Sub Code : 15PHY12/15PHY22

IA Marks:20

Hrs/ Week : 04 Exam Hours : 03

Total Hrs. : 50 Exam Marks : 80

## Module – 1

### Modern Physics and Quantum Mechanics :

Black body radiation spectrum, Assumptions of quantum theory of radiation, Plank's law, Weins law and Rayleigh Jeans law, for shorter and longer wavelength limits. Wave Particle dualism, deBroglie hypothesis. Compton Effect and its Physical significance. Matter waves and their Characteristic properties, Phase velocity and group velocity. Relation between phase velocity and group velocity, Relation between group velocity and particle velocity.

Heisenberg's uncertainty principle and its application, (Non-existence of electron in nucleus).Wave function, Properties and physical significance of wave function, Probability density and Normalization of wave function. Setting up of one dimensional time independent Schrodinger wave equation. Eigen values and Eigen functions. Application of Schrodinger wave equation. Energy Eigen values and Eigen functions for a particle in a potential well of infinite depth and for free particle.

**10 Hours**

## Module – 2

### Electrical Properties of Materials:

Free–electron concept (Drift velocity, Thermal velocity, Mean collision time,Mean free path, relaxation time). Failure of classical free electron theory. Quantum free electron theory, Assumptions, Fermi factor, density of states(qualitative only), Fermi–Dirac Statistics. Expression for electrical conductivity based on quantum free electron theory, Merits of quantum free electron theory.

Conductivity of Semi conducting materials, Concentration of electrons andholes in intrinsic semiconductors, law of mass action. Temperature dependence of resistivity in metals and superconducting materials. Effect of magnetic field (Meissner effect).Type-I and Type-II superconductors–Temperature dependence of critical field.BCS theory(qualitative).High temperature superconductors. Applications of superconductors –.Maglev vehicles.

**10 Hours**

## Module – 3

**Lasers and Optical Fibers :**

Einstein's coefficients (expression for energy density).Requisites of a Laser system. Condition for laser action. Principle, Construction and working of$CO_2$ laser and semiconductor Laser. Applications of Laser – Laser welding, cutting and drilling. Measurement of atmospheric pollutants. Holography–Principle of Recording and reconstruction of images,.

Propagation mechanism in optical fibers. Angle of acceptance. Numerical aperture. Types of optical fibers and modes of propagation. Attenuation, Block diagram discussion of point to point communication, applications.

**10 Hours**

## Module – 4

**Crystal Structure :**

Space lattice, Bravais lattice–Unit cell, primitive cell. Lattice parameters. Crystal systems. Direction and planes in a crystal. Miller indices. Expression for inter – planar spacing. Co-ordination number. Atomic packing factors(SC,FCC, BCC). Bragg's law, Determination of crystal structure using Bragg's X–ray difractometer. Polymarphism and Allotropy. Crystal Structure of Diamond, qualitative discussion of Pervoskites.

**10 Hours**

## Module – 5

**Shock waves and Science of Nano Materials:**

Definition of Mach number, distinctions between- acoustic, ultrasonic, subsonic and supersonic waves. Description of a shock wave and its applications. Basics of conservation of mass, momentum and energy -derivation of normal shock relationships using simple basic conservation equations (Rankine-Hugonit equations). Methods of creating shock waves in the laboratory using a shock tube, description of hand operated Reddy shock tube and its characteristics. Introduction to Nano Science, Density of states in 1D, 2D and 3D structures. Synthesis : Top–down and Bottom–up approach, Ball Milling and Sol–Gelmethods.CNT – Properties, synthesis: Arc discharge, Pyrolysis methods, Applications. Scanning Electron microscope: Principle, working and applications.

**10 Hours**

**Text Books**

1. Wiley precise Text, **“Engineering Physics”**, Wiley India Private Ltd., New Delhi. Book series – 2014,
2. Dr.M.N. Avadhanulu, Dr.P.G.Kshirsagar, **“Text Book of Engineering Physics”**, S Chand Publishing, New Delhi – 2012.**Reference Books**

**Reference Books :**

1. Wiley precise Text, **“Engineering Physics”**, Wiley India Private Ltd., New Delhi. Book series – 2014,
2. S.O.Pillai, **“Solid State Physics”**, New Age International. Sixth Edition
3. ChintooS.Kumar ,K.Takayana and K.P.J.Reddy,**“Shock waves made simple”**, Willey India Pvt. Ltd. New Delhi,2014
4. A. Marikani, **“Engineering Physics”**, PHI Learning Private Limited, Delhi–2013
5. Prof. S. P. Basavaraju, **“Engineering Physics”**, Subhas Stores, Bangalore–2
6. V. Rajendran, **“Engineering Physics”**, Tata Mc.Graw Hill Company Ltd., New Delhi - 2012
7. S.ManiNaidu,**“Engineering Physics”**, Pearson India Limited – 2014.

# Module-1

## Modern Physics and Quantum Mechanics

Black body radiation spectrum, Assumptions of quantum theory of radiation, Plank's law, Weins law and Rayleigh Jeans law, for shorter and longer wavelength limits. Wave Particle dualism, deBroglie hypothesis. Compton Effect and its Physical significance. Matter waves and their Characteristic properties, Phase velocity and group velocity. Relation between phase velocity and group velocity, Relation between group velocity and particle velocity.

Heisenberg's uncertainty principle and its application, (Non-existence ofelectron in nucleus).Wave function, Properties and physical significance of wave function, Probability density and Normalization of wave function. Setting up of one dimensional time independent Schrodinger wave equation. Eigen values and Eigen functions. Application of Schrodinger wave equation. Energy Eigen values and Eigen functions for a particle in a potential well of infinite depth and for free particle.

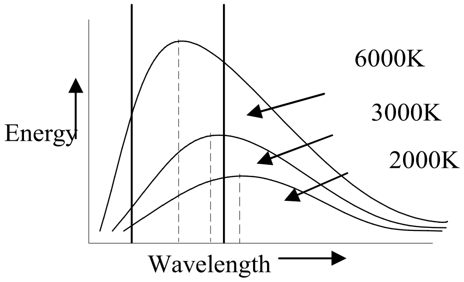
**10 Hours.**

## Content:

- **Black body radiation spectrum**
- **De Broglie's concept of matter waves**
- **Phase Velocity**
- **Group velocity**
- **Relation between phase velocity and group velocity**
- **Heisenberg uncertainty principle**
- **Schrodinger wave equation**
- **Eigen values and Eigen function**
- **Eigen function**

## *Blackbody Radiation spectrum:*

A Blackbody is one which absorbs the entire radiation incident on it and emits all the absorbed radiation when it is more hot. A true blackbody does not exist practically. A blackbody designed by Wein has features very close to the true blackbody. A blackbody at a particular temperature found to emit a radiation of all possible wavelengths. It is a continuous spectrum starting from certain minimum wavelength to maximum wavelength. The maximum intensity corresponds to a particular wavelength. For different temperatures of the black body, there are different curves. As the temperature of the body increases, the wavelength corresponding to maximum intensity shifts towards lower wavelength side. The distribution of energy in black body radiation



Wein's, Rayleigh-Jeans and Planck have given their explanations to account these observed experimental facts as follows:

## *Wein's Displacement Law:*

The law states that "the wavelength of maximum intensity is inversely proportional to the absolute temperature of the emitting body, because of which the peaks of the energy curves for different temperatures get displaced towards the lower wavelength side".

i.e. $\lambda_m \, \alpha \left(\frac{1}{T}\right)$ or $\lambda_m T = \text{constant} = 2.898\times10^{-3}\,\text{mK}$

Wein showed that the maximum energy of the peak emission is directly proportional to the fifth power of absolute temperature.

$E_m \alpha\, T^5$ or $E_m = \text{constant} \times T^5$

***Wein's law:***The relation between the wavelength of emission and the temperature of the source is

$$U_\lambda\, d\lambda = C_1\, \lambda^{-5}\, e^{-\left(\frac{C_2}{\lambda T}\right)}\, d\lambda$$

Where $U_\lambda d\lambda$ is the energy / unit volume in the range of wavelength $\lambda$ and $\lambda+d\lambda$, $C_1$ and $C_2$ are constants.

This is called Wein's law of energy distribution in the black body radiation spectrum.

*Drawbacks of Wein's law:*

Wein's law holds good for the shorter wavelength region and high temperature of the source. It failed to explain gradual drop in intensity of radiation corresponding to longer wavelength greater than the peak value.

1. ***Rayleigh-Jeans Law:***

Rayleigh derived an equation for the blackbody radiation on the basis of principle of equipartition of energy. The principle of equipartition of energy suggests that an average energy kT is assigned to each mode of vibration. The number of vibrations/unit volume whose wavelength is in the range of $\lambda$ and $\lambda+d\lambda$ is given by $8\pi\lambda^{-4}d\lambda$.

The energy/unit volume in the wavelength range $\lambda$ and $\lambda + d\lambda$ is

$$U_\lambda d\,\lambda = 8\pi kT\lambda^{-4}d\lambda$$

Where k is Boltzmann constant= $1.38\text{x}10^{-23}$J/K.

This is Rayleigh-Jeans equation. Accordingly energy radiated by the blackbody decreases with increasing wavelength.

***Drawbacks of Rayleigh-Jeans Law: (or Ultra Violet Catastrophe)***

Rayleigh-Jeans Law predicts to radiate all the energy at shorter wavelength side but it does not happen so. A black body radiates mainly in the infra-red or visible region of electromagnetic spectrum and intensity of radiation decreases down steeply for shorter wavelengths. Thus, the Rayleigh-Jeans Law fails to explain the lower wavelength side of the spectrum. This is referred to as ultra-violet Catastrophe.

## 2. *Planck's Law:*

Planck assumed that walls of the experimental blackbody consists larger number of electrical oscillators. Each oscillator vibrates with its own frequency.

i) Each oscillator has an energy given by integral multiple of hυ where h is Planck's constant & υ is the frequency of vibration.

$$E = nh\upsilon \text{ where } n = 1, 2, 3 \ldots \text{etc.}$$

ii) An oscillator may lose or gain energy by emitting or absorbing respectively a radiation of frequency υ where $\upsilon=\Delta E/h$, ΔE is difference in energies of the oscillator before and after the emission or absorption take place.

Planck derived the law which holds good for the entire spectrum of the blackbody radiation as

$$U_\lambda d\lambda = \frac{8\pi hc}{\lambda^5}\left[\frac{1}{e^{h\nu/kT}-1}\right]d\lambda \quad (\text{since } \upsilon = c/\lambda) \qquad \longrightarrow$$

This is Planck's Radiation Law.

***Reduction of Planck's law to Wein's law and Rayleigh Jeans law:***

***1)*** For shorter wavelengths, $\upsilon = c/\lambda$ is large.

When υ is large, $e^{h\upsilon/kT}$ is very large.

$$\therefore e^{h\upsilon/kT} >> 1$$

$$\therefore (e^{h\upsilon/kT}-1) \approx e^{h\upsilon/kT} = e^{hc/\lambda kT}$$

Substituting in eqn 1:

$$U_\lambda d\lambda = \frac{8\pi hc}{\lambda^5}\left[\frac{1}{e^{hc/\lambda kT}}\right]d\lambda = C_1 \lambda^{-5} e^{\left(\frac{-C_2}{\lambda T}\right)} d\lambda$$

Where $C_1 = 8\pi hc$ and $C_2 = hc/k$

This is the Wein's law of radiation.

***2)*** For longer wavelengths $\upsilon = c/\lambda$ is small.

When υ is small $h\upsilon/kT$ is very small.

Expanding $e^{h\upsilon/kT}$ as power series:

$$e^{h\upsilon/kT} = 1 + h\upsilon/kT + (h\upsilon/kT)^2 + \ldots$$

$$\approx 1 + h\upsilon/kT.$$

$\because$ If $h\upsilon/kT$ is small, its higher powers are neglected.

$$\therefore\ e^{h\upsilon/kT} - 1 = \frac{h\nu}{kT} = \frac{hc}{\lambda kT}$$

Substituting in eqn 1:

$$U_\lambda d\lambda = \left[\frac{8\pi hc}{\lambda^5\left(\frac{hc}{\lambda kT}\right)}\right]d\lambda$$

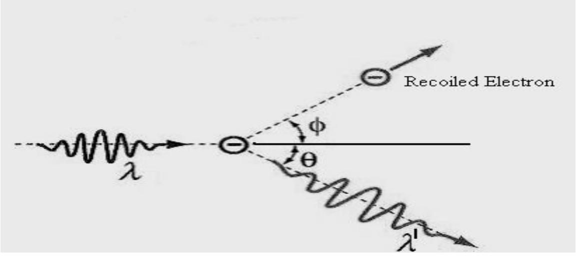
$$= \left[\frac{8\pi kT}{\lambda^4}\right]d\lambda$$

This is Rayleigh Jeans Law of Radiation.

***Compton Effect:***

The scattering of a photon by an electron is called as Compton effect or Compton scattering.

When a photon of wavelength ‘λ’ is scattered by an electron in the direction making an angle ‘θ’ with the direction of incidence, the wavelength of the scattered photon increases. Its wavelength is λ'. The electron recoils in a direction making an angle ‘φ’ with the incident direction of photon. The difference in the wavelength (λ'-λ) is called the Compton shift. Compton found that λ' is independent of the target material, but depends on the angle of scattering.



If λ is the wavelength of the incident photon, its energy E is given by E=hc/λ where ‘h’ is the Planck’s constant, ‘c’ is the velocity of light, ‘λ’ is the wavelength of the incident photon. If λ' is the wavelength of the scattered photon, its energy E' is given by

$E' = hc/\lambda'$

The energy of the scattered photon is reduced from E to E'. The difference of energy is carried by recoiling electron at an angle 'φ' with the incident direction of photon.

Applying the laws of conservation of energy and conservation of momentum Compton obtained an expression for change in wavelength $\Delta\lambda$ given by $\Delta\lambda = \lambda' - \lambda = \frac{h}{mc}(1-\cos\theta)$Where 'm' is the mass of the electron, h/mc is called as Compton wavelength. Compton Effect explains particle nature of light.

## ***Dual nature of matter (de-Broglie Hypothesis)***

Light exhibits the phenomenon of interference, diffraction, photoelectric effect and Compton Effect. The phenomenon of interference, diffraction can only be explained with the concept that light travels in the form of waves. The phenomenon of photoelectric effect and Compton Effect can only be explained with the concept of *Quantum theory of light.* It means to say that light possess particle nature. Hence it is concluded that light exhibits dual nature namely wave nature as well as particle nature.

## ***de-Broglie's Wavelength:***

A particle of mass 'm' moving with velocity 'c' possess energy given by

$E = mc^2$ → (Einstein's Equation) (1)

According to Planck's quantum theory the energy of quantum of frequency 'υ'is

$E = h\upsilon$ → (2)

From (1) & (2)

$mc^2 = h\upsilon = hc/\lambda$ since $\upsilon = c/\lambda$

$\lambda = hc/mc^2 = h/mc$

$\lambda = h/mv$ since $v \approx c$

## *Relation between de-Broglie wavelength and kinetic energy*

Consider an electron in an electric potential V, the energy acquired is given by

$$E = eV = \frac{1}{2} m\text{v}^2 = \frac{p^2}{2m}$$

Where 'm' is the mass, 'v' is the velocity and 'p' is the momentum of the particle. 'e' is charge of an electron.

$$p = \sqrt{2meV} = \sqrt{2mE}$$

The expression for de-Broglie wavelength is given by

$$\lambda = \frac{h}{p} = \frac{h}{m\text{v}} = \frac{h}{\sqrt{2meV}} = \frac{h}{\sqrt{2mE}}$$

## *de-Broglie Wavelength of an Accelerated Electron:*

An electron accelerated with potential difference 'V' has energy 'eV'.If 'm' is the mass and 'v' is the velocity of the electron.

Then $eV = 1/2(mv^2) \rightarrow (1)$

If 'p' is the momentum of the electron, then p=mv

Squaring on both sides, we have

$p^2 = m^2v^2$

$mv^2 = p^2/m$

Using in equation (1) we have

$eV = p^2/(2m)$ or $p = \sqrt{(2meV)}$

According to de-Broglie $\lambda = h/p$

Therefore $\lambda = \left[\frac{h}{\sqrt{2meV}}\right] = \frac{1}{\sqrt{V}}\left[\frac{h}{\sqrt{2me}}\right]$

$$\lambda = \frac{1}{\sqrt{V}}\left[\frac{6.626\times10^{-34}}{\sqrt{2\times9.11\times10^{-31}\times1.602\times10^{-19}}}\right]$$

$$\boxed{=\frac{1.226\times10^{-9}}{\sqrt{V}}}\text{m} \quad \text{or} \quad \lambda = \frac{1.226}{\sqrt{V}}\ \text{nm}$$

## ***Characteristics of matter waves:***

1. Waves associated with moving particles are called matter waves. The wavelength '$\lambda$' of a de-Broglie wave associated with particle of mass 'm' moving with velocity 'v' is

   $\lambda = h/(mv)$

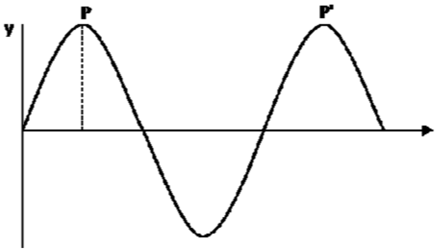
2. Matter waves are not electromagnetic waves because the de Broglie wavelength is independent of charge of the moving particle.
3. The velocity of matter waves ($v_P$) is not constant. The wavelength is inversely proportional to the velocity of the moving particle.
4. Lighter the particle, longer will be the wavelength of the matter waves, velocity being constant.
5. For a particle at rest the wavelength associated with it becomes infinite. This shows that only moving particle produces the matter waves.

## ***Phase velocity and group velocity:***

A wave is represented by the equation:

$y = A\sin(\omega t\text{-}kx)$

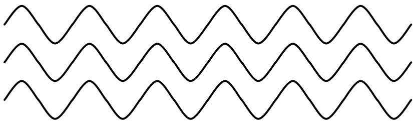
Where 'y' is the displacement along Y-axis at an instant t, '$\omega$' is the angular frequency, 'k' is propagation constant or wave number. 'x' is the displacement along x-axis at the instant 't'.



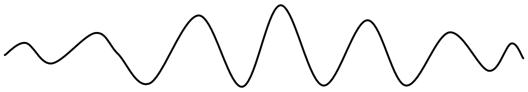
If 'p' is the point on a progressive wave, then it is the representative point for a particular phase of the wave, the velocity with which it is propagated owing to the motion of the wave is called *phase velocity.*

The phase velocity of a wave is given by $v_{phase} = (\omega / k)$.

***Group velocity:***



***Individual Waves***



***Amplitude variation after Superposition***

A group of two or more waves, slightly differing in wavelengths are super imposed on each other. The resultant wave is a packet or wave group. The velocity with which the envelope enclosing a wave group is transported is called *Group Velocity*.

Let $y_1 = A\sin(\omega t - kx) \rightarrow (1)$ and $y_2 = A\sin[(\omega+\Delta\omega)t - (k+\Delta k)x] \rightarrow (2)$

The two waves having same amplitude & slightly different wavelength. Where $y_1$ & $y_2$ are the displacements at any instant'$t$', '$A$' is common amplitude, '$\Delta\omega$' & '$\Delta k$' are difference in angular velocity and wave number are assumed to be small. '$x$' is the common displacement at time '$t$'

By the principle of superposition

$$y = y_1 + y_2$$

$$y = A\sin(\omega t - kx) + A\sin\{(\omega+\Delta\omega)t - (k+\Delta k)x\}$$

But, $\sin a + \sin b = 2\cos\left(\frac{a-b}{2}\right)\sin\left(\frac{a+b}{2}\right)$

$$y = 2A\cos\left[\left(\frac{\Delta\omega}{2}\right)t - \left(\frac{\Delta k}{2}\right)x\right]\sin\left[\left(\frac{2\omega+\Delta\omega}{2}\right)t - \left(\frac{2k+\Delta k}{2}\right)x\right]$$

Since $\Delta\omega$ and $\Delta k$ are small

$$2\omega + \Delta\omega \approx 2\omega \text{ and } 2k + \Delta k \approx 2k.$$

$$\therefore\ y = 2A\cos\left[\left(\frac{\Delta\omega}{2}\right)t - \left(\frac{\Delta k}{2}\right)x\right]\sin(\omega t - kx) \rightarrow (3)$$

From equations (1) & (3) it is seen the amplitude becomes

$$2A\cos\left[\left(\frac{\Delta\omega}{2}\right)t - \left(\frac{\Delta k}{2}\right)x\right]$$

The velocity with which the variation in amplitude is transmitted in the resultant wave is the group velocity.

$$v_{group} = \frac{(\Delta\omega/2)}{(\Delta k/2)} = \frac{\Delta\omega}{\Delta k}$$

In the limit $\frac{\Delta\omega}{\Delta k} \rightarrow \frac{d\omega}{dk}$

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

***__Relation between group velocity and phase velocity:__***

The equations for group velocity and phase velocity are:

$$v_{group} = \frac{d\omega}{dk} \rightarrow (1)\ \& v_{phase} = \frac{\omega}{k} \rightarrow (2)$$

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

$$\omega = k\, v_{phase}$$

$$v_{group} = \frac{d\omega}{dk} = \frac{d}{dk}(k v_{phase})$$

$$v_{group} = v_{phase} + k\frac{dv_{phase}}{dk}$$

$$v_{group} = v_{phase} + k\left(\frac{dv_{phase}}{d\lambda}\right)\left(\frac{d\lambda}{dk}\right) \rightarrow (3)$$

We have $k = (2\pi/\lambda)$

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

$$k\frac{d\lambda}{dk} = \left(\frac{2\pi}{\lambda}\right)\left(-\frac{\lambda^2}{2\pi}\right) = -\lambda$$

Using this in eqn (3)

$$v_{group} = v_{phase} - \lambda\frac{dv_{phase}}{d\lambda}$$

This is the relation between group velocity and phase velocity.

