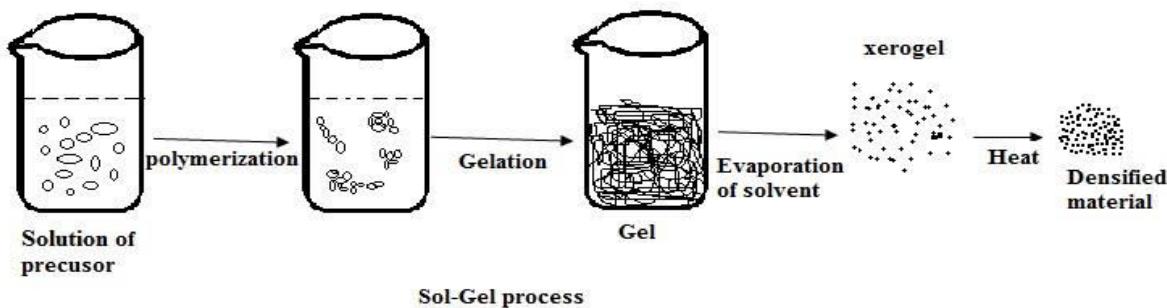
Working:

- The given material is crushed into small grain size and fed into the chamber.
- The cylindrical chamber is rotated around its own axis, the ball get carried upwards. But under gravity, they drop down and hit the sample with the high speed.
- This happens repeatedly and the material to get reduced to nanosize particles.
- However The speed of rotation must be less than a critical speed beyond which , the balls, instead of falling down , will be carried along the periphery of the chamber all along. Then the material misses the hit & reduction in size stops before attaining the nanoparticle size.
- Ball milling method is employed while producing metallic and ceramic nanomaterials. When the milling time is around 20-200 hours, it will be called high energy ball milling which is capable of causing structural changes as chemical reaction. **Advantages:**
 - 1) This method is suitable for large scale production at low cost.
 - 2) It can be used to grind material irrespective of hardness.
 - 3) Nanopowders of 2-20 nm size can be produced by using this technique and size of nanopowder depends on the speed of rotation of the balls. **Disadvantages:**
- 1) The shape of the nanomaterials produced by this method is irregular.
- 2) Many contaminates are inserted from ball and milling additives during this technique.
- 3) Crystal defects are produced during ball milling.

Sol –gel method:

- * Sols are solid particles suspended in liquid medium.
 - *Gels comprise of long networks of particles like polymers in which, the interspaces form pores that contain liquid.
 - *In the gel phase, both the liquid and the solid are dispersed in each other so that, the Material possesses the character of both the solid and the liquid phases.
- “Sol-gel is a process in which, precipitated tiny solid particles agglomerate to form long networks which are spread continuously throughout a liquid in the form of a gel”.***

- In sol-gel method, precursors which have a tendency to form gel are chosen (Precursors: is a substance that leads to the formation of the desired substance after a certain chemical process.)
- A solution of the precursor is obtained by dissolving it in a suitable solvent.
- The precursors are generally inorganic metal salts or alkoxides which undergo hydrolysis. By polycondensation process, nucleation of solid particles starts and sols are formed.



- Then the sols undergo polymerization (i.e., forming continuous network of particles) which in turn turns the solution into a gel.
- The sol-gel is then centrifuged from which a form of gel called Xerogel, which has zero or only traces of the dispersion medium, is obtained.
- The Xerogel is then dried by heating it up to a temperature of 800°C during which time, the pores of the gel network collapse. This is called densification after which we obtain the desired nanomaterials.

Advantages:

- 1) Highly pure and uniform nanostructures can be obtained in sol-gel processing,
- 2) It is a least expensive technique with fine control of the products chemical composition.
- 3) With this method, powder, fiber, thin film, coating can be made. 4) Moderate temp are sufficient for drying or calcinations of the sample

Carbon nanotubes:

“A carbon nanotube is a sheet of carbon atoms joined in a pattern of hexagonal, rolled into a cylinder.”

In the year 1991, a Japanese researcher Iijima of NEC, was synthesizing C_{60} fullerene by striking an electric arc between two graphite rods. He found that, needle like cylinder tubes of graphite sheet were formed on the graphite electrodes. He named those tubes as “nanotubes”

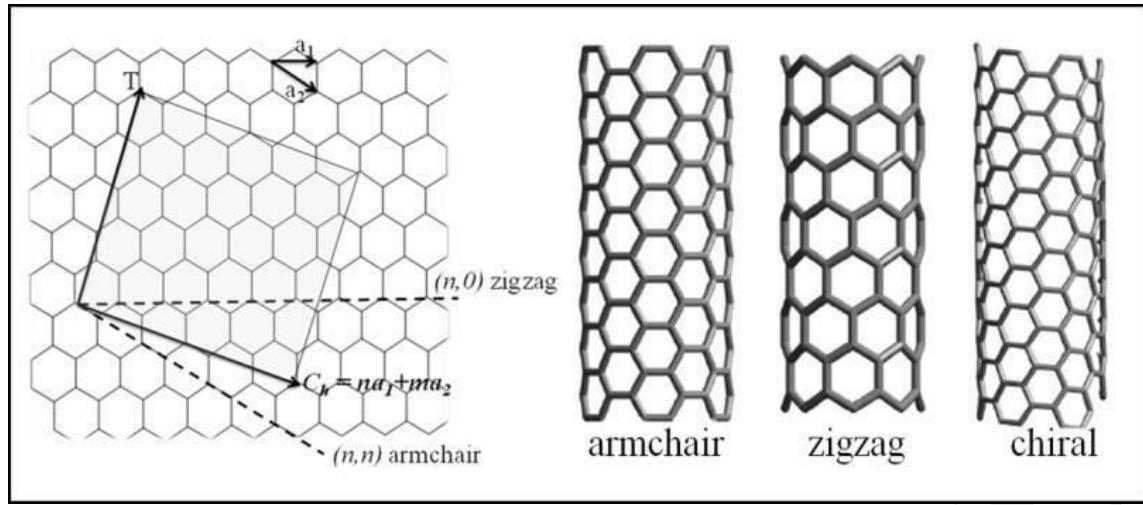
Types of the carbon nano tubes (CNTs):

- 1) Single wall nanotubes (SWNT); in these tube one or both the ends either open, or closed by half fullerene as cap. If there is only one layer of graphite sheet, then it is called single walled nanotubes.
- 2) Multiwalled nanotubes (MWNT): This can be considered as nanotubes with in nanotubes. Or bigger ones enclosing the smaller ones layer.

The nanotubes conducting properties depend upon how the two ends of the sheet meet along, it can happen in 3 different ways leading to 3 different varieties. The resulting molecular structures are defined by roll-up vector, denoted by T. T signifies the axis about which the sheet is rolled. Fig 7.

- If T is parallel to C-C bonds, then it is “**armchair**” structure. fig 8
- There are two more structures in which the nanotubes are found” **zigzag**” structure and “**Chiral**” structure. To obtain these 2 structures the graphite sheet is to be rolled with T at certain angles to C-C bond. Fig 9,& 10.
- All nanotubes with armchair structure conduct like metals.
- The other two structures, depending on the actual angles made by T with respect to the bond angle, the conducting property also varies.

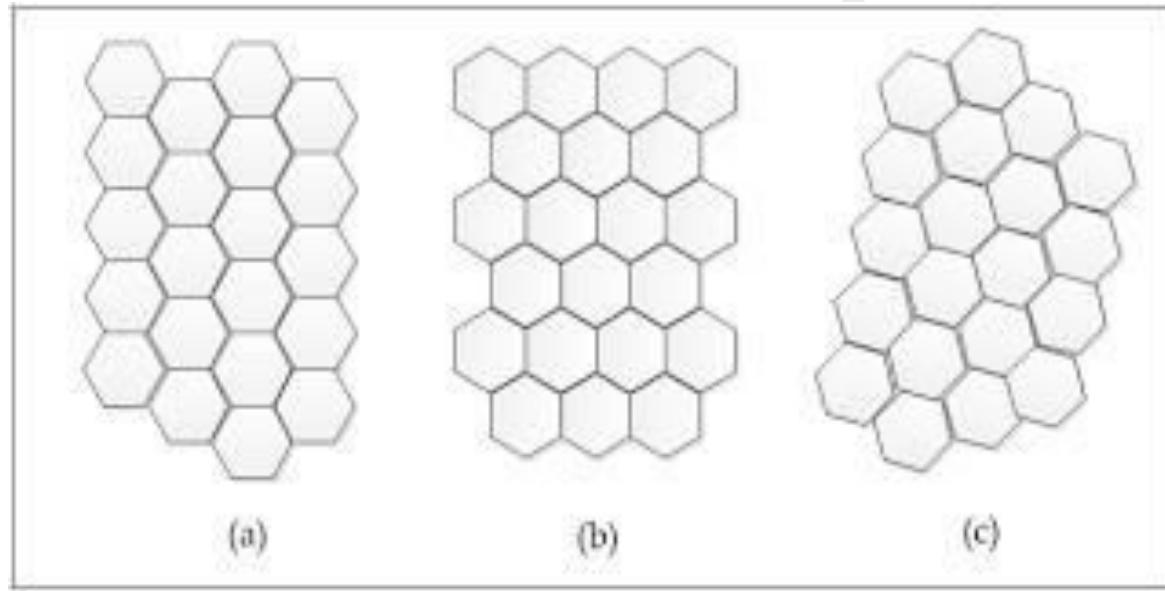
About one third of all zigzag and Chiral nanotubes conduct like metals , and remaining two third exhibit less conductivity (like semiconductors).



a) Armchair

b) zigzag

c) Chiral



Properties of carbon nanotubes:

- 1) **Thermal;** carbon nanotubes are very good conductors of heat, their thermal conductivity are more than twice that of diamond.
- 2) **Electrical;** Electrical properties depend on number of free electrons, collision of electrons, and dimensions of material. At the nano scale the dimension are altered. Carbon nanotubes have found to be metallic or semiconducting depending on their structure. The tube length and diameter are also responsible for change in electrical property.