***<u>Relation between group velocity and particle velocity:</u>***

The equation for group velocity is

$$v_{group} = \frac{d\omega}{dk} \rightarrow (1)$$

But $\omega = 2\pi\upsilon = 2\pi(E/h) \rightarrow (2)$

$$d\omega = \frac{2\pi}{h}dE \rightarrow (3)$$

We have $k = 2\pi/\lambda = 2\pi(p/h) \rightarrow (4)$

$$dk = \frac{2\pi}{h}dP \rightarrow (5)$$

Dividing eqn (3) by (5) we have

$$\frac{d\omega}{dk} = \frac{dE}{dP} \rightarrow (6)$$

But we have $E = P^2/(2m)$, Where ‘P’ is the momentum of the particle.

$$\frac{dE}{dP} = \frac{2P}{2m} = \frac{P}{m}$$

Using the above in eqn (6)

$$\frac{d\omega}{dk}=\frac{P}{m}$$

But p = $mv_{particle}$, Where '$v_{particle}$' is the velocity of the particle.

$$\frac{d\omega}{dk}=\frac{mv_{particle}}{m}=v_{particle} \rightarrow (7)$$

From eqn (1) & (7), we have

$$v_{group}=v_{particle} \rightarrow (8)$$

∴ The de Broglie's wave group associated with a particle travels with a velocity equal to the velocity of the particle itself.

***Relation between velocity of light, group velocity and phase velocity:***

We have $v_{phase} = \omega/k$

Using the values of 'ω' and 'k' from eqn (2) & (4) we have

$$v_{phase}=\frac{E}{P}=\frac{mc^2}{mv_{particle}}=\frac{c^2}{v_{particle}} \rightarrow (9)$$

From eqn (8) $v_{group}=v_{particle}$

$$\therefore v_{phase}\times v_{group}=c^2$$

This is the relation of velocity of light with phase velocity & group velocity.

Since $v_{group}$ is same as $v_{particle}$& the velocity of material particle can never be greater than or even equal to c, which shows that phase velocity is always greater than c.

## Introduction: Classical Mechanics - Quantum Mechanics

Mechanics is the branch of Physics which deals with the study of motion of objects. The study of motion of objects started from 14th Century. Leonardo da Vinci, Galileo and Blaisepascal were the beginners. Their study did not have any logical connection to each other. In the 17th Century Newton consolidated the ideas of previous workers in addition to his own. He gave a unified theory which accounted for all types of motions of bodies on common grounds. His work "Principia mathematica" was published in the year 1687. Newton's three laws of motion were included in his work. 1687 year was recognized as the birth of Mechanics. These laws were important in the wider fields of study in Physics. For example electrodynamics by Maxwel. By the end of 19th Century in the mind of scientific community it was that the knowledge of mechanics is complete and only refinement of the known is required.

In the last part of 19th Century the study of Blackbody radiation became an insoluble puzzle. It was much against the confidence and belief of many investigators. Newtonian mechanics failed to account the observed spectrum.In December 1900 Max Planck explained the blackbody spectrum by introducing the idea of quanta. This is the origin of "Quantum Mechanics". Whatever studies were made in mechanics till then was called classical mechanics. From 1901 onwards quantum mechanics has been employed to study mechanics of atomic and subatomic particles. The concept of quantization of energy is used in Bohr's theory of hydrogen spectrum. In 1924 de-Broglie proposed dual nature of matter called de Broglie hypothesis. Schrodinger made use in his work the concepts of wave nature of matter and quantization of energy. The work of Schrodinger, Heisenberg, Dirac and others on mechanics of atomic and subatomic particles was called Quantum Mechanics.

## Difference between Classical Mechanics and Quantum Mechanics

According to Classical mechanics it is unconditionally accepted that the position, mass, velocity, acceleration etc., of a particle or a body can be measured accurately, which is true as we observe in every day. The values predicted by classical mechanics fully agree with measured values.

Quantum mechanics has been built upon with purely probabilistic in nature. The fundamental assumption of Quantum mechanics is that it is impossible to measure simultaneously the position and momentum of a particle. In quantum mechanics the measurements are purely probable. For example the radius of the first allowed orbit of electron in hydrogen atom is precisely 5.3 x $10^{-11}$m. If a suitable experiment is conducted to measure the radius, number of values are obtained which are very close to 5.3 x $10^{-11}$m. This type of uncertainty makes classical mechanics superior to quantum mechanics. The accurate values declared by classical mechanics are found to be true in day to day life. But in the domain of nucleus, atoms, molecules etc., the probabilities involved in the values of various physical quantities become insignificant and classical mechanics fails to account such problems.

**Heisenberg's Uncertainty Principle:**

According to classical mechanics a particle occupies a definite place in space and possesses a definite momentum. If the position and momentum of a particle is known at any instant of time, it is possible to calculate its position and momentum at any later instant of time. The path of the particle could be traced. This concept breaks down in quantum mechanics leading to Heisenberg's Uncertainty Principle according to which "It is impossible to measure simultaneously both the position and momentum of a particle accurately. If we make an effort to measure very accurately the position of a particle, it leads to large uncertainty in the measurement of momentum and vice versa.

If $\Delta x$ and $\Delta P_x$ are the uncertainties in the measurement of position and momentum of the particle then the uncertainty can be written as

$$\Delta x \,.\, \Delta P_x \geq (h/4\pi)$$

In any simultaneous determination of the position and momentum of the particle, the product of the corresponding uncertainties inherently present in the measurement is equal to or greater than h/4π.

Similarly, 1) $\Delta E . \Delta t \geq h/4\pi$ This equation represents uncertainty in energy and time. ΔE is uncertainty in energy,Δt is the uncertainty in time.

2) $\Delta L . \Delta \theta \geq h/4\pi$ This equation represents uncertainty in angular momentum(ΔL) and angular displacement(Δθ)

## ***Application of Uncertainty Principle:***

### ***Impossibility of existence of electrons in the atomic nucleus:***

According to the theory of relativity, the energy E of a particle is: $E = mc^2 = \frac{m_o c^2}{\sqrt{1-(\mathrm{v}^2/c^2)}}$

Where '$m_o$' is the rest mass of the particle and 'm' is the mass when its velocity is 'v'.

$$\text{i.e. } E^2 = \frac{m_o^2 c^4}{1-(\mathrm{v}^2/c^2)} = \frac{m_o^2 c^6}{c^2 - \mathrm{v}^2} \rightarrow (1)$$

If 'p' is the momentum of the particle:

$$\text{i.e. } p = m\mathrm{v} = \frac{m_o \mathrm{v}}{\sqrt{1-(\mathrm{v}^2/c^2)}}$$

$$p^2 = \frac{m_o^2 \mathrm{v}^2 c^2}{c^2 - \mathrm{v}^2}$$

Multiply by $c^2$

$$p^2c^2 = \frac{m_o^2 \mathrm{v}^2 c^4}{c^2 - \mathrm{v}^2} \rightarrow (2)$$

Subtracting (2) by (1) we have

$$E^2 - p^2c^2 = \frac{m_o^2 c^4 (c^2 - \mathrm{v}^2)}{c^2 - \mathrm{v}^2}$$

$$E^2 = p^2c^2 + m_o^2c^4 \rightarrow (3)$$

Heisenberg's uncertainty principle states that

$$\Delta x \,.\, \Delta P_x \geq \frac{h}{4\pi} \rightarrow (4)$$

The diameter of the nucleus is of the order $10^{-14}$m. If an electron is to exist inside the nucleus, the uncertainty in its position $\Delta x$ must not exceed $10^{-14}$m.

i.e. $\Delta x \leq 10^{-14}$m

The minimum uncertainty in the momentum

$$(\Delta P_x)_{\min} \geq \frac{h}{4\pi\ (\Delta x)_{\max}} \geq \frac{6.63\times10^{-34}}{4\pi\times10^{-14}} \geq 0.5 \times 10^{-20} \text{ kg.m/s} \rightarrow (5)$$

By considering minimum uncertainty in the momentum of the electron

i.e., $(\Delta P_x)_{\min} \geq 0.5 \times 10^{-20}$ kg.m/s = p → (6)

Consider eqn (3)

$E^2 = p^2c^2 + m_o^2c^4 = c^2(p^2+m_o^2c^2)$

Where $m_o = 9.11 \times 10^{-31}$ kg

If the electron exists in the nucleus its energy must be

$E^2 \geq (3 \times 10^8)^2[(0.5 \times 10^{-20})^2 + (9.11 \times 10^{-31})^2(3 \times 10^8)^2]$

i.e. $E^2 \geq (3 \times 10^8)^2[0.25 \times 10^{-40} + 7.4629 \times 10^{-44}]$

Neglecting the second term as it is smaller by more than the 3 orders of the magnitude compared to first term.

Taking square roots on both sides and simplifying

$$E \geq 1.5 \times 10^{-12} \text{ J} \geq \frac{1.5\times10^{-12}}{1.6\times10^{-19}} \text{ ev} \geq 9.4 \text{ Mev}$$

If an electron exists in the nucleus its energy must be greater than or equal to 9.4Mev. It is experimentally measured that the beta particles ejected from the nucleus during beta decay have energies of about 3 to 4 MeV. This shows that electrons cannot exist in the nucleus.

## ***Wave Function:***

A physical situation in quantum mechanics is represented by a function called wave function. It is denoted by 'ψ'. It accounts for the wave like properties of particles. Wave function is obtained by solving Schrodinger equation. To solve Schrodinger equation it is required to know

1) Potential energy of the particle

2) Initial conditions and

3) Boundary conditions.

There are two types of Schrodinger equations:

**1)** ***The time dependent Schrodinger equation:*** It takes care of both the position and time variations of the wave function. It involves imaginary quantity *i*.

The equation is: $$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi}{dx^2}+V\psi=-\frac{ih}{2\pi}\frac{d\psi}{dt}$$

**2)** ***The time independent Schrodinger equation*****:** It takes care of only position variation of the wave function.

The equation is: $$\frac{d^2\psi}{dx^2}+\frac{8\pi^2 m}{h^2}(E-V)\psi=0$$

### ***Time independent Schrodinger wave equation***

Consider a particle of mass 'm' moving with velocity 'v'. The de-Broglie wavelength 'λ' is

$$\lambda = \frac{h}{mv}=\frac{h}{P}\rightarrow (1)$$

Where 'mv' is the momentum of the particle.

The wave eqn is

$$\psi = Ae^{i(kx-\omega t)} \rightarrow (2)$$

Where 'A' is a constant and 'ω' is the angular frequency of the wave.

Differentiating equation (2) with respect to 't' twice

$$\frac{d^2\psi}{dt^2} = -A\omega^2 e^{i(kx-\omega t)} = -\omega^2\psi \quad \rightarrow (3)$$

The equation of a travelling wave is

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

Where 'y' is the displacement and 'v' is the velocity.

Similarly for the de-Broglie wave associated with the particle

$$\frac{d^2\psi}{dx^2} = \frac{1}{\mathrm{v}^2}\frac{d^2\psi}{dt^2} \rightarrow (4)$$

where 'ψ' is the displacement at time 't'.

From eqns (3) & (4)

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

But ω = 2πυ and v =υ λ where 'υ' is the frequency and 'λ' is the wavelength.

$$\frac{d^2\psi}{dx^2} = -\frac{4\pi^2}{\lambda^2}\psi \text{ or } \frac{1}{\lambda^2} = -\frac{1}{4\pi^2\psi}\frac{d^2\psi}{dx^2} \rightarrow (5)$$

$$K.E = \frac{1}{2}m\mathrm{v}^2 = \frac{m^2\mathrm{v}^2}{2m} = \frac{P^2}{2m} \rightarrow (6)$$

$$= \frac{h^2}{2m\lambda^2} \rightarrow (7)$$

Using eqn (5)

$$K.E = \frac{h^2}{2m}\left(-\frac{1}{4\pi^2\psi}\right)\frac{d^2\psi}{dx^2} = -\frac{h^2}{8\pi^2 m\psi}\frac{d^2\psi}{dx^2} \rightarrow (8)$$

Total Energy E = K.E + P.E

$$E = -\frac{h^2}{8\pi^2 m\psi}\frac{d^2\psi}{dx^2} + V$$

$$E - V = -\frac{h^2}{8\pi^2 m\psi}\frac{d^2\psi}{dx^2}$$

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

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

This is the time independent Schrodinger wave equation.

***Physical significance of wave function:***

***Probability density:***If ψ is the wave function associated with a particle, then $|\psi|^2$ is the probability of finding a particle in unit volume. If 'τ' is the volume in which the particle is present but where it is exactly present is not known. Then the probability of finding a particle in certain elemental volume dτ is given by $|\psi|^2 d\tau$. Thus $|\psi|^2$ is called probability density. The probability of finding an event is real and positive quantity. In the case of complex wave functions, the probability density is $|\psi|^2 = \psi * \psi$ where ψ* is Complex conjugate of ψ.

***Normalization:***

The probability of finding a particle having wave function 'ψ' in a volume 'dτ' is '$|\psi|^2 d\tau$'. If it is certain that the particle is present in finite volume 'τ', then

$$\int_0^\tau |\psi|^2 d\tau = 1$$

If we are not certain that the particle is present in finite volume, then

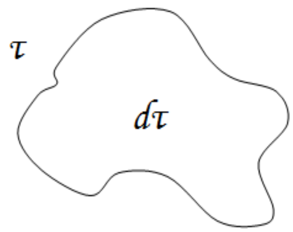
$$\int_{-\infty}^{\infty} |\psi|^2 d\tau = 1$$

In some cases $\int |\psi|^2 d\tau \neq 1$ and involves constant.

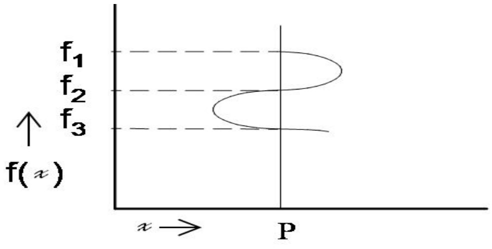
The process of integrating the square of the wave function within a suitable limits and equating it to unity the value of the constant involved in the wavefunction is estimated. The constant value is substituted in the wavefunction. This process is called as normalization. The wavefunction with constant value included is called as the normalized wavefunction and the value of constant is called normalization factor.

***__Properties of the wave function:__***

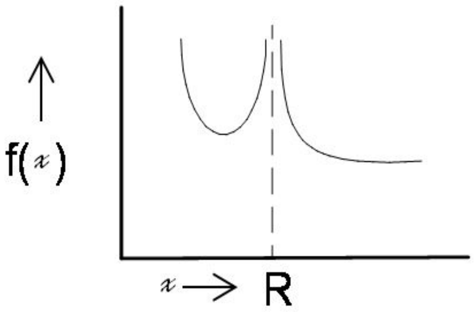
A system or state of the particle is defined by its energy, momentum, position etc. If the wave function 'ψ' of the system is known, the system can be defined. The wave function 'ψ' of the system changes with its state. To find 'ψ' Schrodinger equation has to be solved. As it is a second order differential equation, there are several solutions. All the solutions may not be correct. We have to select those wave functions which are suitable to the system. The acceptable wave function has to possess the following properties:



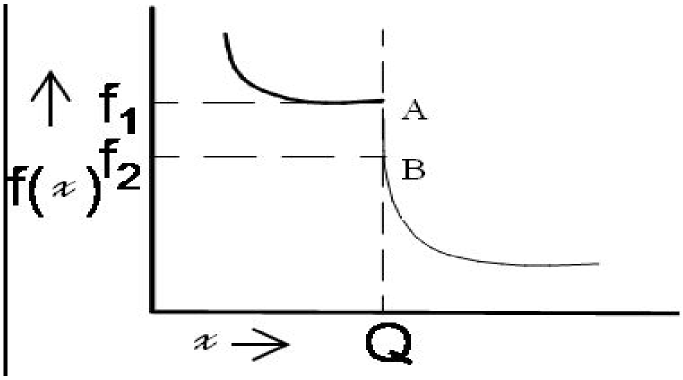
1) **__'ψ' is single valued everywhere:__** Consider the function $f(x)$ which varies with position as represented in the graph. The function f(x) has three values $f_1$, $f_2$ and $f_3$ at $x = p$. Since $f_1 \neq f_2 \neq f_3$ it is to state that if $f(x)$ were to be the wave function. The probability of finding the particle has three different values at the same location which is not true. Thus the wave function is not acceptable.



2) **__'ψ' is finite everywhere__:** Consider the function $f(x)$ which varies with position as represented in the graph. The function $f(x)$ is not finite at $x$=R but $f(x)=\infty$. Thus it indicates large probability of finding the particle at a location. It violates uncertainty principle. Thus the wave function is not acceptable.



3) **<u>'ψ' and its first derivatives with respect to its variables are continuous everywhere</u>:** Consider the function f( $x$ ) which varies with position as represented in the graph. The function f( $x$ ) is truncated at $x$ =Q between the points A & B, the state of the system is not defined. To obtain the wave function associated with the system, we have to solve Schrodinger wave equation. Since it is a second order differential wave equation, the wave function and its first derivative must be continuous at x=Q. As it is a discontinuous wave function, the wave function is not acceptable.



4) For bound states 'ψ' must vanish at potential boundary and outside. If 'ψ*' is a complex function, then ψ* ψ must also vanish at potential boundary and outside.

The wave function which satisfies the above 4 properties are called *Eigen functions*.

***<u>Eigen functions:</u>***

Eigen functions are those wave functions in Quantum mechanics which possesses the properties:

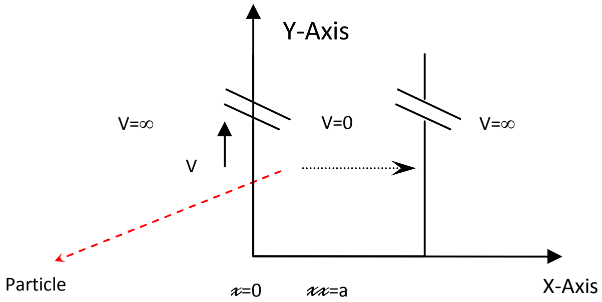
1. They are single valued.
2. Finite everywhere and
3. The wave functions and their first derivatives with respect to their variables are continuous.

**_Eigen values:_**

According to the Schrodinger equation there is more number of solutions. The wave functions are related to energy E. The values of energy $E_n$ for which Schrodinger equation solved are called Eigen values.

**_Application of Schrodinger wave equation:_**

*Energy Eigen values of a particle in one dimensional, infinite potential well (potential well of infinite depth) or of a particle in a box.*



Consider a particle of a mass 'm' free to move in one dimension along positive $x$ -direction between $x$ =0 to $x$ =a. The potential energy outside this region is infinite and within the region is zero. The particle is in bound state. Such a configuration of potential in space is called infinite potential well. It is also called particle in a box. The Schrödinger equation outside the well is

$$\frac{d^2\psi}{dx^2}+\frac{8\pi^2 m}{h^2}(E-\infty)\psi = 0 \rightarrow (1) \qquad \because V = \infty$$

For outside, the equation holds good if ψ = 0 & $|\psi|^2 = 0$. That is particle cannot be found outside the well and also at the walls

The Schrodinger's equation inside the well is:

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi = 0 \rightarrow (2) \qquad \because V = 0$$

$$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi}{dx^2} = E\psi \rightarrow (3)$$

This is in the form $\hat{H}\psi = E\psi$

This is an Eigen-value equation.

Let $\frac{8\pi^2 m}{h^2}E = k^2$ in eqn (2)

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

The solution of this equation is:

$$\psi = C \cos kx + D \sin kx \rightarrow (4)$$

at $x = 0 \rightarrow \psi = 0$

$$0 = C \cos 0 + D \sin 0$$

$\therefore$ C = 0

Also $x = a \rightarrow \psi = 0$

$$0 = C \cos ka + D \sin ka$$

But C = 0

$\therefore$ D sin ka = 0 (5)

D≠0 (because the wave concept vanishes)

i.e. ka = *n*π where *n* = 0, 1, 2, 3, 4… (Quantum number)

$$k = \frac{n\pi}{a} \rightarrow (6)$$

Using this in eqn (4)

$$\psi_n = D\sin\frac{n\pi}{a}x \rightarrow (7)$$

Which gives permitted wave functions.

To find out the value of D, normalization of the wave function is to be done.

i.e. $\int_0^a |\psi_n^2| dx = 1 \rightarrow (8)$

using the values of $\psi_n$ from eqn (7)

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

$$D^2\int_0^a \left[\frac{1-\cos(2n\pi/a)x}{2}\right]dx = 1$$

$$\sin^2\theta = \left(\frac{1-\cos 2\theta}{2}\right)$$

$$\frac{D^2}{2}\left[\int_0^a dx - \int_0^a \cos\frac{2n\pi}{a}xdx\right] = 1$$

$$\frac{D^2}{2}\left[x - \frac{a}{2n\pi}\sin\frac{2n\pi}{a}x\right]_0^a = 1$$

$$\frac{D^2}{2}[a-0] = 1$$

$$\frac{D^2}{2}a = 1$$

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

Hence the normalized wave functions of a particle in one dimensional infinite potential well is:

$$\psi_n = \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x \rightarrow (9)$$

***Energy Eigen values:***

From Eq. 6 &2

$$\frac{8\pi^2 m}{h^2}E = k^2 = \frac{n^2\pi^2}{a^2}$$

Implies $E = \frac{n^2h^2}{8ma^2}$

## Alternative Method (Operator method)

Energy Eigen values are obtained by operating the wave function ‘$\psi$’ by the energy operator (Hamiltonian operator).

$$\hat{H} = -\frac{h^2}{8\pi^2 m}\frac{d^2}{dx^2} + V$$

Inside the well 0 < x < a, V=0

$$\hat{H} = -\frac{h^2}{8\pi^2 m}\frac{d^2}{dx^2} \rightarrow (10)$$

The energy Eigen value eqn is

$$\hat{H}\psi = E\psi \rightarrow (11)$$

From equation (10) and (11)

$$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi_n}{dx^2} = E\psi$$

i.e. $$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi_n}{dx^2} = E\psi_n \rightarrow (12)$$

It is the Eigen value equation.

Differentiating eqn (9)

$$\frac{d\psi_n}{dx} = \sqrt{\frac{2}{a}}\frac{n\pi}{a}\cos\frac{n\pi}{a}x$$

Differentiating again

$$\frac{d^2\psi_n}{dx^2} = -\sqrt{\frac{2}{a}}\left(\frac{n\pi}{a}\right)^2 \sin\frac{n\pi}{a}x$$

$$\frac{d^2\psi_n}{dx^2} = -\left(\frac{n\pi}{a}\right)^2 \psi_n$$

Using this eqn. in (12)

$$\frac{h^2}{8\pi^2 m}\left(\frac{n\pi}{a}\right)^2 \psi_n = E\psi_n$$

$$E = \frac{n^2h^2}{8ma^2} \rightarrow (13)$$

It gives the energy Eigen values of the particle in an infinite potential well.

n = 0 is not acceptable inside the well because $\psi_n = 0$. It means that the electron is not present inside the well which is not true. Thus the lowest energy value for $n = 1$ is called zero point energy value or ground state energy.

i.e. $E_{\text{zero-point}} = \frac{h^2}{8ma^2}$

The states for which n >1 are called exited states.