An insulator can become a conductor at the nano scale. 3)

Mechanical:

*Mechanical properties of nanoparticles are decided by the size of the nanoparticles, surface atoms, etc.

*The carbon nanotubes are highly elastic. The young's modulus is a measure of the elasticity. The young's modulus of carbon nanotubes is about 1800Gpa where it is about 210Gpa for steel.

*carbon nanotubes exhibit large strength in tension. They are about twenty times stronger than steel.

* The carbon nanotubes strength is of about 45Gpa.but steel is 2Gpa.

*the carbon nanotubes can withstand larger strains then steel. They can be bent without breaking.

4) **Chemical;** a change in number of atoms on surface can change the chemical properties like catalytic activity, combustion, etc

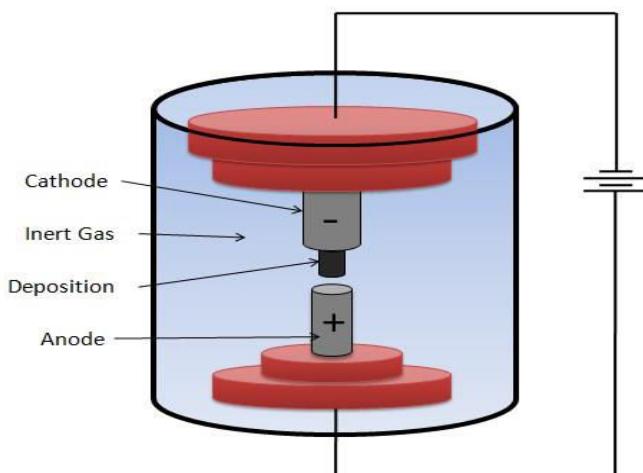
*CNTs are chemically more inert compared to other forms of carbon.

5) **Physical:** CNTs have very high strength to weight ratio, they have low density.

Synthesis of carbon nanotubes:

1) Arc discharge method

2) Pyrolysis method **Arc discharge Method:**

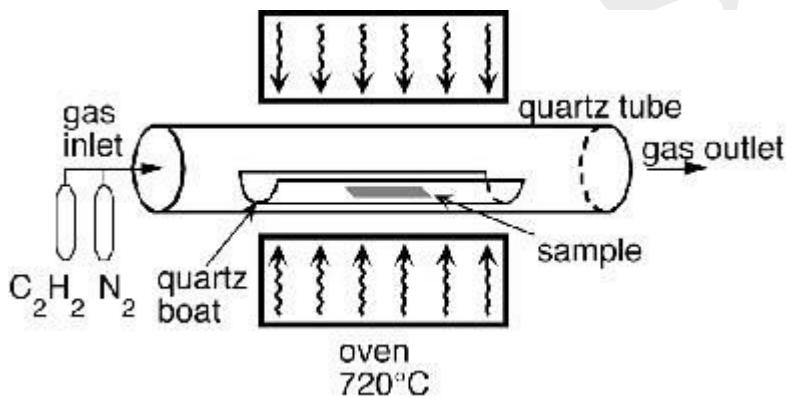


- It consists of a vacuum chamber in which two graphite rods are mounted on the two supports.
- The gap between two graphite rods is about 1-2 mm.
- The chamber is evacuated by using a vacuum pump, and a methane gas at certain pressure is introduced into the chamber.
- The two rods are maintained at a suitable dc potential difference to enable the discharge.
- On the application of the voltage, the arc discharge starts. Carbon evaporates from the anode.
- Some part of the evaporated carbon, deposits on the cathode tip layer. This is called hard deposit. And the rest condenses on the other parts of the cathode (called cathode soot) and on the walls of the chamber (called chamber soot). Both the cathode soot and the chamber soot yield, either single -walled or multi -walled carbon nano tubes.

- If the nickel, cobalt, iron catalyst is used in the central region of the positive electrode, single walled nanotubes are formed.
 - In the absence of catalyst between two graphite electrodes multi –walled nanotubes are formed.
 - Whereas the hard deposit does not yield any carbon nanotubes.
 - Through this method can produce large quantities of nanotubes,
 - It involves purification of the soot by oxidation, centrifugation, filtration and acid treatment.
 - However the resulting products will be highly impure, as, 60-70% .if pure graphite rods are used means >95% products will get.
- *This is a bottom-up approach in nanotechnology

Pyrolysis method (fabrication of carbon nanotubes using chemical vapour deposition.):

Pyrolysis is the decomposition of a chemical compound of higher molecular weight into simpler compounds by heating in the absence of oxygen (high temp), so that no oxidation occurs. It takes place at a temp in the range of 400°C to 800°C .