***__Wave functions, probability densities and energy levels for particle in an infinite potential well__:***

Let us consider the most probable location of the particle in the well and its energies for first three cases.

***__Case I → n=1__***

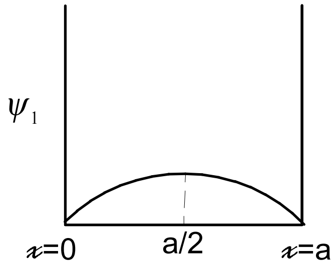
It is the ground state and the particle is normally present in this state.

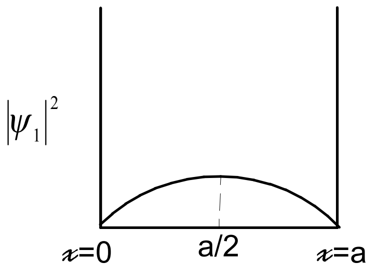
The Eigen function is

$\psi_1 = \sqrt{\frac{2}{a}} Sin\frac{\pi}{a}x \because$ from eqn (7)

$\psi_1 = 0$ for $x = 0$ and $x = a$

But $\psi_1$ is maximum when $x = a/2$.





The plots of $\psi_1$ versus x and $|\psi_1|^2$ verses x are shown in the above figure.

$|\psi_1|^2 = 0$ for $x = 0$ and $x = a$ and it is maximum for $x = a/2$. i.e. in ground state the particle cannot be found at the walls, but the probability of finding it is maximum in the middle.

The energy of the particle at the ground state is

$$E_1 = \frac{h^2}{8ma^2} = E_0$$

***<u>Case II → n=2</u>***

In the first excited state the Eigen function of this state is

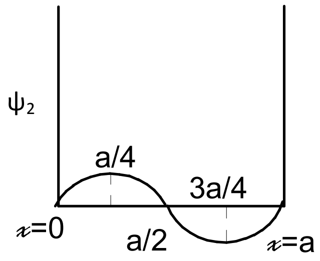
$$\psi_2 = \sqrt{\frac{2}{a}} Sin \frac{2\pi}{a} x$$

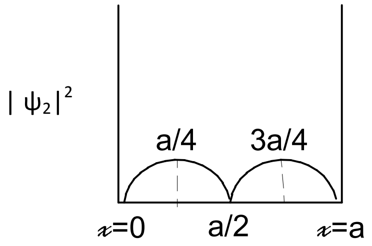
$\psi_2 = 0$ for the values $x = 0, a/2, a$.

Also $\psi_2$ is maximum for the values $x = a/4$ and $3a/4$.

These are represented in the graphs.

$|\psi_2|^2 = 0$ at $x = 0, a/2, a$, i.e. particle cannot be found either at the walls or at the centre. $|\psi_2|^2 = \text{maximum } for\ x = \frac{a}{4}, x = \frac{3a}{4}$





The energy of the particle in the first excited state is $E_2 = 4E_0$.

***Case III*** → n=3

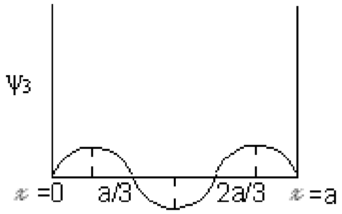
In the second excited state,

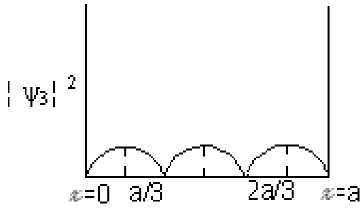
$$\psi_3 = \sqrt{\frac{2}{a}} Sin \frac{3\pi}{a} x$$

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

$\psi_3$ is maximum for $x$ = a/6, a/2, 5a/6.

These are represented in the graphs.





$|\psi_3|^2 = 0$ for $x$ = 0, a/3, 2a/3 and a. $|\psi_3|^2 = \text{maximum } for\ x = \frac{a}{6}, x = \frac{a}{2}, x = \frac{5a}{6}$

The energy of the particle in the second excited state is $E_3 = 9\ E_0$.

## ***Energy Eigen values of a free particle:***

A free particle is one which has zero potential. It is not under the influence of any force or field i.e. V = 0.

The Schrodinger equation is:

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi = 0$$

or $$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi}{dx^2} = E\psi$$

This equation holds good for free particle in free space in which V = 0.

With the knowledge of the particle in a box or a particle in an infinite potential well V = 0 holds good over a finite width ‘a’ and outside V = ∞. By taking the width to be infinite i.e. a = ∞, the case is extended to free particle in space. The energy Eigen values for a particle in an infinite potential well is

$$E = \frac{n^2 h^2}{8ma^2}$$

Where n =1, 2, 3, …

$$n = \frac{2a}{h}\sqrt{2mE}$$

Here when ‘E’ is constant, ‘n’ depends on ‘a’ as a→∞ *n*→∞. It means that free particle can have any energy. That is the energy Eigen values or possible energy values are infinite in number. It follows that energy values are continuous. It means that there is no discreteness or quantization of energy. Thus a free particle is a *‘Classical entity’*.

# Module– 2

# Electrical properties of materials

## Electrical properties of materials:

Free–electron concept (Drift velocity, Thermal velocity, Mean collision time, Mean free path, relaxation time). Failure of classical free electron theory. Quantum free electron theory, Assumptions, Fermi factor, density of states(qualitative only), Fermi–Dirac Statistics. Expression for electrical conductivity based on quantum free electron theory, Merits of quantum free electron theory.

Conductivity of Semi conducting materials, Concentration of electrons and holes in intrinsic semiconductors, law of mass action.

Temperature dependence of resistivity in metals and superconducting materials. Effect of magnetic field (Meissner effect).Type-I and Type II superconductors–Temperature dependence of critical field.BCS theory(qualitative).High temperature superconductors. Applications of superconductors –Maglev vehicles.

**10 Hour**

## Content:

- **Quantum free electron theory- assumptions**
- **Fermi energy**
- **Density of states**
- **Temperature dependence of resistivity of metals**
- **Conductivity of Semi conducting materials**
- **Hall effect**
- **BCS theory**
- **Maglev vehicles and Squid**

## Free electron concept:

*[Drude Lorentz theory, classical free electron theory]*

The stable configuration of a solid is due to the arrangement of atoms and the distribution of electrons in the atom. In metals, bulk state of the metallic elements are crystalline involving a geometric array of atoms in a space lattice, within these atoms the nuclei are surrounded by electrons. The electrons in the inner orbits which are bound to the nuclei form core electrons which cannot be disturbed easily ,those electrons which are in the outer orbits and loosely bound to the nuclei can be disturbed easily and are called valence electrons.

In metals, due to close packing of atoms the boundaries of neighbouring atoms overlap. Due to this, the valence electrons find continuity from one atom to the other and thereby they are not confined to their parent atom. These electrons are free to move within the metal and hence are called free electrons. As these electrons are responsible for electrical conduction in solid, they are also called as conduction electrons.

## Classical Free Electron Theory.

To account for the electrical conduction in metals P.Drude proposed in 1900 the free electron theory of metals. In 1909 H.A.Lorentz extended the theory of Drude. As the theory is based on classical laws and Maxwell - Boltzmann statistics it is also called as classical-free electron theory. The basic assumption in this theory is that a metal consists of a large number of free electrons which can move about freely throughout the body of the metal.

### Assumptions:

1. All metals contain a large number of free electrons which move freely through the positive ionic core of the metals.

Under the application of an applied field these electrons are responsible for electrical conduction and hence called conduction electrons.

2. The free electrons are treated as equivalent to gas molecules and have three degrees of freedom and are assumed to obey Kinetic Theory of Gases.

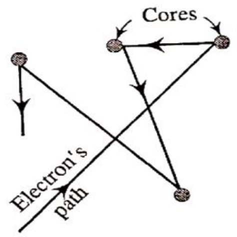
In the absence of an electric field, the kinetic energy associated with an electron at a temperature T is given by (3/2) kT, where k is the Boltzmann constant.

$$\therefore \frac{1}{2} m v_{th}^2 = \frac{3}{2} kT$$

Where $v_{th}$ is the thermal velocity same as root mean square velocity.

3. The electrons travel under a constant potential inside the metal due to the positive ionic cores but stay confined within its boundaries.
4. The interaction between free electrons and positive ion cores and free electrons themselves are considered to be negligible [or ignored]
5. The electric current in a metal due to an applied field is a consequence of the drift velocity in a direction opposite to the direction of the field.

**Mean collision time: (τ)**



*"The average time that elapses between two consecutive collisions of an electron with the lattice points is mean collision time."*

$\tau = -$ Where λ - mean free path

v -total velocity of the electrons due to the combined effect of thermal and drift velocities.

**Note :** As $V_d << V_{th}$

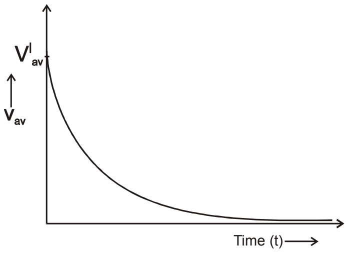
$V_{av} = V = V_{th}$

**Mean free path: (λ)**

*"The average distance travelled by an electron between the successive collisions with the lattice points during their random motion is called mean free path."*

**Relaxation time: ($\tau_r$)**

In the absence of an applied field, the average velocity of the electrons is zero and has some finite value under an applied field.



$v_{av} = 0$ in the absence of the field.

$v_{av} =$ in the presence of electric field.

If the field is turned off suddenly, the average velocity $v_{av}$ reduces exponentially to zero.

Mathematically

$v_{av} = v'_{av}\, e^{-t/\tau_r}$

The time't' is counted from the instant the field is switched off and $\tau_r$ is a constant, called *relaxation time.*

If $t = \tau_r$

Then $v_{av} = v'_{av} e^{-1}$

or $\boxed{v_{av} = \frac{1}{e}\, v'_{av}}$

*"Thus, the* ***relaxation time*** *($\tau_r$) is defined as the time during which the average velocity ($v_{av}$) decreases to $\frac{1}{e}$ times its value at the time when the field is turned off".*

## Drift velocity : $V_d$

Under thermal equilibrium condition, the valence electron in a solid is in a state of random motion. Under a constant field, the electrons will experience a force eE and gets accelerated. An electric field E modifies the random motion and causes the electrons to drift in a direction opposite to that of E. the electrons acquire a constant average velocity in the field. This velocity is called the drift velocity, $V_d$.

*"The average velocity with which free electrons move in a steady state opposite to the direction of the electric field in a metal is called* ***drift velocity".***

## Expression for drift velocity:

If a constant electric field E is applied to the metal the electron of mass m and charge e will experience a force, F= - eE.

F= - eE driving force on the electron which results in the drift velocity $v_d$,

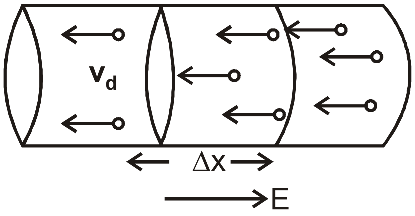
Then the resistance force offered to its motion is

$F_r = \frac{mv_d}{\tau}$ where $\tau$ mean collision time

In the steady state,

$F_r = F$

i,e, $\frac{mv_d}{\tau} = eE$



$$\boxed{V_d = \left(\frac{eE}{m}\right)\tau}$$

**Note :** Current density, $J = \frac{I}{A}$

$$\boxed{J = nev_d} \qquad \boxed{I = nAev_d}$$

**Electrical conductivity in metals**

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

Thus conductivity is proportional to the number of electrons per $m^3$.

**Mobility of electrons: μ**

This measures the ease with which the electrons can drift in a material under the influence of an electric field

*"The mobility of electrons is defined as the magnitude of the drift velocity acquired by the electrons per unit applied field".*

$$\mu = \frac{v_d}{E} \text{.........} (1)$$

From ohm's law

$$\sigma E = J$$

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

$$= \frac{I}{AE} \qquad \text{because, } J = \frac{I}{A}$$

$$= \frac{nev_d A}{AE}$$

$$\sigma = ne\mu$$

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

Greater the value of conductivity (σ), greater is the value of mobility (μ)

## Failures of classical free electron theory:

Electrical and thermal conductivities can be explained from classical free electron theory. It fails to account the facts such as specific heat, temperature dependence of conductivity and dependence of electrical conductivity on electron concentration.

### (a)Specific heat capacity

The molar specific heat of metal at constant volume is

$$C_v = \frac{3}{2}R$$

But experimentally the contribution to the specific heat capacity by the conduction electrons is found to be

$$C_v = 10^{-4}\,RT$$

Thus the predicted value is much higher than the experimental value. Further the theory indicates no relationship between the specific heat capacity and temperature. Experimentally however, the specific heat capacity is directly proportional to the absolute temperature.

### (b) Dependence of electrical conductivity on temperature:

According to the main assumptions of the classical free electron theory.

$$\frac{3}{2}kT = \frac{1}{2}mv_{th}^2$$

$$\therefore v_{th} = \sqrt{\frac{3kT}{m}}$$

$$v_{th} \propto \sqrt{T}$$

The mean collision time $\tau$ is inversely proportional to the thermal velocity.

$$\tau \propto \frac{1}{v_{th}}$$

$$\therefore \tau \propto \frac{1}{\sqrt{T}}$$

Electrically conductivity $\sigma$ is given by

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

$$\therefore \sigma \propto \tau \propto \frac{1}{\sqrt{T}}$$

$$\boxed{\sigma_{theory} \propto \frac{1}{\sqrt{T}}} \rightarrow \text{Theoretically obtained}$$

But experimentally it is found that $\boxed{\sigma_{exp} \propto \frac{1}{T}}$

Again it is found that the prediction of the theory is not matching with the experimental results.

**(c) Dependence of electrical conductivity on electron concentration:**

According to classical theory electrical conductivity σ is given by.

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

Therefore $\sigma \propto n$

This means that divalent and trivalent metals, with larger concentration of electrons should possess much higher electrical conductivity than monovalent metals, which is contradiction to the observed fact. Where experimentally it is found that as 'n' increases, σ is not found to increase. The conductivity of monovalent metals [E.g. copper, silver] is greater than that of divalent and trivalent metals [E.g.: zinc, aluminium].

***NOTE:[****The electron concentrations for zinc and cadmium are $13.1\times10^{28}/m^3$ and $9.28\times10^{28}/m^3$ which are much higher than that for copper and silver, the values of which are $8.45\times10^{28}/m^3$ and $5.85\times10^{28}/m^3$ respectively. Zinc and cadmium which are divalent metals have conductivities $1.09\times10^7/\Omega m$ and $0.15x10^7/\Omega m$. These are much lesser than that of monovalent metals copper and silver, the values of which are $5.88x10^7/\Omega m$ and $6.3x10^7/\Omega m$ respectively****.]***

## Quantum free electron theory:

To account for the failures of classical free electron theory Arnold Sommerfeld came up with quantum free electron theory. The theory extensively uses *Pauli's Exclusion Principle* for restricting the energy values of electron. But the main assumptions of classical free electron theory are retained.

### Assumptions:

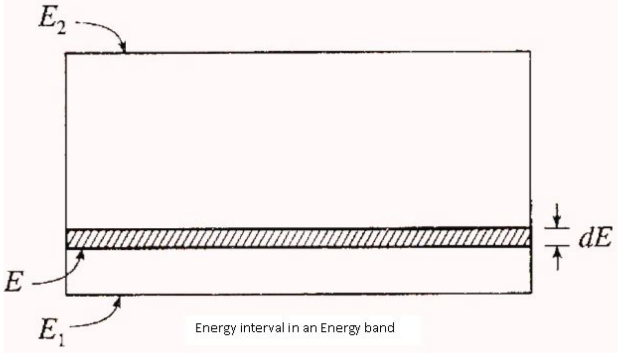
1. The energy values of the conduction electrons are quantized. The allowed energy values are realized in terms of a set of energy values.

2. The distribution of electrons in the various allowed energy levels occur as per Pauli's exclusion principle and also obey the Fermi – Dirac quantum statistics.
3. The field due to positive ion core is constant throughout the material. So electrons travel in a constant potential inside the metal but stay confined within its boundaries.
4. Both the attraction between the electrons and the lattice points, the repulsion between the electrons themselves is ignored and therefore electrons are treated free.

**Density of states, g(E):**

There are large numbers of allowed energy levels for electrons in solid materials. A group of energy levels close to each other is called as energy band. Each energy band is spread over a few electron-volt energy ranges. In 1mm$^3$ volume of the material, there will be a more than a thousand billion permitted energy levels in an energy range of few electron-volts. Because of this, the energy values appear to be virtually continuous over a band spread. To represent it technically it is stated as density of energy levels. The dependence of density of energy levels on the energy is denoted by g (E). The graph shows variation of g (E) versus E. It is called density of states function.

*"It is the number of allowed energy levels per unit energy interval in the valance band associated with material of unit volume". In an energy band as E changes g (E) also changes.*



Energy interval in an Energy band

Consider an energy band spread in an energy interval between $E_1$ and $E_2$. Below $E_1$ and above $E_2$ there are energy gaps. g (E) represents the density of states at

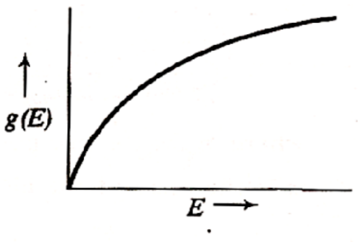
E. As dE is small, it is assumed that g (E) is constant between E and E+dE. The density of states in range E and (E+dE) is denoted by g(E)dE.

Density of states is given by, **g(E) dE =** ——— **dE**

$$\boxed{g(E) = C E^{\frac{1}{2}} dE}$$

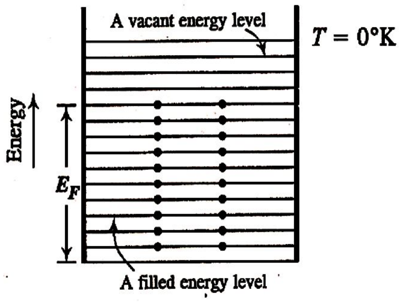
Where c= ——— is a constant.

It is clear g (E) is proportional to in the interval dE



DENSITY OF STATES

**Fermi energy ($E_F$):** In a metal having N atoms, there are N allowed energy levels in each band. In the energy band the energy levels are separated by energy differences. It is characteristic of the material. According to Pauli's exclusion principle, each energy level can accommodate a maximum of two electrons, one with spin up and the other with spin down. The filling up of energy levels occurs from the lowest level. The next pair of electrons occupies the next energy level and so on till all the electrons in the metal are accommodated. Still number of allowed energy levels, are left vacant. This is the picture when there is no external energy supply for the electrons.



FERMI ENERGY

"*The energy of the highest occupied level at absolute zero temperature (0K) is called the Fermi energy and the energy level is called Fermi level*". It is denoted by '$E_f$'

$$\text{Fermi energy}, E_{Fo} = \frac{h^2}{8m}\left(\frac{3n}{\pi}\right)^{2/3}$$

$$E_{Fo} = Bn^{2/3}$$

Where $B = \frac{h^2}{8m}\left(\frac{3}{\pi}\right)^{2/3}$ is a constant = $5.85\times10^{-38}$J

Fermi energy $E_F$ at any temperature, T in general can be expressed in terms of $E_{Fo}$ through the relation

$$E_F = E_{Fo}\left[1 - \frac{\pi^2}{12}\left(\frac{kT}{E_{Fo}}\right)^2\right]$$

Except at extremely high temperature, the second term within the brackets is very small compared to unity. Hence at ordinary temperature the values of $E_{Fo}$ can be taken to be equal to $E_F$.

ie, $\mathbf{E_F = E_{Fo}}$

Thus at a temperature the Fermi ($E_F$) is nothing but the fermi energy at absolute temperature($E_{Fo}$).

## Fermi-Dirac statistics:

Under thermal equilibrium the free electrons acquire energy obeying a statistical rule known as Fermi-Dirac statistics. Fermi-Dirac distribution deals with the distribution of electrons among the permitted energy levels. The permitted energy levels are the characteristics of the given material. The density of the state function g (E) changes with energy in a band. The number of energy levels in the unit volume of the material in the energy range E & (E+dE) is g (E)dE.

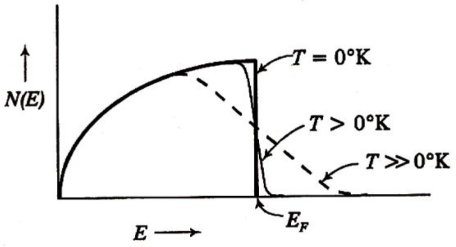
Each electron will have its own energy value which is different from all others except the one with opposite spin. The number of electrons with energy range E & (E+dE) in unit volume is N(E)dE which is the product of the number of energy levels in the same range and the fermi factor.

$\therefore$ N (E) dE = f(E) ×g(E)dE.

But f(E) and g(E) at a temperature T changes only with E. That is, N(E)dE at a given temperature change with E.

The plot of N(E)dE versus E represents the actual distribution of electrons among the available states for the material at different temperatures. The distribution is known as Fermi–Dirac distribution. Fermi-Dirac distribution represents the detailed distribution of electrons among the various available energy levels of a material under thermal equilibrium conditions.

Fermi-Dirac distribution can be considered in the following three conditions: At T=0K, at T> 0K and T>>0K.The plot of N(E) versus E for all the three cases is in the fig.



FERMI-DIRAC DISTRIBUTION AT DIFFERENT TEMPERATURES

**Fermi factor,f (E):**The electrons in the energy levels far below Fermi level cannot absorb the energy above absolute zero temperature. At ordinary temperature because there are no vacant energy levels above Fermi level into which electrons could get into after absorbing the thermal energy. Though the excitations are random, the distributions of electrons in various energy levels will be systematically governed by a statistical function at the steady state.

The probability f(E) that a given energy state with energy E is occupied at a steady temperature T is given by, $f(E)=\frac{1}{e^{\frac{(E-E_F)}{kT}}+1}$ f(E) is called the Fermi factor.

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

**(i) Probability of occupation for $E<E_f$ at T = 0°K**

When T=0°K &$E<E_f$

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

$$= \frac{1}{0+1}$$

f(E) = 1 for E < $E_F$

Hence,f(E) = 1 means the energy level is certainly occupied, & E<$E_F$ applies to all the levels below $E_F$.