- It consists of a quartz tube kept in a furnace. The quartz tube is connected to sources of acetylene (C_2H_2) and nitrogen.
 - The substrate containing cobalt and nickel which act as catalyst is kept in a quartz plate. The quartz tube is provided with an outlet for the gas. The temperature in the quartz tube is maintained at about $400^{\circ}\text{C} - 800^{\circ}\text{C}$.
 - Due to the high temperature in the quartz tube, acetylene breaks down into carbon atoms. When these carbon atoms come near the substrate, they get absorbed and get converted into nanotubes due to the presence of catalyst. This method produces multi-walled nanotubes.
 - To produce single walled nano –tubes, a methane or carbon monoxide source is used instead of acetylene. The temp for these sources is maintained at about 1200°C .
- *Pyrolysis is a bottom-up method..

Applications:

- 1) Using semiconductor nanotubes, it has been possible to make electronic components such as transistors and electronic logic gates which could be used for computing purposes.
- 2) CNTs are used to make high quality tennis rackets to build aircrafts and making micro mechanical systems(MEMS)
- 3) CNTs are used to develop flat panel displays for television and computer monitors.
- 4) CNTs are used in the tips for atomic force microscope probes.
- 5) CNTs are used to develop light weight shield for electromagnetic radiation 6) They are used in chemical sensors to detect gas.
- 7) They are also used in batteries (can store lithium).
- 8) Sensors: used in smoke detectors, gas sensors
- 9) Cosmetics: sun screen lotions containing nano TiO₂ provide enhanced sun protection factor. The added advantage of nano skin blocks arises they protect the skin by sitting onto it rather than penetrating into the skin, thus they block uv radiation effectively for prolonged duration
- 10) Based on optical property.
Used in optical detector, imaging solar cell

Scanning electron microscope (SEM):

- A microscope is basically an instrument which provides a magnified image of an object.
- SEM is the kind of microscope that uses a beam of electrons to create a magnified image of the specimen. **Principle:**

The principle used in the working of an SEM is the wave nature of electron. An electron accelerated under a potential difference of V volts behave like a wave nature of light

$$\lambda = \frac{h}{\sqrt{meV}} = \frac{1.226}{\sqrt{V}} \text{ nm}$$

this is the basic principle made use of in the working of all kinds of electron microscope.

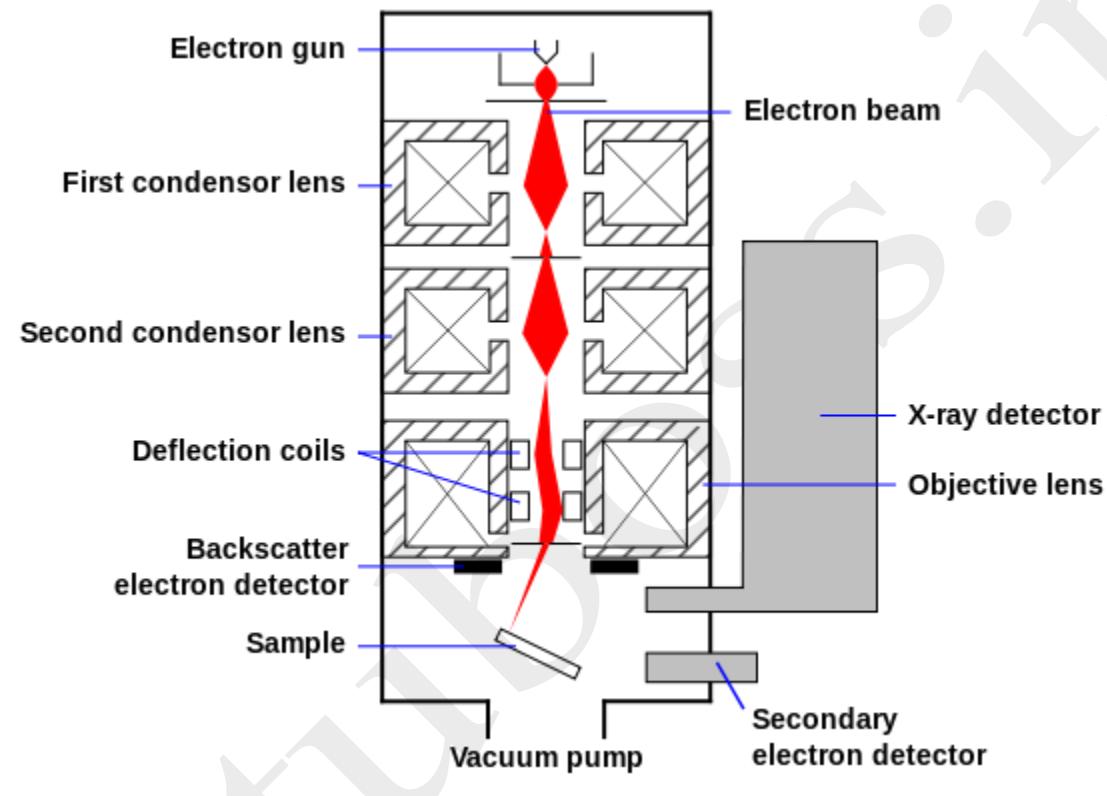
Construction:

- The apparatus consists of an highly evacuated chamber inside which there is an electron gun at the top, which consists of the filament and the anode.
- It consists of two magnetic lenses, 1) one is the condensing lens 'C' and other one is the objective lens 'O' (these are actually a pair of current carrying coils which provide magnetic field between them).
- A scan coil is accompanies the lens 'O'.
- A flat surface called stage is provided at the bottom portion of the apparatus to place the specimen under study.
- There are 3 types of detectors in the apparatus, they are back scattered electron detectors, secondary electron detectors, x-ray detectors.
- The electrons incident on the sample are called primary electrons, out of these, some of them will be scattered by the sample and some of them knockout the electrons from the atoms in the specimen those which are scattered by the sample are back scattered electrons. and the one which are knocked off from the atoms are called secondary electrons

Working:

- The sample is to be placed on the specimen stage after which, inside the chamber is evacuated by connecting it to a high vacuum pump.
- Electrons are emitted by the filament by thermionic emission.
- A suitable + ve potential is applied to the anode with respect to the filament.
- The accelerated electrons from the electron gun passes through the condensing lens C. Converges the beam and the beam passes through the objective aperture, hence the size of the beam can be controlled. a thinner beam enters into the field of objective lens O. the objective lens focuses the beam onto the desired part of the specimen.

- A set of coils called scan coils placed along with the objective lens, enable the beam to scan. The specimen in a particular way called raster. The scan coils are connected to a raster scan generator which directs the beam onto a spot the specimen.
- Upon incidence, electrons are scattered out from the specimen, the back scattered electrons, secondary electrons and the X-ray emitted are detected by the respective detectors. As the case happens to be and a corresponding signal is produced. The signal is converted into a micro spot of corresponding brightness on a screen (which resembles the one in a TV)
- The beam focus is shifted to the next adjacent spot in order, where again dwells momentarily – and so on. This way image is built on the screen point to point.



Applications:

- SEM is used to study biological specimens like pollen grains.
- Crystalline structure.
- SEM is used in forensic investigations.
- SEM is used to study external morphology of biological organisms in the sub microscope.
- SEM is used to study properties like hardness and melting point of elements and compounds in the sample.
- SEM it can be also used to study the properties like reflectivity and roughness of the sample.

Vtuboss.in

Shock waves:

Mach number:

In aerodynamics the speeds of bodies moving in a fluid medium are classified into different categories on the basis of Mach number.

It is defined as “The ratio of the speed of the object to the speed of sound in the given medium”.

$$\text{Mach number} = \frac{\text{object speed}}{\text{speed of sound in the medium}}$$

$$M = \frac{v}{a}$$

Where, M= Mach number

V= object speed a =

Speed of sound in the medium

Note* It does not have any unit. It is a pure number.

Distinction between Acoustic, ultrasonic, Subsonic and Supersonic waves:

Acoustic waves: These are longitudinal waves that travel in a medium with the speed of sound in that medium .These waves can propagate in solids, liquids and gases.

Acoustic waves can be classified into the following three types depending upon their frequency.

- 1) Infrasonic: These acoustic waves have frequency less than 20HZ. The human ear cannot detect these waves.
- 2) Audible: These acoustic waves have frequency between 20HZ to 20KHZ. The human ear is sensitive to these waves. They cause sensation of hearing in human beings.
- 3) Ultrasonic: These acoustic waves have frequency more than 20KHZ. The human ear is not sensitive to these waves. *An acoustic wave is sound wave.
 * It moves with a speed of 333m/s in air at STP
 *Sound waves have frequencies between 20HZ to 20KHZ.
 * Amplitude of Acoustic wave is very small.

Ultrasonic waves: Ultrasonic waves are pressure waves having frequencies beyond 20KHZ. But they travel with the same speed as that of sound .The Mach number =1

- Amplitude of ultrasonic wave is also small.

Subsonic wave: If the speed of mechanical wave or body moving in the fluid is lesser than that of sound, such a speed is referred to as subsonic wave. The Mach number <1.

Ex: The vehicles such as motor cars, trains, flight of birds is also subsonic.

- For a body moving with subsonic speed, the sound emitted by it manages to move ahead and away from the body since it is faster than the body.

Supersonic waves: Supersonic waves are mechanical waves which travel with speeds greater than that of sound.i.e. with speed for which, Mach number >1

A body with supersonic speed zooms ahead by piercing its own sound curtain, leaving behind a series expanding sound waves with their centers displaced continuously along its trajectory.

Today's fighter planes can fly with supersonic speed .Amplitude of supersonic waves will be high it affects the medium in which it is travelling.

Shock waves:

- Any fluid that propagates at supersonic speeds, gives rise to a shock wave.
- Shock waves are produced in nature during earth quakes (as seismic waves which travel with speeds ranging from 2km/s to 8km/s).
- When lightning strikes.

Shock waves can be produced by a sudden dissipation of mechanical energy in a medium enclosed in a small space.

“A shock wave is a surface that manifests as a discontinuity in a fluid medium in which it is propagating with supersonic speed”.

They are characterized by sudden increase in pressure, temperature and density of the gas. Through which it propagates.

Shock waves are as strong or weak depending on the magnitude of the instantaneous change in pressure and temperature in the medium

Ex: The shock waves created by the explosion of crackers, bursting of an automobile tire, during lighting thunder, during nuclear explosion.

- For strong shock waves mach no is high.
- For weaker shock waves the mach no is low(lesser than 1) **Applications of Shock waves:**
 - They are used in the treatment of kidney stones.
 - Cell information
 - Wood preservation
 - Use in pencil industry
 - Gas dynamic studies
 - Shock waves assisted needle less drug delivery ➤ Treatment of dry bore wells.

Basic of conservation of mass, momentum, and energy.

Conservation means the maintenance of certain quantities unchanged during physical process.

- Conservation laws apply to closed systems.
- A closed system is the one that does not exchange any matter with the outside and is not acted on by outside forces.

The conservation of mass, momentum and energy are the three fundamentals principles of classical physics.

1) Law of conservation of mass:

“The total mass of any isolated system remains unchanged and is independent of any chemical and physical changes that could occur within the system”

Or

“The total mass of a system remains constant as mass can neither be created nor destroyed”

2) Law of conservation of momentum:

“In a closed system the total momentum remains a constant”

Or “When two objects collides in an

isolated system, the total momentum of the objects before collision =the total momentum of the objects after collision”

3) Law of conservation of Energy:

“The total energy of a closed system remains constant and is independent of any changes occurring within the system”

Types of shock waves:

- **Stationary shock wave:** In a stationary shock wave, the shock front remains stationary with respect to fixed observer.
- **Moving shock wave:** such shock waves travel in fluids which are either stationary or move with small speeds with respect to the observer.
- **Normal shock wave:** if the shock wave is perpendicular to the flow of gas, it is known as normal shock wave.
- **Oblique shock wave:** if the shock wave is at some angle (other than 90^0) to the flow of gas it is known as oblique shock waves.

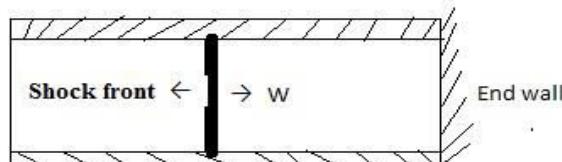
Derivation of normal shock relationship using simple basic conservation equations (Rankine-Hugonit equations):

Consider a shock wave propagating with a speed W in a shock tube.

The conditions of the shock wave at the downstream end can be determined by solving the equations for conservation of mass, momentum and energy, as applied to the shock region. These equations are known as Rankine-Hugonit relations.

* Consider two regions with reference to the shock front, one which is head of the shock front and the other behind it.

*Both the regions are at far enough distance from the shock front so that equilibrium conditions prevail the two regions where, the physical conditions such as pressure, density etc. are uniform.



Let us consider pressure (P_1) temperature (T_1), density (ρ_1), and enthalpy (h_1) before creation of the shock wave.

Similarly (P_2), (T_2), (ρ_2) and (h_2) be the corresponding values after creation of the shock wave.

Then the three conservation relations which correspond to the conservation laws.

$$\rho_1 u_1 = \rho_2 u_2 \quad \text{----- (1) conservation of mass}$$

Where u_1 is the velocity of the fluid ahead of the shock.
 u_2 is the velocity of the fluid following shock

$$P_1 + \rho_1 u_1^2 = P_2 + \rho_2 u_2^2 \quad \text{----- (2) conservation momentum}$$

$$\text{And} \quad h_1 + \frac{u_1^2}{2} = h_2 + \frac{u_2^2}{2} \quad \text{----- (3) conservation of energy}$$

These 3 equations along with the equation of states

$$PV=RT \text{----- (4)}$$

Lie at the roots of all the aerodynamic problems and applications.

Using the above equations, the following normal shock relations called Rankine-Hugoniot equations can be derived in which P_5 and T_5 represent pressure and temperature at the downstream and behind the reflected shock wave.

$$1) \frac{P_2}{P_1} = [1 + \frac{2\gamma}{\gamma+1} (m^2 - 1)]$$

$$\frac{\gamma+1}{\gamma-1} \frac{p_2}{p_1}$$

$$2) \frac{T_2}{T_1} = \frac{P_2}{P_1} \left[\frac{1 + \gamma(-\gamma + 1)}{1 + \gamma(\gamma + 1)} \right]$$

$$PP_{25} = ($$

$$\frac{3(\gamma\gamma - 11)\rho}{pp_1 \frac{2^2}{\gamma-1} + \frac{-(\gamma(\gamma + 11))}{p}}$$

3)

$$\frac{\gamma+1}{\gamma-1} \frac{p_5}{p_2}$$

$$4) \frac{T_5}{T_2} = \frac{P_5}{P_2} \left[\frac{1 + \gamma(-\gamma + 1)}{1 + \gamma(\gamma + 1)} \right]$$

Methods of creating shock waves in the laboratory using a shock tube:

Shock waves can be created in the laboratory by

- (a) Using a Reddy shock tube
- (b) Detonation
- (c) Very high pressure gas cylinder
- (d) Combustion
- (e) Using small charge of explosives.