∴ At T=0°K, all the energy levels *below* the Fermi level are *all occupied.*

**(ii) Probability of occupation for E > $E_F$ at T= 0°K**

When T =0°K & E > $E_F$

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

f(E) = 0 for E > $E_F$

∴ At T=0°K all the energy levels *above* Fermi level are *unoccupied.*

In view of the above two cases, at T=0°K the variation of f(E) for different energy values, becomes a step function as in fig.

**(iii) Probability of occupation at ordinary temperatures.**

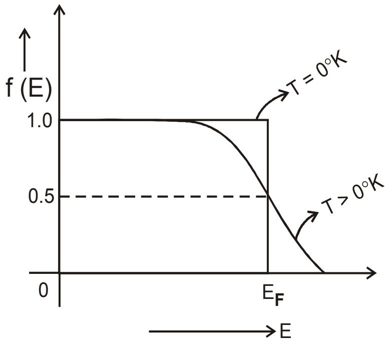
At ordinary temperatures, though the value of probability remains 1 for E<< $E_F$ it starts decreasing from 1 as the values of E become closer to $E_F$.

At E = $E_F$&T > 0° k

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

$$= \frac{1}{1+1}$$

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



Further, for E>$E_f$, the probability value falls off to zero rapidly. Thus plot of f(E) Vs E at different temperatures is as in figure.

**Fermi Temperature:**

*"Fermi temperature is the temperature at which the average thermal energy of the free electron in a solid becomes equal to the Fermi energy at 0°K".*But the thermal energy possessed by electrons is given by the product of kT.

It means when T = $T_F$, $kT_F = E_{F0}$ is satisfies.

But all practical purposes, $\mathbf{E_F = E_{F0}}$

$\therefore$ $\mathbf{T_F} = \frac{E_F}{k}$

Fermi temperature is only a hypothetical concept because even at ordinary temperature it is not possible for electrons to receive thermal energy in a magnitude of $E_F$. For example at $E_F = 3eV$, $T_F = 34800$ K which is quite exaggerated to realize.

**<u>Fermi Velocity</u>**:*"The Velocity of the electrons which occupy the fermi level is called fermi velocity $V_F$".*

$$\therefore E_F = \frac{1}{2} m v_F^2$$

$$\mathbf{V_F} = \left( \frac{2E_F}{m} \right)^{1/2}$$

**<u>Expression for Electrical conductivity in metals</u>**

According to Sommerfeld's quantum free electron theory, the free electrons obey Fermi-Dirac Statistics as compared to gas molecules which are known to obey Maxwell- Boltzmann statistics. Hence by applying F-D statistics and by using the Boltzmann transport equation the expression for electrical conductivity is

$$\boldsymbol{\sigma} = \frac{\mathbf{ne^2\,\lambda}}{\mathbf{m^* V_f}}$$

Where $m^*$ is the effective mass of an electron.

The expression for electrical resistivity is

$$\boldsymbol{\rho} = \frac{\mathbf{m^* V_f}}{\mathbf{ne^2\,\lambda}}$$

**Merits of Quantum Free Electron Theory:**

**a) Specific heat:**

According to classical free electron theory all the free electrons in a metal absorb the heat energy when a metal is heated. It results in a large value of specific heat. But as per quantum free electron theory, only a few electrons that are occupying energy levels close to Fermi energy level $E_F$ absorb the heat energy to get excited to higher energy levels and contribute for specific heat. Hence the value of specific heat is very small.

According to quantum free electron theory the specific heat of solids is given by

$$C_v = 10^{-4}RT$$

The above result agrees well with the experimentally observed values.

**b) Temperature dependence of electrical conductivity:**

We have, $\sigma = \frac{ne^2\tau}{m*}$

$$\sigma = \frac{ne^2}{m*}\frac{\lambda}{v_f} \text{........... (1)} \qquad \text{Because } \tau = \frac{\lambda}{v_f}$$

As per quantum free electron theory, $E_f$ and $V_f$ are independent of temperature. But λ is dependent on temperature and is explained as.

As the free electrons traverse in a metal they get scattered by vibrating ions of the lattice. The vibrations occur in such a way that the displacement of ions takes place equally in all directions. Hence ions may be assumed to be present effectively in a circular cross section of area $\pi r^2$ which blocks the path of the electrons irrespective of direction of approach [here r is the amplitude of vibration].

The vibrations of larger area of cross section scatter more effectively, thereby reducing λ

$$\Rightarrow \lambda \propto \frac{1}{\pi r^2} \text{......... (2)}$$

But

a) The energy E of the vibrating body is proportional to the square of amplitude

b) E is due to thermal energy.

c) E is proportional to temperature T.

$$\therefore r^2 \propto T$$

$$\therefore \lambda \propto \frac{1}{T} \text{...............(3)}$$

Comparing (1) & (3)

$$\text{Thus} \quad \sigma \propto \frac{1}{T}$$

Thus the exact dependence of σ on T is explained.

**c). Electrical conductivity and electron concentration:**

The free electron model suggests that σ is proportional to electron concentration 'n' but trivalent metals such as aluminum and gallium having more electron concentration than that of monovalent metals, have lower electrical conductivity than monovalent metals such as copper and silver.

According to quantum free electron theory.

$$\sigma = \frac{ne^2}{m}\left(\frac{\lambda}{v_f}\right)$$

It is clear from the above equation that σ depends on both 'n' & the ratio $\left(\frac{\lambda}{v_f}\right)$.

**Expression for Electrical Conductivity of a Semiconductor:**

On the basis of free electron theory, the charge carriers can be assumed to be moving freely inside a semiconductor. Both the holes and the electrons contribute to the conductivity of the semiconductor.

Let us consider to start with, the conductivity in a semiconductor due to the flow of electrons only. Consider a semiconductor of area of cross section A, in which a current I is flowing. Let v be the velocity of electrons. The electrons move through a distance v in one second. As per the assumption of free electron theory, a large number of free electrons flow freely through the semiconductor whose area of cross section is A.

The volume swept by the electrons/second = Av.

If $N_e$ is the number of electrons / unit volume, and e is the magnitude of electric charge on the electron, then, the charge flow/second = $N_eeAv$.

Since charge flow/second is the current I,

$I = N_eeAv$.

$\therefore$ Current density $J = (I/A) = N_eev$ …… (1)

The electron mobility, μe is given by,

$\mu_e = v/E$, …… (2)

Where, E is the electric field.

Substituting for v, from Eq. (2), Eq. (1) becomes,

$$J = N_e\, e\, (\mu_e E) \quad \text{…… (3)}$$

But the ohm's law, is given by the equation,

$J = \sigma E$ where σ is the conductivity of the charge carriers.

If $\sigma_e$ is the conductivity due to electrons in the semiconductor material, then ohm's law becomes,

$$J = \sigma_e E \,, \qquad \ldots\ldots (4)$$

Comparing Eqs (3) and (4),

conductivity of electrons is given by,

$$\sigma_e = N_e e\mu_e \qquad \ldots\ldots (5)$$

Now let us consider the contribution of holes to the conduction of electricity. If $\sigma_h$ is the conductivity due holes, $N_h$ is the number of holes/unit volume and $\mu_h$ is the mobility of holes, then in similarity to Eq (5), the equation for conductivity due to holes can be written as,

$$\sigma_h = N_h e \mu_h \qquad \ldots\ldots (6)$$

The total conductivity for a semiconductor is given by the sum of $\sigma_e$ and $\sigma_h$ .

i.e, $\sigma = \sigma_e + \sigma_h = N_e e \mu_e + N_h e \mu_h$

$$\boldsymbol{\sigma = e (N_e \mu_e + N_h \mu_h)} \qquad \ldots\ldots (7)$$

***For an Intrinsic Semiconductor (Pure Semiconductor)***

In the case of intrinsic semiconductor, the number of holes is always equal to the number of electrons. Let it be equal to $n_i$ ,i.e. $N_e = N_h, = n_i$ .

By using Eq. (7), $\sigma_i$ the conductivity of an intrinsic semiconductor can be written as,

$$\boldsymbol{\sigma_i = n_i e (\mu_e + \mu_h)} \qquad \ldots\ldots (8)$$

## Concentration of charge carriers:

***Expressions for electron concentration (Ne) and hole concentration ($N_h$) at a given temperature :***

*"The number of electrons in the conduction band/unit volume of the material is called the electron concentration".* Similarity "*the number of holes in the valence band/unit volume of the material is called the hole concentration".* In general, *"the number of charge carries/unit volume of the material is called carrier concentration".*

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

Consider the evaluation of $N_h$ , the hole concentration in the valence band.

i.e, $\therefore N_h = \frac{4\sqrt{2}}{h^3}(\pi m_h{}^{*} kT)^{3/2} e^{-E_F/kT}$

Both ***Ne*** and ***$N_h$*** are dependent on Fermi enery ($E_F$)

## Law of mass action for semiconductors:

We have for electron concentration $N_e$ and hole concentration $N_h$ , the equations,

$$\therefore\ N_e = \frac{4\sqrt{2}}{h^3}(\pi m_e{}^{*}kT)^{3/2}e^{\left(\frac{E_F-E_g}{kT}\right)} \qquad \text{and,}$$

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

In the above expressions, we see the dependence of both $N_e$&$N_h$ on $E_F$. Let us consider the product $N_e$&$N_h$.

$$N_e\,N_h = \frac{32}{h^6}(\pi kT)^3(m_e * m_h *)^{3/2}e^{E_g/kT}$$

The above equation shows that the product $N_e\ N_h$ does not depend on $E_F$, but remains a constant at a given temperature for the given semiconductor.

$$\therefore \mathbf{N_e\ N_h = a\ constant.}$$

This condition is applicable for both extrinsic and intrinsic semiconductors.

For an intrinsic semiconductor, $N_e = N_h = n_i$ where, ni is the intrinsic charge carrier density.

Then $N_e N_h = n^2_i$ = a constant.

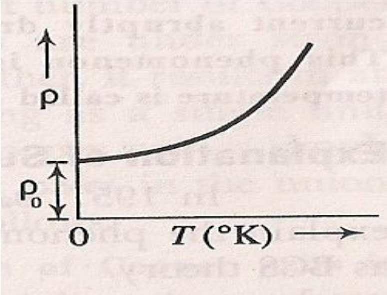
The above equation is called the law of mass action for semiconductors. *"The law says that, for a given semiconductor material either extrinsic or intrinsic, the product of the charge carrier concentration remains a constant at any temperature, even if the doping is varied".*

## Superconductivity

Super conductivity is the phenomenon observed in some metals and materials. Kammerlingh Onnes in 1911 observed that the electrical resistivity of pure mercury drops abruptly to zero at about 4.2K .This state is called super conducting state. The material is called superconductor .The temperature at which superconductivity is attained is called critical temperature $T_c$.

### *Temperature dependence of resistivity of a metal:*

All metals are good conductors of electricity. The electrical conductivity of metal varies with the temperature. The electrical resistance of a metal, to the flow of current, is due to scattering of conduction electrons by lattice vibrations. When the temperature increases the amplitude of lattice vibrations also increases, thereby increasing the resistance. The dependence of resistance of metal (non-superconducting state) on temperature is shown in figure. The resistance decreases with temperature and reaches a minimum value known as residual resistance, at T = 0K. The residual resistance at T = 0K is due to impurities in the metal.



DEPENDENCE OF ρ ON T

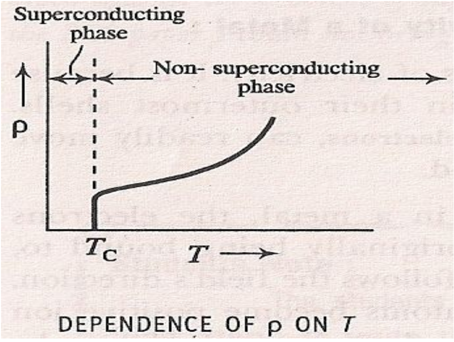
The variation is expressed by Matthiessen's rule

$$\boldsymbol{\rho = \rho_o + \rho(T)}$$

Where 'ρ' is the resistivity of the given material, '$\rho_o$'is the residual resistivity and 'ρ(T)' is the temperature dependent part of resistivity called ideal resistivity.

***Temperature dependence of resistivity of a superconductor:***

The resistance of a superconductor in the non-superconducting state decreases with temperature and the electrical resistivity of some of the metals and alloys vanish entirely below a certain temperature. *"The resistance offered by certain materials to the flow of electric current abruptly drop to zero below a threshold temperature. This phenomenon is called* ***superconductivity*** *and threshold temperature is called "critical temperature." "The temperature at which a material undergoes transition from normal state to superconducting state losing its resistivity is called the* ***critical temperature or transition temperature Tc****".*Above the transition temperature, the substance is in the normal state and below it will be in superconducting state. The critical temperature is different for different superconducting materials. It is not very sensitive to the presence of small amount of impurities.



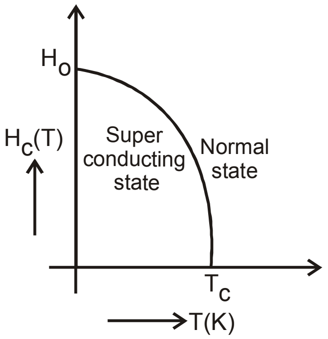
## ***BCS Theory*** **(Explanation of superconductivity)*:***

Bardeen, Cooper and Schrieffer (BCS) in 1957 explained the phenomenon of superconductivity based on the formation of cooper pairs. It is called BCS theory. It is a quantum mechanical concept.

During the flow of current in a superconductor, when an electron approaches a positive ion lattice of the metal there is a Coulomb force of attraction between the electron and the lattice ion and thus ion core is set in motion causing lattice distortion. Smaller the mass of the positive core, larger will be the distortion. The lattice vibrations are quantized in a terms of *Phonons.* Now another electron passing by this distorted lattice will interact with it and thus the energy of this electron is also reduced. This interaction is looked upon as if the two electrons interact via the phonon field, (because the lattice vibrations are quantized and quanta of these vibrations are *phonons*) resulting in lowering of energy for the electrons. Due to this interaction an apparent force of attraction develops between the electrons and they tend to move in pairs. *This interaction is strongest when the two electrons have equal and opposite spins and momenta.*This leads to the formation of cooper pairs. *"**Cooper pairs** are a bound pair of electrons formed by the interaction between the electrons with opposite spin and momenta in a phonon field".*

At normal temperatures the attractive force is too small and pairing of electrons does not take place.At lower temperature that is below the critical temperature the apparent force of attraction exceeds the Coulomb force of repulsion between two electrons leading to the formation of cooper pairs. According to quantum mechanics a cooper pair is treated as single entity. A wave function is associated with each such cooper pair and wave functions associated with similar cooper pairs start overlapping which extends over a million pairs and hence virtually over the entire volume of the superconductor. Finally large number of cooper pairs forms a union one aiding the motion of the other. So the entire union of cooper pairs will therefore move as one unit. The resistance experienced by any one cooper pair is overcome by the co-operative action of the other pairs in the union. Ultimately when electrons flow in a material in the form of cooper pairs do not encounter scattering. The resistance vanishes and conductivity is very large and thus the phenomenon superconductivity.

### **Effects of magnetic field(*critical field $H_c$*):**



The superconducting state of a metal exits only in a particular range of temperature and field strength. The condition for the superconducting state to exist in the metal is that some combination of temperature and field strength should be less than a critical value. Super conductivity will disappear if the temperature of the specimen is raised above its $T_c$ or if sufficiently strong magnetic field is employed. *"The minimum magnetic field required to destroy the superconductivity in the material is called **critical field $H_c$**".*

The critical field as a function of temperature is nearly parabolic and can be reasonably represented by

$\mathbf{H_c = H_o\left(1 - \left(\frac{T^2}{T_C{}^2}\right)\right)}$Where $H_o$ is the critical magnetic field at 0° K.

By applying magnetic field greater than $H_o$, the material can never become superconductor whatever may be the low temperature. The critical field need not be external but large current flowing in superconducting ring itself can produce critical field and destroys superconductivity.

### **Meissner effect:**

A superconducting material kept in a magnetic field expels the magnetic flux out of its body when it is cooled below the critical temperature and thus becomes perfect diamagnetic. This effect is called Meissner effect.

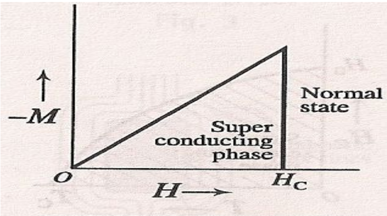
### **Type of superconductors**

### **1.Type I superconductors:**

These materials exhibit complete Meissner effect and have well defined critical field $H_c$. These are perfect diamagnetic in the superconducting state and possesses negative magnetic moment.

The material remains in the superconducting when the field is less than the critical field. It expels the magnetic lines of force from the body of the mater immediately after $H_c$ the material transits to normal state and the flux penetrates the material i.e. Meissner effect is absent. $H_c$ is of the order of 0.1 T or less. Since $H_c$ very low, even weak magnetic field can destroy the phenomenon. As weak magnetic field can penetrate the material more easily and they are also called *soft superconductor.*

| Element | $T_c$ (K) |
|---|---|
| Aluminium | 1.196 |
| Cadmium | 0.52 |
| Gallium | 1.09 |
| Indium | 3.40 |
| Tin | 3.72 |
| Mercury | 4.12 |
| Lead | 7.175 |

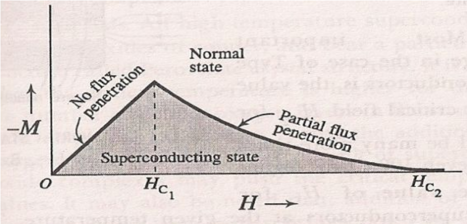


DEPENDENCE OF MAGNETIC MOMENT ON H

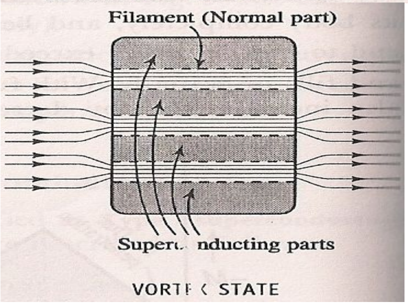
## 2.Type II Superconductors:

These materials are having two critical fields $H_{c1}$ and $H_{c2}$. For the field less then$H_{c1}$ (lower critical field), it expels the magnetic field completely and there is no flux penetration. It becomes a perfect diamagnetic and the material is in the super conducting state. After $Hc_1$ the flux penetrates and partially fills the body of the material through channels called filaments. As the field is increased these filaments broaden and by $Hc_2$ (the material possesses both normal and superconducting state, hence the state is called *'Mixed State'.* This is also referred to as '*vortex state'* where the material is in a magnetically mixed state but electrically it is a superconductor. After $Hc_2$ the material transits to normal state and the resistance is finite. Type II superconductors can carry larger currents when the magnetic field is between $Hc_1$ and $Hc_2$.

$Hc_2$ the upper critical field is many a folds greater than $Hc_1$ the lower critical field. Only strong magnetic field of the order of 10T can penetrate the material hence these are called hard super conductor. Type-II superconductors are used in the manufacturing of the superconducting magnets of high magnetic fields above 10 Tesla.



DEPENDENCE OF MAGNETIC MOMENT ON *H*



VORTEX STATE

| Element | $T_c$ (K) |
|---|---|
| Tantalum | 4.5 |
| Thallium | 2.4 |
| Niobium | 9.3 |

## High temperature superconductors

Superconductors with a transition temperature above 100˚K are known as high temperature superconductors. In 1987 it was shown that materials such as $YBa_2Cu_3O_7$-x,(x≤0.1) have critical temperature which is well above that of liquid nitrogen (77K). Hence they do not require liquid helium at all for cooling. These compounds are known as 1-2-3 compound as the constituent present are in the ratio 1, 2 & 3.

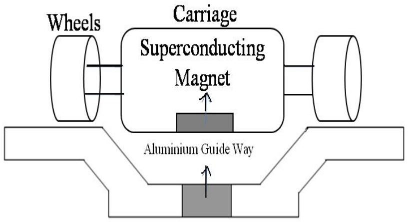
These are not metals or inter metallic compound, they are oxides classified as ceramics. All high temperature superconductors are different types of oxides of copper, and bear a particular type of crystal structure called Perovskites crystal structure. The number of copper layers increases the Tc value increases. The current in the high $T_C$ materials is direction dependent. It is strong in parallel to copper-oxygen planes and weak in perpendicular to copper-oxygen planes.

High Tc materials are Type-II superconductors and they are brittle and not easily formed into wires, unable to carry large currents and unstable over long periods. The formation of electron pairs is not due to interaction of electron lattice as in the BCS theory. Still it is not clear what does cause the formation of pairs. Research is being conducting in this direction. The above said difficulties are not there with recent high temperature super conductors where the rare earth elements are replaced by Bismuth or Thallium (around 100K).Today one cannot rule out the possibility of room temperature superconductivity.

## ***Applications of Superconductors:***

***Magnetically Levitated Vehicles (Maglev vehicles):*** Magnetically levitated vehicles are called Maglev vehicles. The magnetic levitation is based on the principle of Meissner effect. The repulsion between the two strong fields produced by the superconducting magnet and electric current levitates the vehicle and is set afloat. The afloating of the vehicles by this principle is called *Magnetic Levitation.*

The superconducting magnet is kept inside the vehicle and the electric current flows in the Aluminium guide way. Once the magnetic field in the vehicle is switched on is repelled by the magnetic field of the guide way. As it is about to levitate, the guide way propels the vehicle forward by the segments provided in the Aluminium guide way. The vehicle is provided with retractable wheels. Initially the vehicle runs on the guide way, once it is levitated in air the wheels are retracted into the body. The height to which the vehicle is levitated above guide way is about 10 to 15cm. While stopping, the wheels are drawn out and the vehicle slowly settles on the guide way by running a distance. Since such vehicles float under magnetic effect, they do not have friction, less power consumption, and noiseless travel.



# Module-3

## Lasers and Optical Fibers

Einstein's coefficients (expression for energy density).Requisites of a Laser system. Condition for laser action. Principle, Construction and working of $CO_2$ laser and semiconductor Laser. Applications of Laser – Laser welding, cutting and drilling. Measurement of atmospheric pollutants. Holography–principle of Recording and reconstruction of images.

Propagation mechanism in optical fibers. Angle of acceptance. Numerical aperture. Types of optical fibers and modes of propagation. Attenuation, Block diagram discussion of point to point communication, applications.

**10 Hour**

# Content:

- **Einstein's coefficients**
- **Essential requisites of a laser system**
- **Population inversion and metastable state**
- **$Co_2$ laser**
- **Semiconductor laser**
- **Applications of laser**
- **Holography**
- **Numerical aperture**
- **attenuation**

## Introduction:

The word Laser stands for ***L**ight **A**mplification by **S**timulated **E**mission of **R**adiation.* It is a device which amplifies light. It has properties like Coherence, Unidirectional, Monochromatic, Focusability, etc.

**Interaction of an electromagnetic wave with matter** requires certain conditions. The interaction leads to transition of an atom or a molecule from one energy state to another. If the transition is from lower state to higher state it absorbs the incident energy. If the transition is from higher state to lower state it emits a part of its energy.

If $\Delta E$ is the difference between the two energy levels,

Then $\Delta E = (E_2 - E_1)$ Joule

According to Max Planck, $\Delta E = h\nu = (E_2 - E_1)$

$\nu = (E_2 - E_1)/h$ Hz.

Three types of interactions, which are possible:

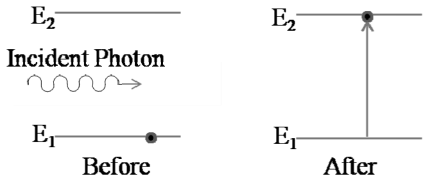
1) Induced absorption/ Stimulated absorption/absorption
2) Spontaneous emission
3) Stimulated emission.

Emission or Absorption takes through quantum of energy called photons. $h\nu$ is called quantum energy or photon energy.

$h = 6.626\times10^{-34}$ Joules is Planck's constant and '$\nu$' is the frequency.

### 1) *Induced absorption/ Stimulated absorption/absorption:*

Induced absorption is the absorption of an incident photon by system as a result of which the system is elevated from a lower energy state to a higher state, wherein the difference in energy of the two states is the energy of the photon Consider the system having two energy states $E_1$ and $E_2$, $E_2 > E_1$. When a photon of energy $h\nu$ is incident on an atom at level $E_1$, the atom goes to a higher energy level by absorbing the energy.



When an atom is at ground level ($E_1$), if an electromagnetic wave of suitable frequency $\nu$ is applied to the atom, there is possibility of getting excited to higher level ($E_2$). The incident photon is absorbed. It is represented as

$$\text{Atom} + \text{Photon} \rightarrow \text{Atom}^*$$

The frequency of the absorbed photon is

$$\nu = (E_2 - E_1)/h.$$

The rate of absorption is proportional to $N_1U_\nu$

Where '$N_1$' is the number density of the lower energy state, '$U_\nu$' is the energy density of incident radiation.

Rate of induced absorption $\alpha$ $N_1U_\nu$

Rate of absorption = $B_{12}N_1U_\nu$

Where '$B_{12}$' is the proportionality constant called Einstein Coefficient of induced absorption.

### 1. ***Spontaneous Emission:***

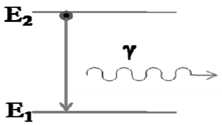
The emission of a photon by the transition of a system from a higher energy state to a lower energy state without the aid of an external energy is called spontaneous emission. Let '$E_1$' and '$E_2$' be two energy levels in a material, such that $E_2>E_1$. $E_1$ is ground level and $E_2$ is the higher level. $h\nu=E_2-E_1$ is the difference in the energy. The atom at higher level ($E_2$) is more unstable as compared to that at lower level ($E_1$).

In spontaneous emission atom emits the photon without the aid of any external energy. It is called spontaneous emission. The process is represented as

$$\text{Atom}^* \rightarrow \text{Atom} + \text{Photon}$$

The photons emitted in spontaneous emission may not have same direction and phase similarities. It is incoherent.

Ex: Glowing electric bulbs, Candle flame etc.



Spontaneous emission depends on $N_2$ which is the number of atoms present in the higher level.

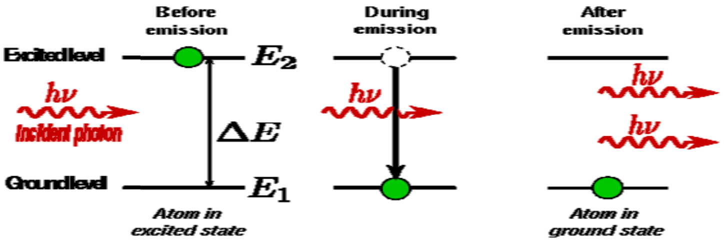
The rate of spontaneous emission $\alpha$ $N_2$

The rate of spontaneous emission= $A_{21}N_2$

Where '$A_{21}$'is the proportionality constant called Einstein coefficient of spontaneous emission.

2. ***Stimulated Emission:***

Stimulated emission is the emission of a photon by a system under the influence of a passing photon of just the right energy due to which the system transits from a higher energy state to a lower energy state.



$$E_2 - E_1 = \Delta E = h\nu$$

The photon thus emitted is called stimulated photon and will have the same phase, energy and direction of movement as that of the passing photon called the stimulation photon.

Initially the atom is at higher level $E_2$. The incident photon of energy hν forces the atom to get de-excited from higher level $E_2$ to lower level $E_1$. i.e. $h\nu=E_2-E_1$ is the change in energy.

The incident photon stimulates the excited atom to emit a photon of exactly the same energy as that of the incident photons. The emitted two photons have same phase, frequency, direction and polarization with the incident photon. This kind of action is responsible for lasing action.

$\text{Atom}^* + \text{Photon} \rightarrow \text{Atom} + (\text{Photon} + \text{Photon})$

The rate of stimulated emission is directly proportional to $N_2U_\nu$, where '$N_2$' is the number of atoms present in the higher energy level and '$U_\nu$' is the energy density.

The rate of stimulated emission $\alpha$ $N_2U_\nu$

The rate of stimulated emission = $B_{21}N_2U_\nu$,

where '$B_{21}$' is the proportionality constant called Einstein's Coefficient of stimulated emission.

**<u>Einstein's A & B Coefficients(Expression for energy density)</u>**

Consider two energy states $E_1$ and $E_2$ of a system of atoms. Let $N_1$ and $N_2$ be the no of atoms ( no. density population) in the energy states $E_1$ and $E_2$ respectively.

(Let Uν be the energy incident / unit volume). Let radiations of wavelength in the range λ and λ + dλ be incident on the system of atoms.

Let be Uν the energy incident / unit volume of the system. Then Uνdν represents the energy density of frequency ν let us consider.

1. **The Case of Induced absorption:**

In the case of induced absorption (when) an atom in the ground state. When absorbs a radiation of frequency $\nu = \frac{E_2 - E_1}{h}$ then it makes transients the level $E_2$.

No. of such absorption per unit time per unit volume is called Rate of absorption.

The rate of absorption = $B_{12}N_1U\nu$.

Where $B_{12}$ is the proportionality constant called Einstein coefficient of induced absorption.

**2. Spontaneous Emission:**

An atom in the excited state $E_2$ makes transition to ground state $E_1$ by the emission of photon of frequency ν. No. of such spontaneous emissions per unit time per unit volume is called Rate of spontaneous emission. Which is proportional to the no. density in the higher energy state $N_2$.

The rate of spontaneous emission $\alpha\ N_2$

Rate of spontaneous emission = $A_{21}N_2U\nu$.

Where $A_{21}$ is called Einstein coefficient of spontaneous emission.

**3. Stimulated emission:**

When a radiation of frequency v incident on an atom in the state $E_2$. Which stimulate the atom to make downward transition and causes the emission of stimulated photons.

The rate of stimulated emission $\alpha\ N_2$.

Rate of stimulated emission = $B_{21}U_\nu N_2$

Where $B_{21}$ is the constant of proportionality called the Einstein coefficient of stimulated emission. And $N_2$ is the No, density in the higher energy state $E_2$. At thermal equilibrium.

At thermal equilibrium,

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

$$B_{12}N_1U_\nu = A_{21}N_2 + B_{21}N_2U_\nu$$

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

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

i.e, $$U_\nu = \frac{A_{21}}{B_{21}}\left[\frac{N_2}{\left(\frac{B_{12}}{B_{21}}N_1 - N_2\right)}\right]$$

$$= \frac{A_{21}}{B_{21}}\left[\frac{1}{\left(\frac{B_{12}N_1}{B_{21}N_2}\right) - 1}\right] \qquad \rightarrow (1)$$

By Boltzmann's law,

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

i.e., $N_1/N_2 = e^{h\nu/KT}$

Eqn. (1) becomes $$U_\upsilon = \frac{A_{21}}{B_{21}}\left[\frac{1}{\left(\frac{B_{12}}{B_{21}}e^{\left(\frac{h\upsilon}{kT}\right)}-1\right)}\right] \rightarrow (2)$$

By Planck's law, $$U_\upsilon = \frac{8\pi h\upsilon^3}{c^3}\left[\frac{1}{\left(e^{\left(\frac{h\upsilon}{kT}\right)}-1\right)}\right] \rightarrow (3)$$

Comparing equation (2) & (3)

$\frac{A_{21}}{B_{21}} = 8\pi h\nu^3/c^3$ & $\frac{B_{12}}{B_{21}} = 1$ i.e. $B_{12} = B_{21}$

The probability of induced adsorption is equal to the stimulated emission.

Because of the of identity, the subscripts could be dropped and $A_{21}$&$B_{21}$ can be represented as A & B. Therefore the equation for energy density at thermal equilibrium is,

$$U_\upsilon = \frac{A}{B}\left[\frac{1}{\left(e^{\left(\frac{h\upsilon}{kT}\right)}-1\right)}\right]$$

***Conclusions of Einstein co-efficient:***

***Dependence of nature of emission on frequency:***

Consider $\frac{A_{21}}{B_{21}} = 8\pi h\nu^3/c^3 \rightarrow (1)$

If $A_{21}$ has high value, the probability of spontaneous emission is high. If $B_{21}$ has high value, the probability of stimulated emission is high.

**Further** $\frac{A_{21}}{B_{21}} \alpha\, \nu^3$

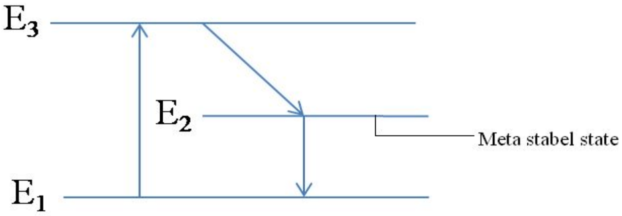
Since $\nu = \Delta E/h$, in normal condition, the energy difference between the two levels $E_1$ and $E_2$ is large

$\frac{A_{21}}{B_{21}} >> 1$ or $A_{21} >> B_{21}$

Thus the probability of spontaneous emission is more than the stimulated emission.

## Condition for laser action:

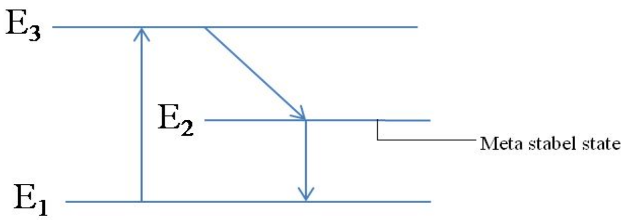
1. ***Meta Stable State:*** *"It is the state in which the atoms or molecules stay for an unusually long time of the order of* $10^{-3}$ *to* $10^{-2}$ *second."*



This state plays an important role in lasing action. This property helps in achieving population inversion, In excited state other than metastable atom stay of order of $10^{-8}$ second.

2. ***Population Inversion:*** *"It is the state of the system at which the population of a particular higher energy level is made to be greater than that of the lower energy level."*

Let $E_1$, $E_2$, $E_3$ be the energy levels of the system $E_3>E_2>E_1$. $E_2$ is the metastable state of the system. Atoms get excited from the state $E_1$ to $E_3$ by means of external source and stay there for short time. These atoms undergo spontaneous transitions to $E_2$ and $E_1$. The atoms at the state $E_2$ stay for longer time. A stage is reached in which the number of atoms at state $E_2$ is more than the number of atoms at $E_1$ which is known as population inversion.



***Note:***

***Pumping:*** ***"The process of producing population inversion is called pumping."*** It is the process of exciting atoms from lower energy level to higher energy level. It can be achieved by different methods.

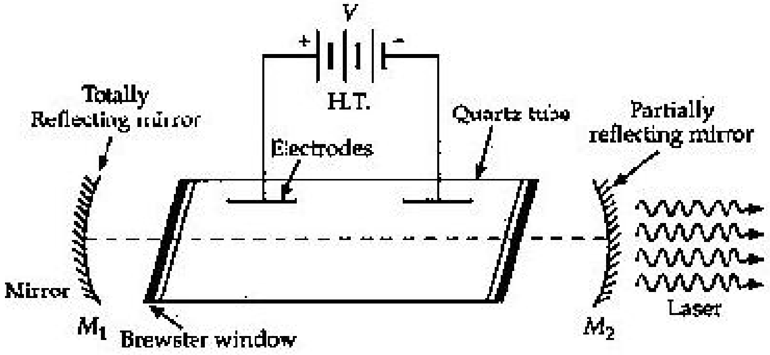
a. ***Optical pumping:*** Using high intensity light or by operating flash tube. Ex:Ruby Laser.
b. ***Electric Discharge:*** By applying very high potential between the plates of discharge tube gas gets discharge leads to pumping. Ex: Argon Laser.
c. ***Atom-Atom Collision:*** Excited atoms collide with other types of atom and transfer its energy to bring other atoms to excited state. Ex: He-Ne Laser.
d. ***Chemical Method:*** Exothermic chemical reactions liberate energy. This liberated energy is used in pumping the atoms. Ex: Dye Laser.
e. ***Using Current :*** In semiconductor diode laser the tuning of current input brings the charge carriers to achieve population inversion.

**Requisites of a Laser System:**

1) **The excitation source for pumping action**: "*It is the external source which provides energy in an appropriate form for pumping the atoms to higher energy levels*".
2) **Activemedium:** "*The quantum system in which the pumping &lasing actions occur, is called an active system*".
3) **Laser cavity(Resonator):** "*Is an active medium bounded by two mirrors*".

## Carbon dioxide ($CO_2$) laser:

### Construction:



Carbon dioxide laser consists of a discharge tube having a diameter of 2.5cm and a length of about 5m. The discharge tube is filled with a mixture of carbon dioxide, nitrogen and helium gases in the ratio of 1:2:3 with traces $H_2$of water vapour. Pressures maintained are about 6 -17 torr.

Two optically plane mirrors, one fully silvered and other one half silvered are fixed on either side of the tube normal to its axis. There is 100% reflectivity from the fully silvered mirror and polarised laser light comes out from the half silvered mirror.

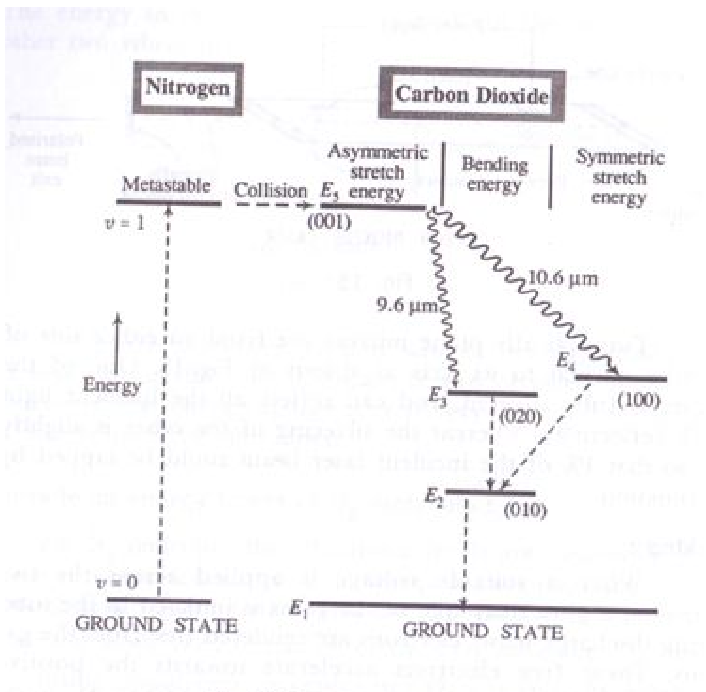
### Working:

When a suitable voltage is applied across the two electrodes a glow discharge of the gasses is initiated in tube .During the discharge many electrons are set free from gas atoms and move towards positive electrode at which time they begin to collide with $N_2$and $O_2$ molecules in their path, which excites $N_2$ molecules are excited to the first vibrational level V=1 which is a metastable state of $N_2$molecule

$$e_1 + N_2 \rightarrow e_2 + N_2^*$$

Where $e_1$ and $e_2$ are the energy values of the electrons before and after the collision respectively, and $N_2$and $N_2^*$are the energy values the $N_2$molecules in the ground state i.e, V=0 & V=1 state.

Likewise, many of the $CO_2$ molecules will also be raised to their (001) energy state (which is not metastable state).For **$N_2$**molecules since V=1 is the metastable state ,the molecules remain there for relatively long time which leads to increase of population in V=1 state so that when **$N_2$** molecule in the metastable state collides with



$CO_2$ LASER ENERGY LEVEL DIAGRAM

$CO_2$ molecules in the ground state ,because of matching of energy levels, resonant energy transfer takes place from the **$N_2$** to $CO_2$ molecule .which elevated to the (001) state whereas ,$N_2$molecule returns to the ground state .

i.e, **$N_2$***+$CO_2$ ->**$N_2$**+$CO_2$*

Where, $CO_2$ and $CO_2$* are energies of $CO_2$molecule in the ground and excited state respectively.

Thus the population of the (001) or $E_5$ level of $CO_2$increases rapidly which leads the population inversion. Let us denotes ground state,(010),(020),(100) and (001) states as $E_1$,$E_2$,$E_3$,$E_4$ and $E_5$ levels respectively as shown in figure. Once the population inversion is established between $E_5$ level with respect to the $E_3$ & $E_4$ levels then two laser transition takes place within $CO_2$ gas.

Those transitions are

1. Transition from E5 to E4 which gives the radiation of wavelength 10.6μm, which is comes under far infrared(IR) region.

2. Another transition from E5 to E3 level which gives rise to radiation of wavelength 9.6μm which is also comes under far IR region.

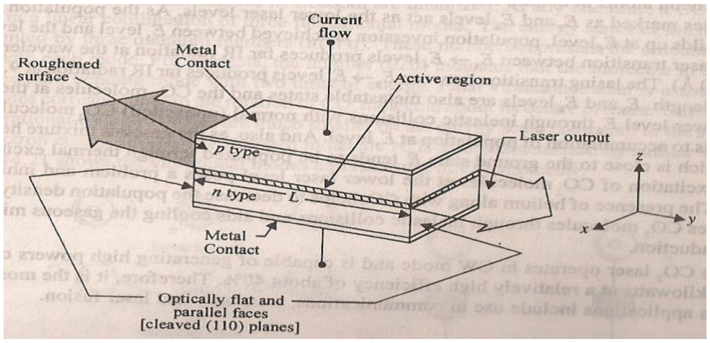
The $CO_2$ molecules in the E2 level undergo collision with He & $H_2O$ vapour molecules efficiently & come down to the ground state.$CO_2$ laser operates with an efficiently of 30% power output of few kilo watts can be continuously maintained in a medium.

## ***Gallium-Arsenide Laser: Semiconductor laser:***

A Semiconductor diode laser is a specially fabricated p-n junction device that emits coherent light when it is forward biased. The wavelength of the emitted photon depends upon the activation energy of the crystal.

**Construction:** A schematic diagram of semiconductor laser is as shown in the figure. The gallium arsenide laser diode is a single crystal of GaAs consists of heavily doped P-N sections. The n-section formed by doping of tellurium and P-section formed doping with zinc and doping concentration is very high is of the order of $10^{17}$ to $10^{19}$atoms/cm$^3$.The overall size of the diode is very small and each of its side is of the order of 1mm.

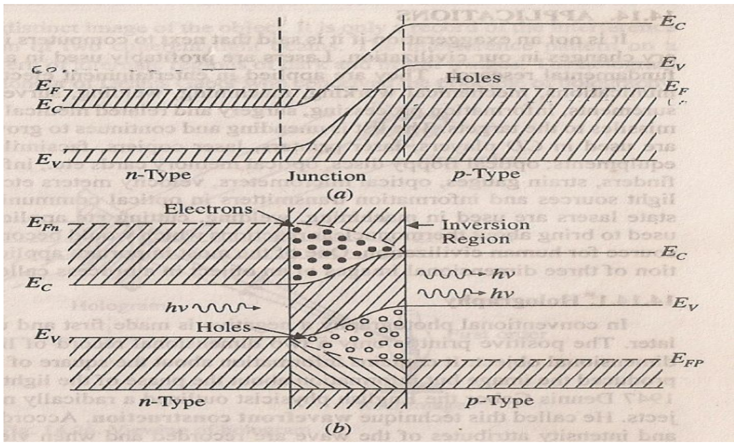
The p-n junction layer of the width varying 1μm to 100μm .Its depending upon the diffusion and temperature conditions that exist at the time of fabrications



***Cross sectional view of p-n junction diode laser.***

A pair of parallel planes of the crystal are polished at right angles to the p-n layer .these planes play the role of reflecting mirrors. These planes provides sufficient reflection to sustain the lasing action through feedback. The other two remaining sides perpendicular to the junction are roughened to suppress reflections of photons ,so that they will not develop the lasing action. The end surfaces of the p and n sections parallel to the plane of the junction are contact with electrodes through which forward bias voltage is applied.

**Working:** The energy band diagram of heavily doped pn-junction is as shown unbiased condition. At thermal equilibrium, the Fermi level is uniform across the junction. Because of very high doping on n-side, Fermi level is pushed into the conduction band and electrons occupy the portion of the conduction band lying below the Fermi level. On P-side, the Fermi level lies within the valence band and holes occupy the portion of the valence band that lies above the Fermi level. When the junction is forward biased electrons and holes are injected into the junction region in high concentrations. At low forward current, the electron-holes recombination results in spontaneous emission of photons and the junction acts as a LED. As the forward current is increased gradually and when it reaches a threshold value the carrier concentration in the junction region there will be large concentrations of electrons within the band. As a result condition of population inversion is attained in the narrow region. This narrow zone in which population inversion occurs is called as an active region, at that stage a photon emitted spontaneously triggers stimulated emission. This stimulated electron-hole recombination produces coherent radiation.



***Energy level diagram of p-n junction diode laser***

***(a) Before biasing (b) After biasing.***

The stimulated electron-hole recombination causes emission of coherent radiation of very narrow bandwidth. At room temperature, GaAs laser emits light of wavelength $9000A^0$ and GaAsP laser radiates at $6500A^0$.