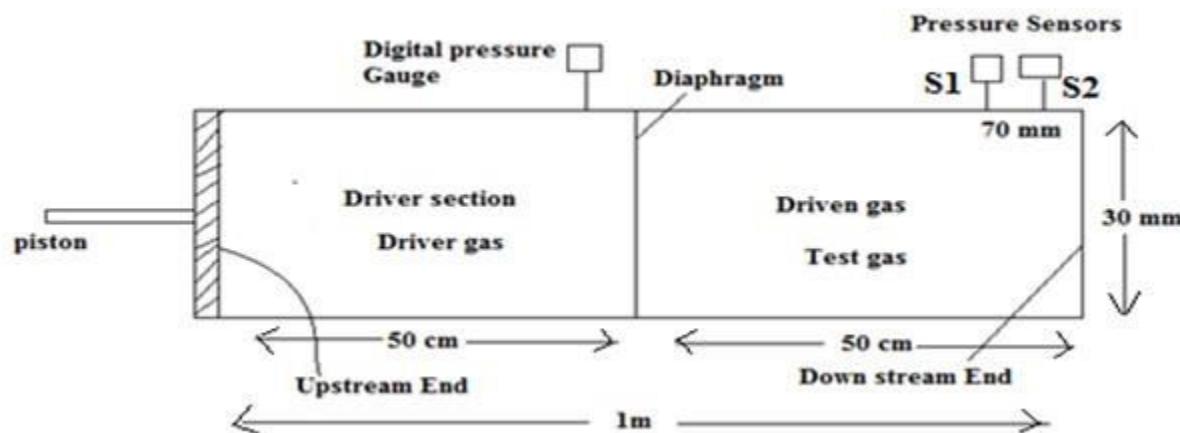
Characteristics of shock tube:

- The Reddy tube operates on the principle of free piston driven shock tube (FPST) ▪ It is a hand operated shock producing device.
- It is capable of producing mach no exceeding 1.5
- The rupture pressure is a function of the thickness of the diaphragm
- Temperature exceeding 900K can be easily obtained by the Reddy tube by using helium as the driver gas and argon as the driven gas. This temperature is useful in the chemical kinetic studies.

Description of hand operated Reddy shock tube:

Reddy tube is a hand operated shock tube capable of producing shock waves by using human energy.

It is a long cylindrical tube with two separated by a diaphragm.
It's one end is fitted with a piston and the other end is closed.



Description:

- ❖ Reddy tube consists of a cylindrical stainless steel tube of about 30mm diameter and length 1m.
- ❖ It is divided into two sections each of length 50cm.
- ❖ One is the driver tube and other one is the driven tube.
- ❖ The sections are separated by a 0.1mm thick aluminium or paper diaphragm.

- ❖ A piston is fitted at the far end of the driver section
- ❖ A digital pressure gauge is mounted in the driver section next to the diaphragm.
- ❖ Two piezoelectric sensors S_1 and S_2 are mounted 70mm apart towards the closed end of the shock tube.
- ❖ A port is provided at the closed end of the driven section for filling the test gas to the required pressure.
- ❖ The driver section is filled with a gas termed as the driver gas which is held at a relatively high pressure due to the compressing action of the piston .the gas in the driven section is termed as driven gas or test gas.

Working:

- ❖ The driver gas is compressed by pushing the piston hard into the driver tube until the diaphragm ruptures.
- ❖ The driver gas rushes into the driven section and pushes the driven gas towards the far downstream end. This generates a moving shock wave that traverses the length of the driven section
- ❖ The shockwave instantaneously raises the temperature and pressure of the driven gas as the shock moves over it.
- ❖ The propagating primary shock wave is reflected from the downstream end. After the reflection, the test gas undergoes compression which boosts its temperature and pressure to still higher values by the reflected shockwaves. This state of high values of pressure and temperature is sustained at the downstream end until an expansion wave reflected from the upstream end of the driver tube arrives there and neutralizes the compressions partially expansion waves are created at the instant the diaphragm is ruptured and they travel in a direction opposite to that of the shock wave.
- ❖ The period over which the extreme temperature and pressure conditions at the downstream end is sustained, is typically in the order of millisecond, however , the actual duration depends on the properties of the driver and test gases and dimension of the shock tube.
- ❖ The pressure rise caused by the primary shock waves and also the reflected shock wave are sensed as signals by the sensors S_1 and S_2 respectively, and they are recorded in a digital cathode ray oscilloscope.
- ❖ Since the experiment involve typically, millisecond duration measurements, the rise time of the oscilloscope should be a few microsecond. Hence an oscilloscope with a band width of 1MHZ or more is required. From the recording in the CRO, the shock arrival times are found out by the associated time base calculations, using the data so obtained, Mach number, pressure and temperature can be calculated.