The wavelength of the emitted laser beam is

$\lambda = \frac{hC}{E_g}$ Where h = Planck's const.

***Advantages of semiconductor laser:***

1. They are compact
2. They are efficient
3. They are highly stable

***Properties of laser:***

1. *Coherence*: The emitted radiation after getting triggered is in phase with the incident radiation.

   *Coherence is of two types*

   a. Temporal or time coherence
   b. Spatial Coherence
2. *Monochromaticity*: The laser beam is highly monochromatic than any other radiations.
3. *Unidirectionality*: Laser beam travels in only one direction. It can travel long distance without spreading.
4. *Focusability*: A laser beam can be focused to an extremely fine spot.
5. *Intensity*: The power output of the laser may vary from few milliwatts to few kilowatts. But this energy is concentrated in a beam of very small cross section. The intensity of laser beam is approximately given by

$$I = \left(\frac{10}{\lambda}\right)^2 P \quad Wm^{-2}$$

Where p is the power radiated by laser.

In case of He-Ne laser, $\lambda = 6328 \times 10^{-10}$m and $P = 10 \times 10^{-3}$W,

the corresponding intensity is

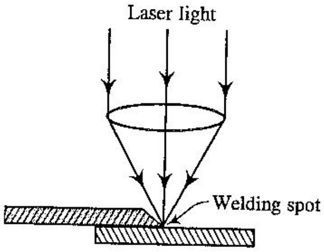
$$I = \left(\frac{1}{6328\times10^{-10}}\right)^2 100\times10^{-3} \quad = 2.5\times10^{11} \quad Wm^{-2}$$

To obtain the above intensity from tungsten bulb, the temperature would have to be raised to $4.6\times10^6$K. The normal operating temperature of the bulb is approximately 2000K.

***<u>Application of laser:</u>***

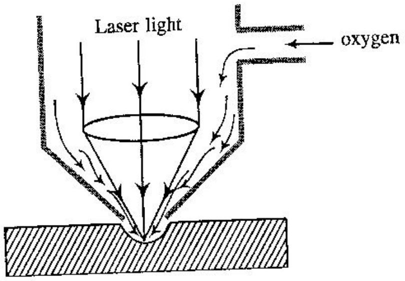
1. ***Laser welding***: Laser beam is allowed to fall on the surface to be welded. The beam is absorbed and the surface starts melting due to the heat generated. The reflectivity and thermal diffusivity of the material are the important factors of welding. The reflectivity is more, the energy released is less. To increase the energy, the surface is coated with either cupric oxide or graphite. During the melting, the impurities accumulate on the surface of the material and it becomes a homogeneous solid structure and forms a stronger joint on cooling.

The laser welding is very narrow and accurate. In laser welding, laser does not have any physical contact with the material to be welded. Hence no contamination occurs. The properties of the material do not change due to welding. Laser welding can be carried out in normal workshop environment.



LASER WELDING

2. ***<u>Laser cutting:</u>*** When the laser is allowed to focus onto a tiny spot, the metal gets vaporized. There will be no physical distortion. $CO_2$ laser is used for the laser cutting. The laser cutting depends upon the input power for the laser beam and inversely proportional to the thickness of the material. It also depends on the nature of the gas used with the laser beam. Oxygen is commonly used gas. The gas is flown coaxially with the beam. The combustion of the gas helps the metal to get vaporized and it reduces the laser power which is required for cutting. Laser cuts the material accurately.

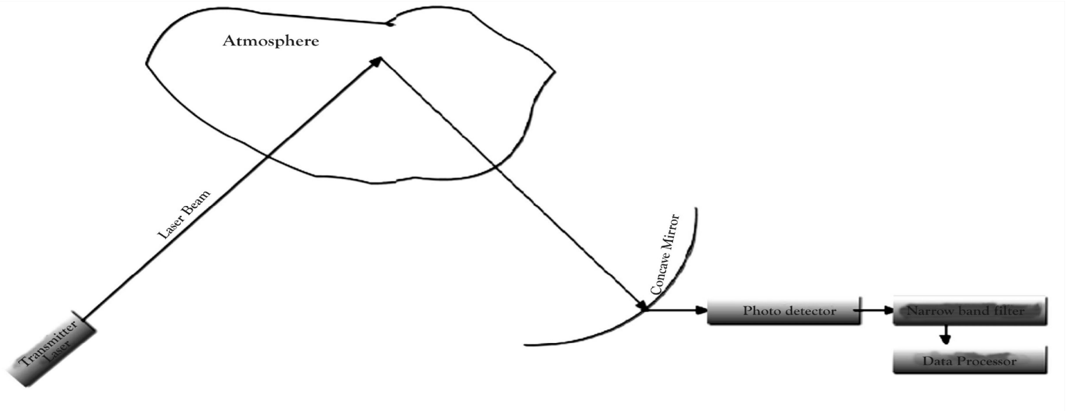


LASER CUTTING

3. ***Drilling:*** Laser beam can drill the hardest material or a brittle material with a hole of diameter 10µm. Laser is used to make holes in gemstones, ceramics, without any damage. Very small dimensional holes can be made by using lasers. No contamination occurs as there is no physical contact.

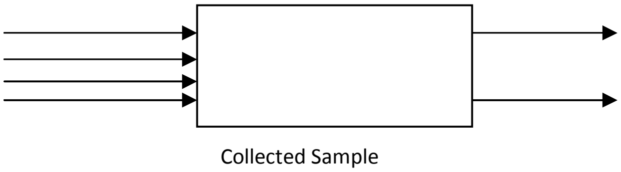
*4.* ***Measurement of pollutants in the atmosphere:*** There are various types of pollutants in the atmosphere which include nitrogen, oxides of carbon monoxide, sulphur dioxide and a number of particulate matters. In conventional technique, samples of the atmosphere are collected at desired heights and the chemical analysis is carried out to find out the composition of the pollutants. Whatever the data obtained in this method is not a real time data. Whereas in the laser technique, the laser senses the atmospheric density variation by scanning the required local region and electronic data processes yield the data, which is a real time data.

In the application of laser for measurement of pollutant, laser is made use of the way as RADAR (Radio Detection and Ranging) system is used. Hence it is often referred as a LIDAR (Light Detection and Ranging) technique. In the LIDAR system, the transmitting part consists of pulsed laser and the receiving part consists of a concave mirror, photo detector and a data processor.



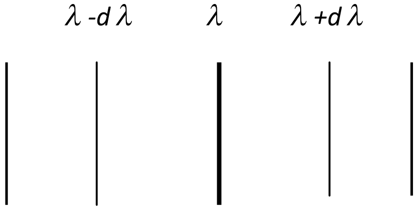
When measurements are carried out, the laser beam undergoes scattering at places in the atmosphere where there is congestion due to higher concentration of particulate matter. The back scattered light is received by the concave mirror. The distance of congestion from the measuring station is calculated on the basis of time delay between the pulse emission and reception of the back scattered light. By scanning the space around the station, the concentration of pollutants can be mapped for different vertical section of the atmosphere. This method cannot provide any information regarding the nature of the scattering particles. As this technique doesn't provide the information regarding the nature of the scattering particles following two more techniques are followed.

1. *Absorption Technique*:



The laser beam is passed through the sample collected from the atmosphere. The transmitted beam is recorded with a detector. While the beam passes through the sample, it undergoes absorption of various degrees depending upon the presence of exact type of chemical substance that the particulate comprise of. Depending upon the characteristic absorption pattern observed in the recording, the composition of the atmospheric pollutants could be determined.

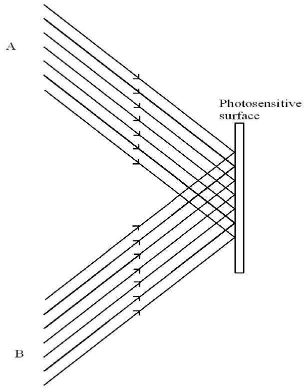
2. *Raman Back Scattering*: Since laser is highly monochromatic, we expect to see only one line in the spectrum. But due to Raman scattering in the spectrum, several lines of low intensity will be seen symmetrically on either side of the incident line. There wavelength values will be close to that of the incident light. These additional spectral lines are called as side bands. Different gasses produce different side bands. The shifts in frequencies are termed as Raman shifts. Thus by observing the Raman spectrum of the back scattered light in the gas sample one can assess the composition of the pollutants.



*Raman Back Scattered Spectrum*

## ***Holography***

Holography is the technique of producing 3-dimentional image of an object on 2-dimentional recording aid, by the phenomenon of interference. A and B are two identical or coherent beams incident on photosensitive surface at different angles. Due to interference effect, interference fringes are recorded on developing the photographic plate.



## ***Principle of Hologram construction:***

Light wave reflected from an object are characterized by their intensity (square of amplitude) and phase. When both intensity and phase attributes of the wave coming from three dimensional object is recorded on a photographic plate, it is called construction of hologram. When recorded photographic plate (hologram) is illuminated by a coherent light source, the three dimensional image of the original object is formed. This formation of image is known as reconstruction process.

## ***Recording phase variation in a Hologram:***

In recording hologram of an object a photographic plate is placed in front of an object at a suitable distance. Consider a coherent light incident on the object. The light reflected from two nearby points on the object travel slightly different distances in reaching the photographic plate due to variation in depth on the object. Thus the two wave fronts arrive at the photographic plate in a slightly different phase. Hence the light reflected from different points on the object will have different phases and interfere with the reference beam. The fringes recorded in the hologram carry information regarding the phase difference.

In holography there are two phases:

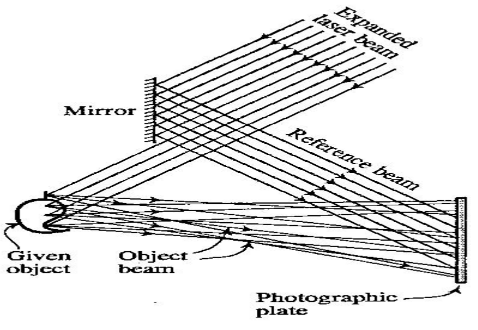
1) Recording
2) Reconstruction of the image.

Recording has two methods

1) Wave front division technique.
2) Amplitude division technique.

### ***1) Recording of the image of an object by wave front division technique***

Expanded coherent laser beam from the laser source is obtained. A portion of it is made to incident on the mirror and other portion is made to incident on the object as shown in the fig.



HOLOGRAM RECORDING

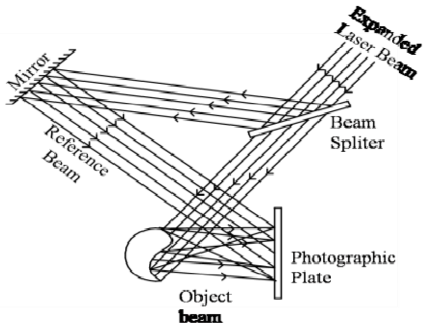
GABOR ZONE PLATE

Photographic plate is placed at a suitable position so that it receives the light reflected from both the mirror and the object. The light reflected from the mirror form a plane wavefront. It is called reference beam. The light reflected from each point on the object form a spherical wavefront. It is called object beam. Thus the interference effects of the two beams are recorded on the photographic plate.

As the spherical wave intersect the plane wave in circular zones, the interference pattern consists of concentric circular rings having constructive and destructive interference. It is called *Gabor Zone plate.*

Hologram consists of number of such zone plates. The centre of each is displaced from the other. In the recorded pattern the neighbouring zones overlap each other and become apparent, once the film is developed. It is called a hologram.

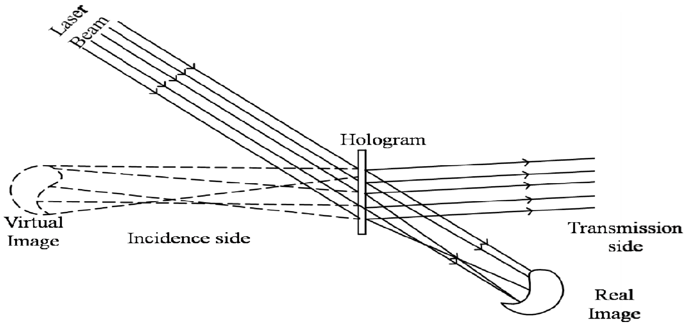
### *2) Recording the image of an object by amplitude division technique:*



Expanded coherent laser beam from the laser source is obtained. It is made to incident on the beam splitter. The beam splitter reflects the portion of the light which is incident on the mirror. The transmitted light from the beam splitter is incident on the object. The reflected plane wavefront from the mirror and reflected spherical wavefronts from different points on the object undergoes interference on the photographic plate kept at a suitable place. The interference fringes are recorded on the photographic plate. The developed photographic plate becomes the hologram of the object.

### *Reconstruction of the image from the hologram:*

Original Laser beam is made to incident on the hologram in the same direction as the reference beam was incident on it at the time of recording. The beam undergoes refraction in the hologram. Secondary wavelets originating from each constituting zone plate interfere constructively and generate real image on the transmission side and virtual image on the incident side.



## Optical Fibers

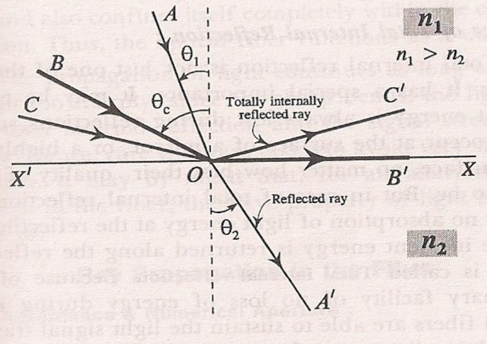
### *Total Internal Reflection:*

When a ray of light travels from denser to rarer medium it bends away from the normal. As the angle of incidence increases in the denser medium, the angle of refraction also increases. For a particular angle of incidence called the "*critical angle*", the refracted ray grazes the surface separating the media or the angle of refraction is equal to 90°. If the angle of incidence is greater than the critical angle, the light ray is reflected back to the same medium. This is called *"Total Internal Reflection".*

In total internal reflection, there is no loss of energy. The entire incident ray is reflected back.

$XX^1$ is the surface separating medium of refractive index $n_1$ and medium of refractive index $n_2$, $n_1 > n_2$.

AO and $OA^1$ are incident and refracted rays. $\theta_1$ and $\theta_2$ are angle of incidence and angle of refraction, $\theta_2 > \theta_1$. For the ray BO, $\theta_c$ is the critical angle. $OB^1$ is the refracted ray which grazes the interface. The ray CO incident with an angle greater than $\theta_c$ is totally reflected back along $OC^1$.



TOTAL INTERNAL REFLECTION

From Snell's law,

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

For total internal reflection,

$$\theta_1 = \theta_c \text{ and } \theta_2 = 90°$$

$$n_1 \sin\theta_c = n_2 \quad \text{(because } \sin 90° = 1\text{)}$$

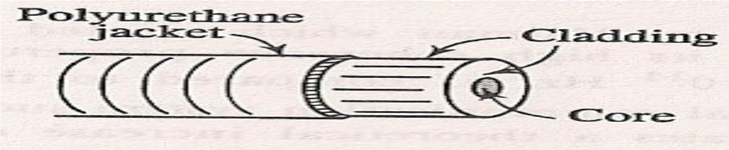
$$\theta_c = \sin^{-1}(n_2/n_1)$$

In total internal reflection there is no loss or absorption of light energy.

The entire energy is returned along the reflected light. Thus is called Total internal reflection.

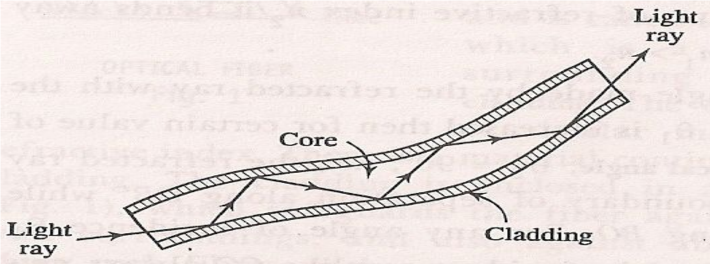
***Optical Fibers:*** They are used in optical communication which on the principle of Total internal reflection(TIR).

Optical fiber is made from transparent dielectrics. It is cylindrical in shape. The inner cylindrical part is called as core of refractive index $n_1$. The outer part is called as cladding of refractive index $n_2$, $n_1 > n_2$. There is continuity between core and cladding. Cladding is enclosed inside a polyurethane jacket. Number of such fibers is grouped to form a cable.



OPTICAL FIBER

The light entering through one end of core strikes the interface of the core and cladding with angle greater than the critical angle and undergoes total internal reflection. After series of such total internal reflection, it emerges out of the core. Thus the optical fiber works as a waveguide. Care must be taken to avoid very sharp bends in the fiber because at sharp bends, the light ray fails to undergo total internal reflection.



FIBER AS A WAVEGUIDE

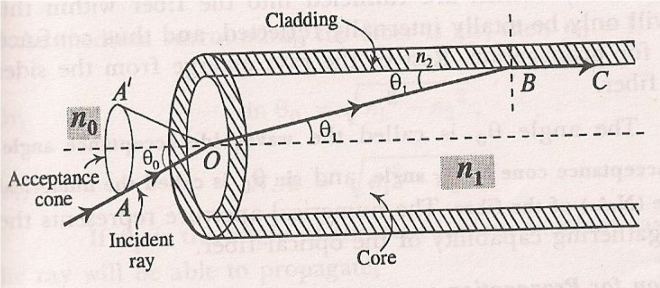
***Angle of Acceptance and Numerical Aperture:***

Consider a light ray AO incident at an angle ‘$\theta_0$’ enters into the fiber. Let ‘$\theta_1$’ be the angle of refraction for the ray OB. The refracted ray OB incident at a critical angle ($90^\circ - \theta_1$) at B grazes the interface between core and cladding along BC. If the angle of incidence is greater than critical angle, it undergoes total internal reflection. Thus $\theta_0$ is called the waveguide acceptance angle and $\sin\theta_0$ is called the numerical aperture.

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

From Snell’s law,

$$n_o \sin\theta_0 = n_1 \sin\theta_1 \qquad \rightarrow (1)$$



ACCEPTANCE CONE

From Snell's law,

At 'B' the angle of incidence is $(90 - \theta_1)$

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

$$n_1\cos\theta_1 = n_2$$

$$\cos\theta_1 = n_2 / n_1 \qquad \rightarrow (2)$$

From eqn.(1)

$$Sin\theta_0 = \frac{n_1}{n_0}\sin\theta_1$$

$$= \frac{n_1}{n_o}\sqrt{1 - cos^2\theta_1} \qquad \rightarrow (3)$$

Using eqn. (2) in (3)

$$Sin\theta_0 = \frac{n_1}{n_0}\sqrt{1 - \frac{n_2^2}{n_1^2}}$$

$$= \frac{\sqrt{n_1^2 - n_2^2}}{n_o} \rightarrow (4)$$

The surrounding medium is air, $n_o = 1$

$$Sin\theta_0 = \sqrt{n_1^2 - n_2^2}$$

Where $Sin\theta_o$ is called numerical aperture.

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

Therefore for any angle of incidence equal to $\theta_i$ equal to or less than $\theta_0$, the incident ray is able to propagate.

$$\theta_i < \theta_0$$

$$\mathrm{Sin}\theta_i < Sin\theta_0$$

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

$sin\theta_i < N.A$ is the condition for propagation.

***Fractional Index Change:*** "*It is the ratio of the refractive index difference between the core and cladding to the refractive index of the core of an optical fiber*".

$$\Delta = \frac{n_1 - n_2}{n_1}$$

***Relation between N.A and Δ:***

Consider $\Delta = \frac{n_1 - n_2}{n_1}$

$$n_1 - n_2 = \Delta n_1$$

We have

$$N.A = \sqrt{n_1^2 - n_2^2} = \sqrt{(n_1 + n_2)(n_1 - n_2)}$$

Considering, $n1 \approx n_2$

$$= \sqrt{(n_1 + n_2)\Delta n_1}$$

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

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

Increase in the value of Δ increases N.A

It enhances the light gathering capacity of the fiber. Δ value cannot be increased very much because it leads to intermodal dispersion intern signal distortion.

***V-number:***

"*The number of modes supported for propagation in the fiber is determined by a parameter called V-number*".

If the surrounding medium is air, then

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

Where ‘d’ is the core diameter, $n_1$ and $n_2$ are refractive indices of core and cladding respectively, ‘λ’ is the wavelength of light propagating in the fiber.

$$V = \frac{\pi d}{\lambda}(NA)$$

If the fiber is surrounded by a medium of refractive index $n_0$, then,

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

For V >1, the number of modes supported by the fiber is given by, number of modes $\approx V^2/2$.

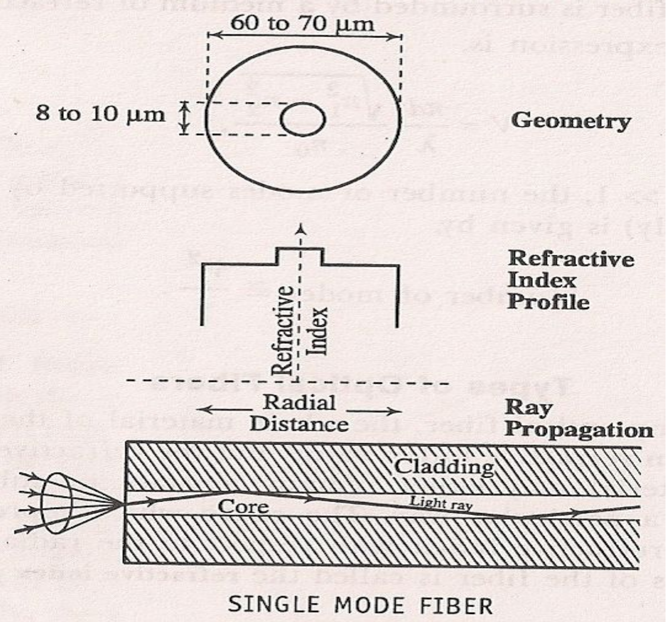
## ***Types of optical fibers:***

In an optical fiber the refractive index of cladding is uniform and the refractive index of core may be uniform or may vary in a particular way such that the refractive index decreases from the axis radialy.

Following are the different types of fibers:

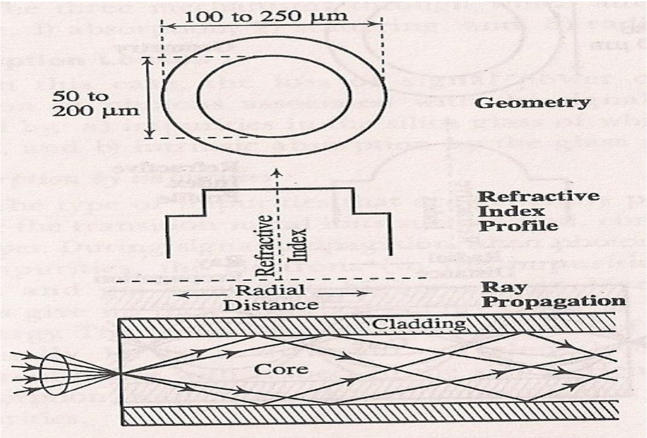
1. Single mode fiber
2. Step index multimode fiber
3. Graded index multimode fiber

***Single mode fiber*****:** Refractive index of core and cladding has uniform value; there is an increase in refractive index from cladding to core. They are used in submarine.



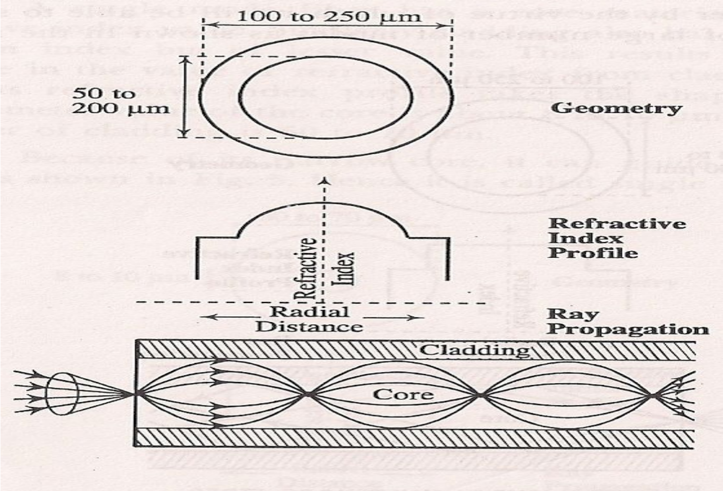
SINGLE MODE FIBER

2. ***Step index multimode fiber:*** It is similar to single mode fiber but core has large diameter. It can propagate large number of modes as shown in figure. Laser or LED is used as a source of light. It has an application in data links.



STEP - INDEX MULTIMODE FIBER

3. ***Graded index multimode fiber:*** It is also called GRIN. The refractive index of core decreases from the axis towards the core cladding interface. The refractive index profile is shown in figure. The incident rays bends and takes a periodic path along the axis. The rays have different paths with same period. Laser or LED is used as a source of light. It is the expensive of all. It is used in telephone trunk between central offices.



GRADED - INDEX MULTIMODE FIBER

## ***Signal distortion in optical fibers:***

The propagation of a signal through the optical fiber involves total internal reflection of light rays many times. Further, the rays are reflected at various angles. The rays reflected at higher angles travel greater distances than the rays reflected at lower angles. As a result, all the rays do not arrive at the end of the fiber simultaneously and the light pulse broadens as it travels through the fiber. Since the output pulse does not match with the input pulse, the signal is said to be distorted.

If white light is used instead of monochromatic light, another kind of distortion occurs. Since radiation of different wavelengths has different velocities, they do not arrive at the output simultaneously. This distortion is called chromatic dispersion.

The signal distortion is quite considerable in multimode step index fibers. In graded index fibers, the light travels with different velocities in different parts of the core as the refractive index varies radially along the core. The rays travel faster near the interface. Hence all the rays arrive at the output almost at the same time and the signal distortion is reduced. In a single mode step index fiber the distortion is less than that in multimode step index fibers.

## ***Signal attenuation in optical fibers:***

Attenuation is the loss of optical power as light travels through a fiber. It is expressed in decibel/kilometre [db/km]. A fiber with lower attenuation will allow more power to reach its receiver than a fiber with higher attenuation. If $P_{in}$ is the input power and $P_{out}$ is the output power after passing through a fiber of length 'L', the mean attenuation constant or coefficient 'α' of the fiber, in units of db/km is given by

$$\alpha = -\frac{10}{L}\log_{10}\left(\frac{p_{out}}{p_{in}}\right)\text{dB/km}$$

Attenuation can be caused by three mechanisms.

**Attenuation coefficient.**

When light travels in a material medium there will always loss in intensity with distance travelled .such a loss in intensity obeys a law is called Lamberts law. or There is loss in its intensity with distance travelled. The intensity loss obeys Lambert's law i.e. from Lambert's law.

$-\ \frac{dP}{dL}\alpha P$ P → initial intensity

L → distance propagated in the medium

-ve sign confirms that it is decrease in power

$$-\frac{dP}{dL} = \alpha\ P \qquad \rightarrow (1)$$

Where α - *attenuation coefficient* or *fibre attenuation coefficient* or *attenuation* or *fibre loss.*

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

Integrating both sides,

$$\int \frac{dp}{p} = -\alpha \int dl$$

$$\int_{P_{in}}^{P_{out}} \frac{dP}{P} = -\ \alpha \int_{o}^{L} dL$$

Where $P_{out}$→ intensity of light received at output

$P_{in}$ → intensity of light launched at input

$$[ln\ P]_{P_{in}}^{P_{out}} = -\ \alpha[L]_{o}^{L}$$

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

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

As the dependence of loss of intensity is logarithmic in nature, α also takes the unit as Bel [as sound intensity variation is also logarithmic whose unit is also Bel]

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

As Bel is larger unit, $\alpha$ is expressed in decibel / kilometre (dB/km)

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

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

Note : * $P_{in}$ & $P_{out}$ expressed in watt
* L in km
Attenuation can be caused by three mechanisms.

**Type of Attenuation in an Optical fiber:**

1.*Absorption losses:*- Absorption of photons by impurities like metal ions such as iron, chromium, cobalt and copper in the silica glass of which the fiber is made of. During signal processing photons interact with electrons of impurity atoms. The atoms are excited and de-excite by emitting photons of different characteristics. Hence it is a loss of energy. The other impurity such as hydroxyl ions (OH) causes significant absorption loss. The absorption of photons by fiber material itself is called intrinsic absorption.

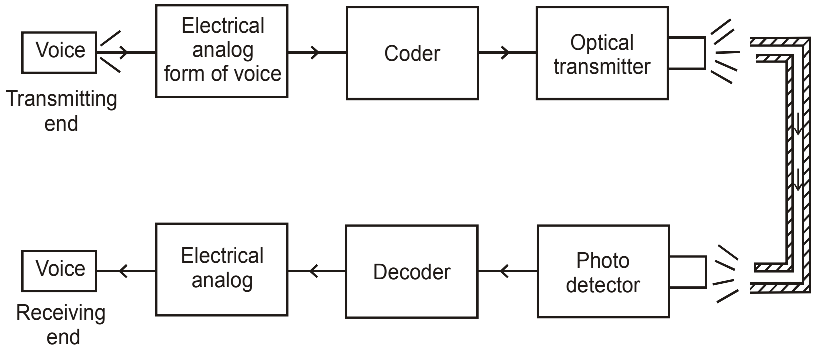
2. *Scattering losses*: When the wavelength of the photon is comparable to the size of the particle then the scattering takes place. Because of the non-uniformity in manufacturing, the refractive index changes with length leads to a scattering. This type of scattering is called as Rayleigh scattering. It is inversely proportional to the fourth power of wavelength. Scattering of photons also takes place due to trapped gas bubbles which are not dissolved at the time of manufacturing.

3. *Radiation losses*: Radiation losses occur due to macroscopic bends and microscopic bends.

a. Macroscopic bending: All optical fibers are having critical radius of curvature provided by the manufacturer. If the fiber is bent below that specification of radius of curvature, the light ray incident on the core cladding interface will not satisfy the condition of TIR. This causes loss of optical power.

b. Microscopic bending: Optical power loss in optical fibers is due to non-uniformity of the optical fibers when they are laid. Non uniformity is due to manufacturing defects and also lateral pressure built up on the fiber. The defect due to non-uniformity (microbendings) can be overcome by introducing optical fiber inside a good strengthen polyurethane jacket.

**Application of optical fiber:( Point to point communication in OF)**



Point of Point optical fibre communication system

A fiber optic communication system is very much similar to a traditional communication system and has three major components. A transmitter converts electrical signals to light signals, an optical fibre transmits the signals and a receiver captures the signals at the other end of the fiber and converts them to electrical signals.

The transmitter consists of a light source supported by necessary drive circuits. First voice is converted into electrical signals using a transducer. It is digitized (converted to binary electrical signals) using a coder. The digitized signal, which carries the voice information, is fed to an optical transmitter. The light source in optical transmitter (LED or laser diode) emits modulated light, which is transmitted through optical fiber. The light emitted by the source is in the IR range with a wavelength of 850nm, 1300nm or 1550nm.

On the other end the modulated light signal is detected by a photo detector is amplified and is decoded using a decoder. The output is fed to a suitable transducers to convert it into an audio or video form.

## ***Advantages of optical communication system:***

1) It carries very large amount of information in either digital or analog form due to its large bandwidth.
2) The materials used for making optical fiber are dielectric nature. So, it doesn’t produces or receives any electromagnetic and R-F interferences.

3) Fibers are much easier to transport because of their compactness and lightweight.
4) It is easily compatible with electronic system.
5) It can be operated in high temperature range.
6) It does not pick up any conducted noise.
7) Not affected by corrosion and moisture.
8) It does not get affected by nuclear radiations.
9) No sparks are generated because the signal is optical signal.

# Module-4

## Crystal Structure

Space lattice, Bravais lattice–Unit cell, primitive cell.Lattice parameters. Crystal systems. Direction and planes in a crystal. Miller indices. Expression for inter – planar spacing. Co-ordination number. Atomic packing factors (SC,FCC, BCC). Bragg's law, Determination of crystal structure using Bragg's X–ray difractometer. Polymarphism and Allotropy. Crystal Structure of Diamond, qualitative discussion of Pervoskites.

**10 Hours**

**Content:**

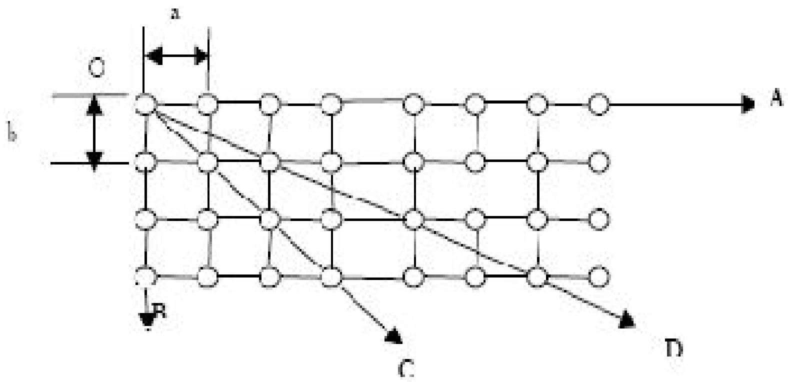
- **Space lattice**
- **Bravais lattice**
- **unit cell**
- **lattice parameters**
- **crystal systems**
- **directions and planes in a crystal**
- **Millar indices**
- **expressions for inter planer**
- **Co-ordination number atomic packing fractor.**
- **Braggs law**
- **Braggs X-Ray spectrometer**
- **Polymorphism and allotropy**

# Crystal Structure

*The solid state*

- Atoms in solids may be randomly positioned (as in a liquid) – Amorphous Solids (e.g. glasses)
- Arranged in an *orderly, repeating pattern* within the material – Crystalline Solids

A crystal is one in which atoms or molecules are in three dimensional periodic arrangement. The periodicity may be same or different in different directions. The periodic positions of the atoms or molecules are called space lattice or crystal lattice. "The geometrical representation of a crystal structure in terms of lattice points is called space lattice".



*How do we describe the arrangement of atoms in crystals?*

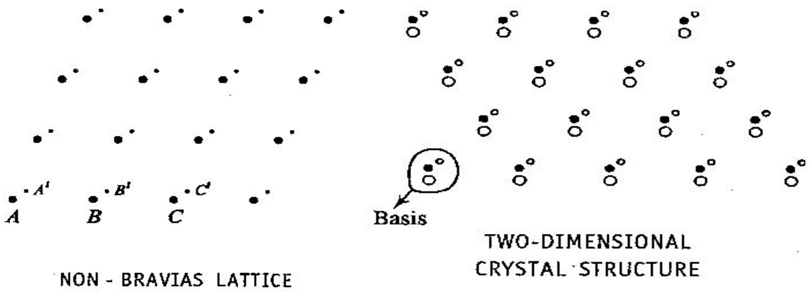
There are two types of lattice

1) Bravais lattice
2) Non Bravais lattice

A Bravais lattice is one in which all the atoms at the lattice points are identical or all the lattice points are equivalent.

A non-Bravais lattice is one in which some of the lattice points are non-equivalent. A non-Bravais lattice is also known as the lattice with a basis. Basis is the set of atoms located near to the Bravais lattice.

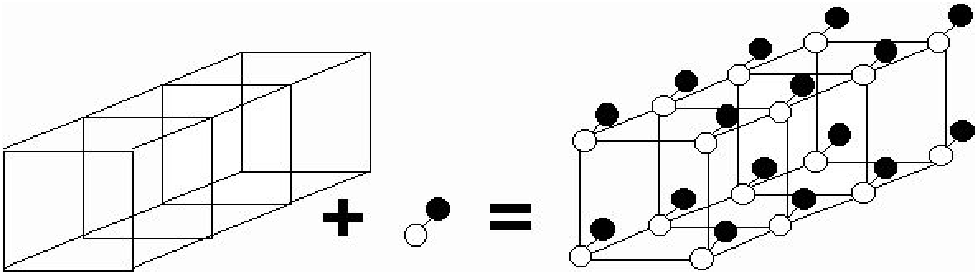
Non Bravais lattice is the superposition of two or more different Bravais lattice. In the diagram, points A, B,C etc., identical points represents Bravais lattice whereas AA`, BB`, CC` etc., which are not identical represents non-Bravais lattice.



NON - BRAVIAS LATTICE

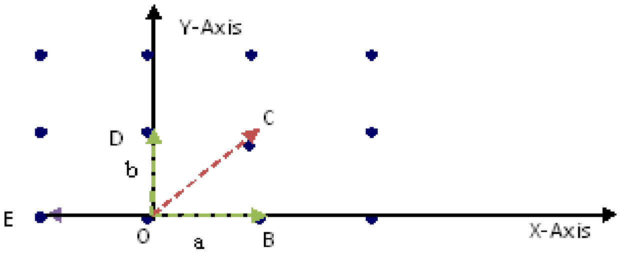
TWO-DIMENSIONAL CRYSTAL STRUCTURE

Space Lattice + Basis = Crystal Structure



**Basis Vectors**

Consider two dimensional arrays of points. Let 'O' be the origin. And be the coordinate vectors.



Two dimensional array of Points

The position or lattice vector R is $R = n_1 a + n_2 b$ where $n_1$ and $n_2$ are integers whose value depends on lattice points.

For B, $(n_1, n_2) = (1,0)$

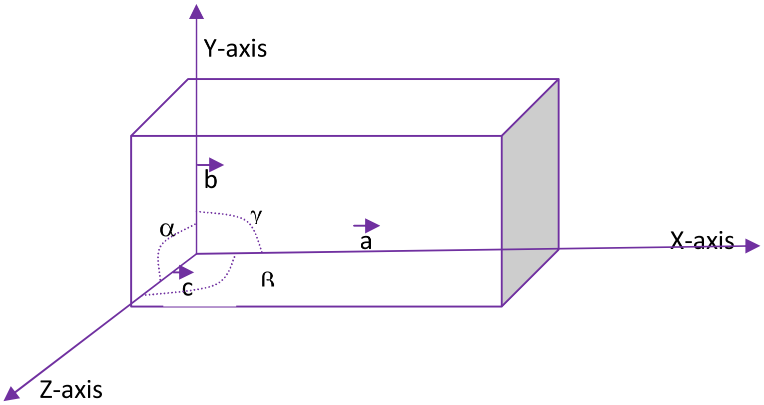
For C, $(n_1, n_2) = (1,1)$

For D, $(n_1, n_2) = (0,1)$

For E, $(n_1, n_2) = (-1,0)$

## ***Unit Cell and Lattice Parameters.***

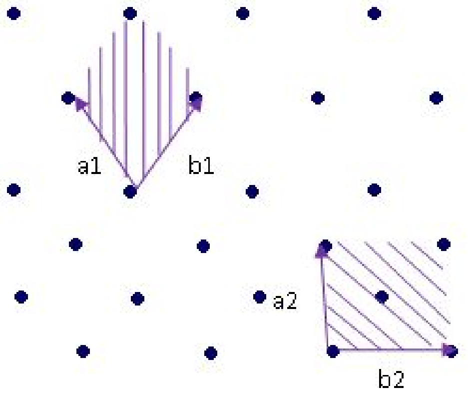
A unitcell is the smallest portion of the space lattice, which on repetition along the direction of three basis vectors generates the space lattice itself. Unit cell has basis vectors$\vec{a}$, $\vec{b}$&$\vec{c}$ and interfacial angles α, β & γ.



The basis vectors $\vec{a}, \vec{b}, \vec{c}$ and interfacial angles α, β & γ are the lattice parameters. Each unit cell has only one lattice point because there are eight points at its corners and each point is shared by eight adjacent cells.

**Primitive cell and non-primitive cell:** Consider, a Bravais lattice in two dimensions as shown in figure. A unit cell with basis vectors $a_1 \& b_1$ has four lattice points at the vertex. It is a primitive cell. The other unit cell with basis vectors $\overrightarrow{a_2}$ and $\overrightarrow{b_2}$ has an additional lattice point at the center along with four points at the corners, which is not the meeting point of the basis vectors. This is non-primitive cell.

A primitive cell is a unit cell with all the points in it are at the vertices. A non-primitive cell is a unit cell which incorporates an integral multiple of primitive cells and is imagined only for the sake of easy visualization of the symmetry in the arrangement of the lattice points.

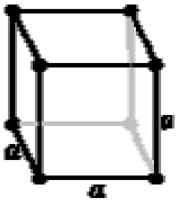
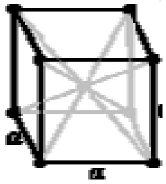
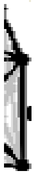


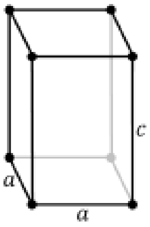
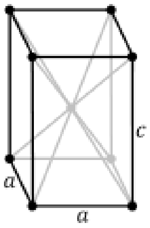
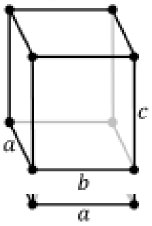
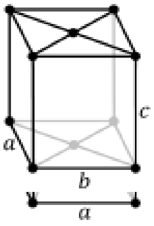
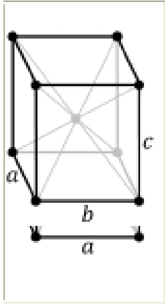
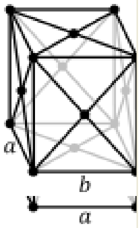
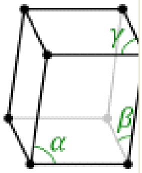
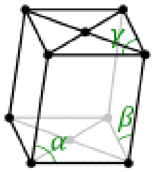
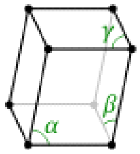
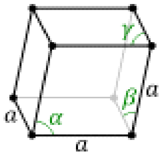
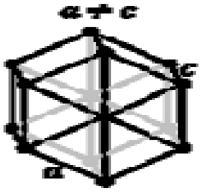
**Crystal systems:**

There are seven crystal systems named on the basis of geometrical shape and symmetry.

The seven crystal systems are further divided into 14 Bravais lattice. The simple lattice has points only at the corners. A body centered lattice has an additional point at the centre of the cell and a face centered lattice has six additional points one on each face. The base centered lattice has two additional points one at the bottom face and other at the top face.

The seven crystal systems and the 14 Bravais lattices are represented in the following table:

| **The seven Crystal systems (From Most symmetric to least symmetric)** | **The 14 Bravais Lattices** | | |
|---|---|---|---|
| 1. Cubic<br>$a=b=c$ ;$\alpha=\beta=\gamma=90^{o}$<br>Ex:- *Au, Cu, NaCl,* $CaF_2$,$NaclO_2$ | simple (SC) Polonium | body-centered (BCC) Iron, Chrominium & Tungsten | face-centered (FCC) NaCL(Halite) or Rock Salt, aluminium, copper, gold |
| |  |  |  |

| | | | | |
|---|---|---|---|---|
| 2. Tetragonal<br>$a=b\neq c$ ; $\alpha=\beta=\gamma=90^{o}$<br>Ex:-$SnO_2$,<br>$TiO_2$,$NiSO_4$. | Simple | body-centered | | |
| |  |  | | |
| 3. Orthorhombic<br>$a\neq b\neq c$ $\alpha=\beta=\gamma=90^{o}$<br>Ex:- KNO3,BaSO4,<br>MgSO4. | Simple | base-centered | body-centered | face-centered |
| |  |  |  |  |
| 4. Monoclinic<br>$a\neq b\neq c$ $\alpha=\gamma=90^{o}\neq\beta$<br>Ex:- $CaSO_4.2H_2O$,<br>$FeSO_4$, $Na_2SO_4$ | Simple | base-centered | | |
| |  |  | | |
| 5. Triclinic<br>$a\neq b\neq c$ $\alpha\neq\beta\neq\gamma\neq 90^{o}$<br>*Ex:-* $K_2Cr_2O_7$,<br>$CuSO_4.5H_2O$ |  | | | |
| 6. Rhombohedral<br>(trigonal)<br>$a=b=c$ $\alpha=\beta=\gamma\neq 90o$<br>Ex:- calcite, quartz, Bi<br>tourmaline, As,Sb, |  | | | |
| 7. Hexagonal<br>$a=b\neq c$ $\alpha=\beta=90^{o}$<br>$\gamma=120^{o}$<br>Ex:-<br>$SiO_2$Zn,Mg,Cd,AgI |  | | | |

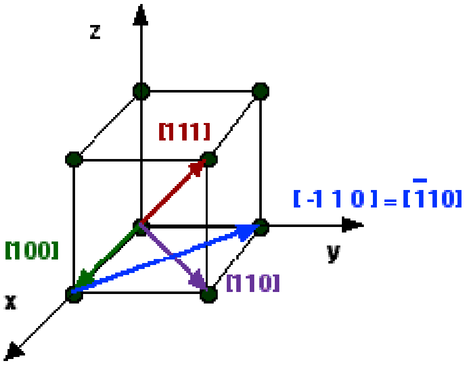
## MILLER INDICES OF DIRECTIONS AND PLANES:

Miller has introduced three numbers to explain the planes and directions in a crystal. These numbers are called Miller indices.