Experimental analysis using Reddy tube:

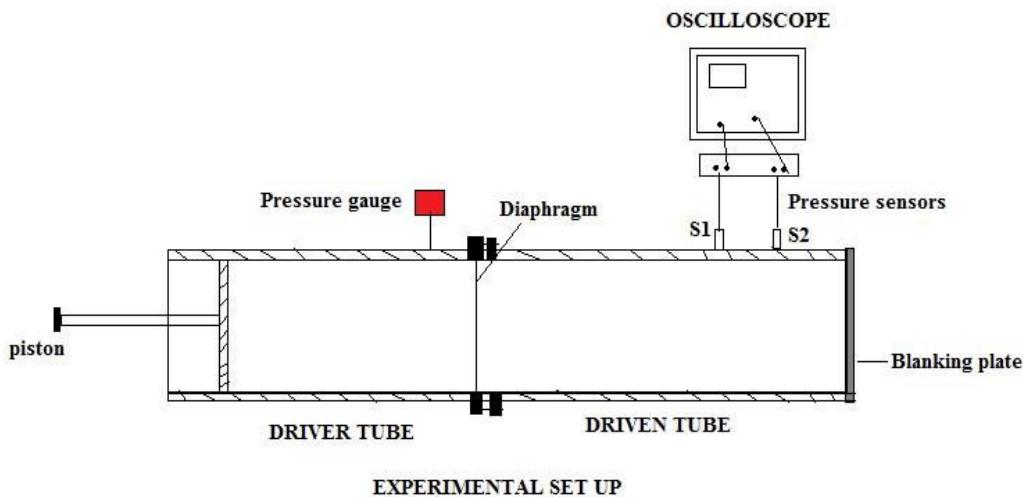
Aim: 1) To determine the speed of the primary shock wave and determine the mach number.

2) To determine ($\frac{P_2}{P_1}$) across the primary shock wave and evaluate P_5 and T_5 across the

Reflected shock wave and compare with the calculated values.

Apparatus: Reddy tube, digital pressure gauges, 2 pressure sensors, oscilloscope, diaphragm, blanking plate, a vacuum pump.

Experimental set up:



Procedure:

- The end of the driven tube is closed with a blanking plate the pressure inside the driven section is reduced by connecting it to a vacuum pump and the value is then closed.
- The diaphragm is fitted into the redy tube, the pressure sensors are connected to the CRO via the coupler and CRO is set for observations.
- The piston is driven hard into the driver tube till the reture sound of the diaphragm is heard. The pressure reading P4 from the pressure gauge in the driver tube is noted.
- Two signals of pressure rise are seen in the CRO display the first one appears when the primary shock passes the first sensor and the second one, when it passes the second sensor.
- From the CRO display, the time taken "t" for the shock to travel between the two pressure sensors is measured the distance x between the two pressure sensors is measured with a graduated scale.
- The experiment is repeated 3 or 4 times and the average value is taken following which the calculations are made.

CALCULATIONS:

- Evaluation of Mach number M Shock speed of primary shock wave $U_s = \frac{x}{t}$

$$\text{Mach number, } M = \frac{u_s}{a}$$

- Calculation of P_2 (First pressure jump)

Given $P_1=1 \text{ bar}$ and $\gamma = 1$

$$P_2 = P_1 \left[1 + \frac{2\gamma}{\gamma+1} (m^2 - 1) \right]$$

3) Calculation of T_2

Given $T_1 = \text{ambient temperature} = 300\text{K}$

$$\frac{\gamma+1}{\gamma-1} \frac{p_2}{p_1} = \frac{PP_{21}}{TT_{21}} \left[\frac{1}{1 + \gamma(-\gamma_1 + 1)} \right]$$

4) Calculations of P_5

$$PP_{52} = \left(\frac{3(\gamma\gamma - 1)}{\rho p p p p_1 221} + \frac{-(\gamma(\gamma + 1))}{\rho} \right)$$

5) Calculations of T_5

$$\frac{\gamma+1}{\gamma-1} \frac{p_5}{p_2} = \frac{PP_{52}}{TT_{52}} \left[\frac{1}{1 + \gamma(-\gamma_1 + 1)} \right]$$

QUESTION BANK

- 1) What is Mach number? Distinguish between Acoustic, ultrasonic, subsonic and supersonic waves.
- 2) Describe the Reddy shock tube with the help of neat Diagram
State the three conservation laws.
- 3)
- 4) Describe the ball milling method and sol-gel method to prepare the nano materials
- 5) Describe the construction and working of a scanning electron microscope.
- 6) Give an account of Rankine –Hugoniot equations.
- 7) Give the graphical representation of density of states with equation for 3D, 2D, 1D and 0D structures.
- 8) Write a note on carbon nanotubes.

- 9) What are the properties of carbon nanotubes?
- 10) Describe arc discharge method of obtaining CNTS with the help of a diagram Write a note on pyrolysis method of obtaining CNTS.