A **Miller indices of direction** is basically a vector between two points in the crystal. Any direction can be defined by following a simple procedure:

1. Choose the position vector, so that it is in convenient position within your chosen co-ordinate system.
2. Find the projection of the vector onto each of the three axes in terms of the unit cell dimensions.
3. To get the Miller Index we express the vector as a set of whole number, and enclose in square brackets.

Example:-



**A cubic unit cell along with miller indices of directions.**

Procedure to find miller indices of planes:

1. Find the intercepts of the planes along x, y and z axis
2. Express the intercepts as multiples of lattice constants a, b, c.
3. Find out the reciprocal of these numbers.
4. Find the least common multiple (LCM) of the denominator and multiply each term with LCM.
5. The result is in the form of h, k, l. are called miller indices, denoted by (h k l)

| Intercepts | Reciprocals | Whole numbers | Miller indices |
|---|---|---|---|
| 2a b c | 1/2 1/1 1/1 | 1 2 2 | (1 2 2) |
| 2a b ∞ | ½ 1/1 1/∞ | 1 2 0 | (1 2 0) |
| a –b 2c | 1/1 -1/1 ½ | 2 $\bar{2}$ 1 | (2 $\bar{2}$ 1) |
| -a 2b –c | -1/1 ½ -1/1 | -2 1 -2 | ($\bar{2}$ 1 $\bar{2}$) |

**Few examples for obtaining the Miller indices**

**Calculation of miller indices**

Following points should be noted

1. The negative digit indicates cutting of axis on the negative side of the origin.
2. Zero index indicates that the plane is parallel to corresponding axis.
3. A parallel set of planes have same miller indices.

Example:

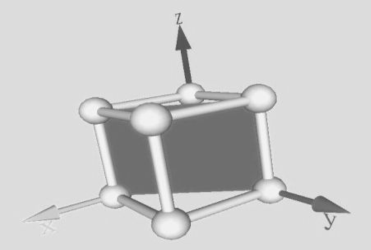
The planes have intercepts 4, 1, 2

1. x:y:z=4:1:2
2. Reciprocals – – –
3. LCM=4
4. 4×– : 4×1 : 4×–

The miller indices are 1, 4, 2 i.e. 1:4:2

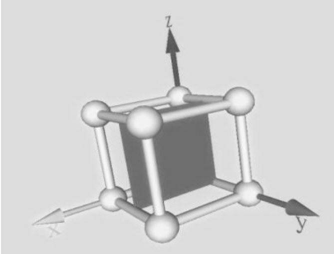
By knowing the Miller indices we can draw the planes within the unit cell. The two Figures shown below gives the idea of drawing the planes with in the unit cell.

1) The Fig. shows the plane with Miller indices (110)



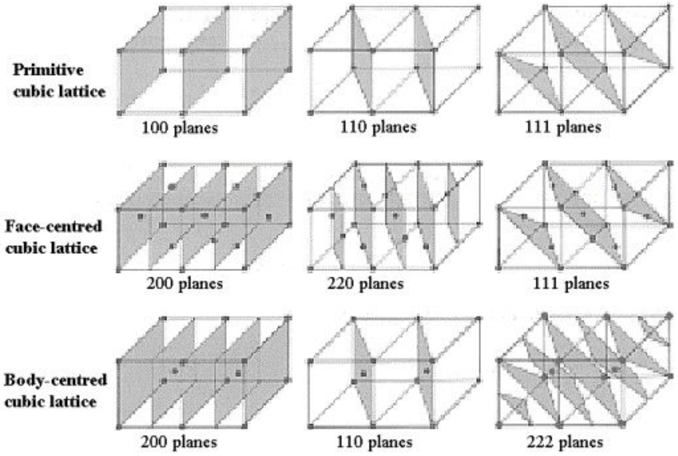
**Plane with Miller indices (110)**

2) The Fig. shows the plane with Miller indices (020)



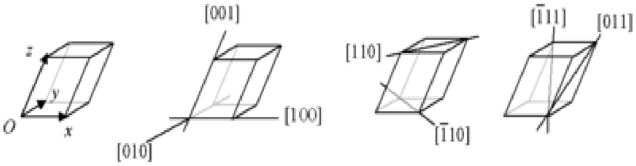
**Plane with Miller indices (020)**

Due to the symmetry of crystal structures the spacing and arrangement of atoms may be the same in several directions. These are known as equivalent directions. A group of equivalent directions is known as a family of directions denoted by < h k l>. Similarly the set of equivalent planes are known as a family of planes is denoted by {h k l}.

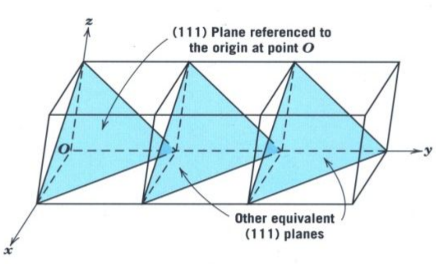


**Miller indices for three types of cubic lattices.**

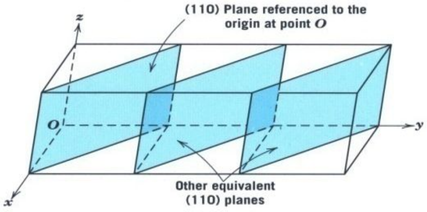
Miller indices of directions



Family of planes is denoted by {h k l} and Family of Directions is denoted by < h k l>



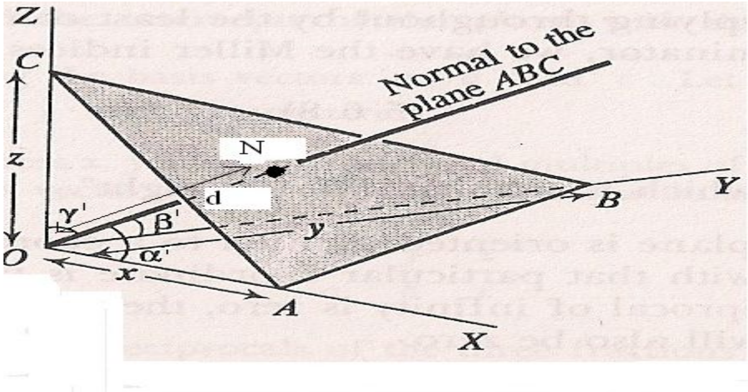
(c)



(b)

**Expression for inter-planar spacing in terms of Miller indices:**

Consider a plane ABC which belongs to a family of planes. h, k, l are the Miller indices of this plane, which represents the set of planes. The perpendicular ON from the origin O to the plane represents the inter-planar spacing d=ON of this family of planes. Let ON make an angle $\alpha^1$, $\beta^1$, $\gamma^1$ with the x, y, z axes respectively.



INTERPLANAR SPACING

The intercepts of the plane on the three axes are

OA= a/h ; OB= a/k ; OC=a/l

Where ‘a’ is the length of the cube edge.

Then from figure, we have

$$\cos\alpha^{1} = \frac{d}{OA} = \frac{d}{a/h} = \frac{dh}{a}$$

$$\cos\beta^1 = \frac{d}{OB} = \frac{d}{a/k} = \frac{dk}{a}$$

$$\cos\gamma^1 = \frac{d}{OC} = \frac{d}{a/l} = \frac{dl}{a}$$

From the figure $ON = \left[x^2 + y^2 + z^2\right]^{\frac{1}{2}}$

$$d = \left[d^2\cos^2(\alpha^1) + d^2\cos^2(\beta^1) + d^2\cos^2(\gamma^1)\right]^{\frac{1}{2}}$$

But, $\left[\cos^2(\alpha^1) + \cos^2(\beta^1) + \cos^2(\gamma^1)\right] = 1$ for the orthogonal coordinates

Substituting the values of cos$\alpha^1$, cos$\beta^1$, cos$\gamma^1$ in equation (2),

We get,

$$\left(\frac{d}{OA}\right)^2 + \left(\frac{d}{OB}\right)^2 + \left(\frac{d}{OC}\right)^2 = 1$$

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

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

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

This is the relation between inter-planar spacing'd' and the edge of the cube 'a'. It should be noted that this formula is applicable only to primitive lattices in cubic, orthorhombic and tetragonal systems.

Spacing between the planes 100, 110 and 111

$d_{hkl} = \frac{a}{\sqrt{\left(h^2 + k^2 + l^2\right)}}$ if h k l= 100, $d_{100} = \frac{a}{\sqrt{\left(1^2 + 0 + 0\right)}} = a$

If h k l=110, $d_{110} = \frac{a}{\sqrt{\left(1^2 + 1^2 + 0\right)}} = \frac{a}{\sqrt{2}}$

$$\text{If h k l=111, } d_{111} = \frac{a}{\sqrt{(1^2+1^2+1^2)}} = \frac{a}{\sqrt{3}}$$

**Expression for space lattice constant 'a' for a cube lattice**

Let 'a' be the lattice constant, 'ρ' be the density of the material and 'n' be the number of molecules in a unit cell.

$$\rho = \frac{\text{Total mass of molecules in a unit cell}}{\text{Volume of the unit cell}}$$

The total mass of the molecules in one kilo mole of substance is equal to the molecular weight of the molecule expressed in kg.

Therefore the mass of each molecule = $M/N_A$

Where $N_A$ is Avagadro number

The total mass of the molecule = $\frac{nM}{N_A}$

For a cubic lattice a=b=c

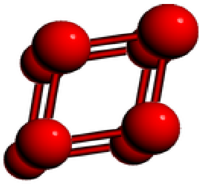
∴ the volume of the unit cell = $a^3$

Hence, the density (ρ)is = $\frac{nM}{a^3 N_A}$

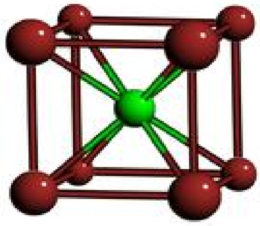
$$a^3 = \frac{nM}{\rho N_A}$$

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

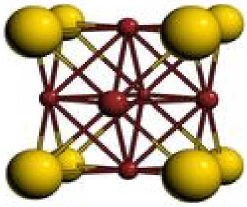
1. **Simple cubic structure (SC):**



## 2. Body centered cubic structure (BCC):



## 3. Face centered cubic structure (FCC):



**Properties of the Unitcell (Cubic)**

**1.Volume of a unit cell:**

The general expression for finding the volume a unit cell is

$$V = abc\left[1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\ \cos\beta\ \cos\gamma\right]^{\frac{1}{2}}$$

Where a,b,c,$\alpha$,$\beta$ and $\gamma$ are called lattice parameters.

For cubic system a=b=c and $\alpha=\beta=\gamma=90^0$.

Therefore $V= a^3$.

1. **Co-ordination number:**

It is the number of nearest neighbour's directly surrounding a given atom well within a crystal.

The co-ordination number for an atom in simple cubic structure is = 6

The co-ordination number for an atom in body centered cubic structure is =8

The co-ordination number for an atom in face centered cubic structure is =12

2. **Number of atoms per unit cell:**

In a unit cell atoms are at the corners, at the center of the faces and at the center of the body.

An atom situated at the corner share 1/8th part to a unit cell.

An atom situated at the face share 1/2 part to a unit cell.

An atom situated at the center of the body share one full part to a unit cell.

1. In a simple cubic structure there are 8 corner atoms.

   ∴ Total share of all the corner atoms/unit cell = (1/8) × 8 =1

   ∴ The number of atoms/unit cell in simple cube = 1
2. In a body centered cubic structure there are 8 corner atoms and an atom at the center of the unit cell.

   ∴ Total share of all the corner atoms per unit cell = (1/8) × 8 = 1

   The share of an atom at the center of the body =1

   ∴ The number of atoms per unit cell in body centered cube = 1+1=2
3. In a face centered cubic structure there are 8 corner atoms and 6 face centered atoms in a unit cell.

   ∴total share of atoms at the corner/unit cell= (1/8) × 8=1

   Total share of atoms at all the faces/unit cell = (1/2) × 6=3

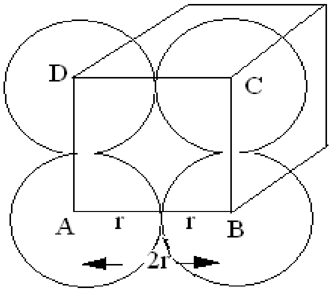
   ∴ The number of atoms/unit cell in face centered cube = 1+3 = 4
4. **Atomic packing factor (APF)**

The fraction of the space occupied by atoms in a unit cell is known as atomic packing factor. It is the ratio of the total volume occupied by the atoms in the unit cell to the total available volume of the unit cell.

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

There is only one lattice point at each of the eight corners of the unit cell. In a simple cubic structure an atom is surrounded by six equidistant neighbors. Hence the co-ordination number is 6. Since each atom in the corner is shared by 8 unit cells, the total number of atoms in one unit cell is (1/8) ×8 = 1

The nearest neighbor distance ‘2r’ is the distance between the centers of two nearest neighboring atoms.



The nearest neighbor distance 2r = a

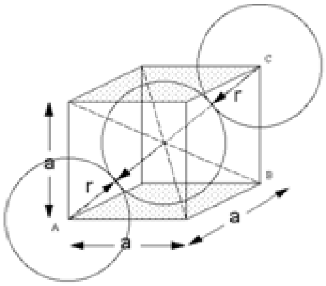
The number of lattice points per unit cell = 1

Volume of all the atoms in a unit cell v = $\frac{4}{3}\pi r^3$

Volume of unit cell = V = $a^3 = (2r)^3$

Packing factor is P.F = $\frac{v}{V} = \frac{4\pi r^3}{3\times 8r^3} = \frac{\pi}{6} = 0.52 = 52\%$

## 2. Body centered cubic structure (BCC):



In a BCC structure eight atoms are present at eight corners and one atom is at the center. The co-ordination number is 8. The number of atoms per unit cell is = [(1/8) × 8]+1 = 2

The lattice constant is

$(AB)^2 = a^2 + a^2 = 2a^2$

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

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

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

Volume of all the atoms per unit cell v = $2\times\left(\frac{4}{3}\pi r^3\right)$

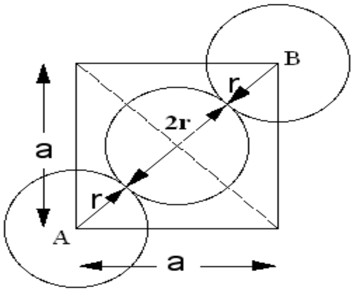
Volume of the unit cell V = $a^3 = \frac{64r^3}{3\sqrt{3}}$

Atomic packing factor = $\frac{v}{V} = \frac{8\pi r^3\times 3\sqrt{3}}{3\times 64r^3} = \frac{\sqrt{3}\,\pi}{8} = 0.68 = 68\%$

## 3. Face centered cubic structure (FCC):

In a FCC structure eight atoms are at the corners of the unit cell and six atoms are present at the center of the six faces. The center atom is surrounded by 12 points. The co-ordination number is 12. Each corner atom is shared by 8 unit cells and the face centered atom is shared by 2 surrounding unit cells.

∴ The number of atoms per unit cell is $= \frac{1}{8} \times 8 + 6 \times \frac{1}{2} = 4$



Atomic radius of face centered cube

AB $= 4r$

$(AB)^2 = a^2 + a^2$

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

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

Nearest neighbor distance $2r = \frac{a\sqrt{2}}{2}$

Volume of all the atoms in unit cell ,$v = 4 \times \left(\frac{4}{3}\pi r^3\right)$

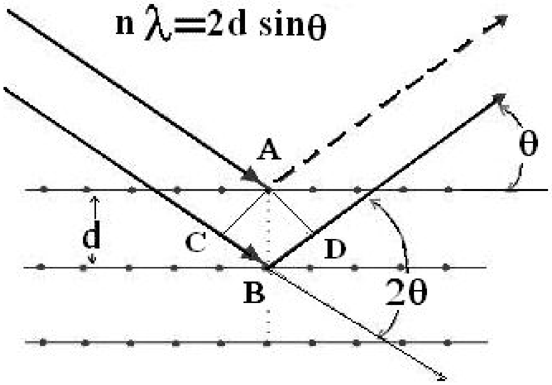
Volume of unit cell, $V = a^3 = \frac{64r^3}{2\sqrt{2}}$

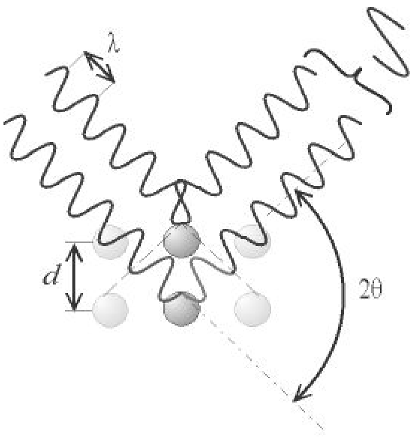
∴ The packing factor $= \frac{v}{V} = \frac{16\pi r^3 \times 2\sqrt{2}}{3 \times 64 r^3} = \frac{\sqrt{2}\,\pi}{6} = \frac{\pi}{3\sqrt{2}} = 0.74 = 74\%$

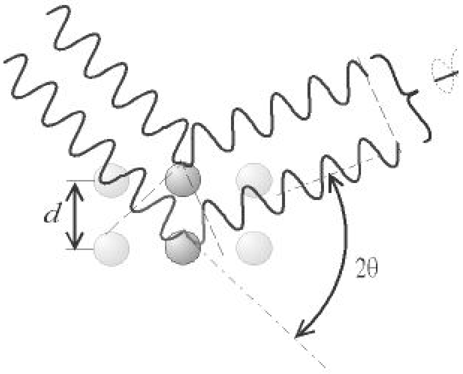
| Parameters | SC | BCC | FCC |
|---|---|---|---|
| Co-ordination number | 6 | 8 | 12 |
| Atomic Radius (r) | $\frac{a}{2}$ | $\frac{\sqrt{3}a}{4}$ | $\frac{\sqrt{2}a}{4}$ |
| Atoms per unit cell | 1 | 2 | 4 |
| Atomic packing factor | $\frac{\pi}{6}$ | $\frac{\sqrt{3}\pi}{8}$ | $\frac{\sqrt{2}\pi}{6}$ |

**Bragg's Law:**

Consider a set of parallel planes called Bragg's planes. Each atom is acting as a scattering center. The intensity of the reflected beam at certain angles will be maximum when the path difference between two reflected waves from two adjacent planes is an integral multiple of λ.







Let 'd' be the distance between two adjacent planes, 'λ' be the wavelength of the incident x-ray, 'θ' be the glancing angle. The path difference between the rays reflected at A & B is given by

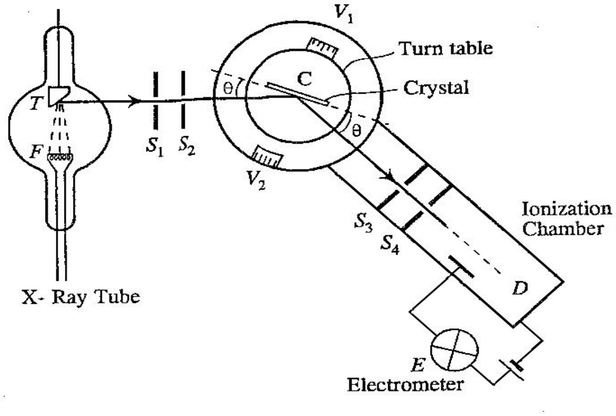
= CB + BD

= d sinθ + d sinθ = 2dsinθ

For the reflected light intensity to be maximum, the path difference 2dsinθ = nλ, where 'n' is the order of scattering. This is called Bragg's law.

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

The schematic diagram of Bragg's x-ray spectrometer is shown in fig. It is used to determine lattice constant and inter-planar distance'd'. It has 1) x-ray source 2) A Crystal fixed on a circular table provided with scale and vernier. 3) Ionization chamber.

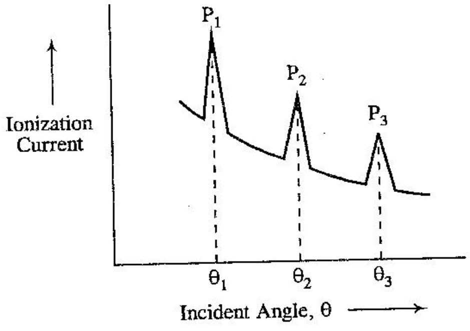


BRAGG'S X–RAY SPECTROMETER

A collimated beam of x-rays after passing the slits $S_1$ and $S_2$ is allowed to fall on a crystal C mounted on a circular table. The table can be rotated about vertical axis. Its position can be measured by vernier $V_1$. An ionization chamber is fixed to the longer arm attached to the table. The position of which is measured by vernier $V_2$. An electrometer is connected to the ionization chamber to measure the ionization current produced by diffracted x-rays from the crystal. $S_3$ and $S_4$ are the lead slits to limit the width of the diffracted beam. Here we can measure the intensity of the diffracted beam.

If x-rays incident at an angle 'θ' on the crystal, then reflected beam makes an angle 2θ with the incident beam. Hence the ionization chamber can be adjusted to get the reflected beam till the ionization current becomes maximum.

A plot of ionization current for different incident angles to study the x-ray diffraction spectrum is shown in fig.



VARIATION OF IONIZATION CURRENT

The rise in Ionization current for different values of ‘θ’ shows that Bragg’s law is satisfied for various values of ‘n’. i.e. $2d\sin\theta = \lambda$ or $2\lambda$ or $3\lambda$ etc. Peaks are observed at $\theta_1$, $\theta_2$, $\theta_3$ etc. with intensities of $P_1$, $P_2$,$P_3$etc.

i.e. $2d\sin\theta_1 : 2d\sin\theta_2 : 2d\sin\theta_3 = \lambda : 2\lambda : 3\lambda$

The crystal inter-planer spacing‘d’ can be measured using $2d\sin\theta = n\lambda$

If $d_1$, $d_2$, $d_3$ be the inter-planar spacing for the planes (100), (110) & (111) respectively.

It can be shown -

For cubic crystal: $d_1:d_2:d_3 = 1:\frac{1}{\sqrt{2}}:\frac{1}{\sqrt{3}}$

For FCC : $d_1:d_2:d_3 = 1:\frac{1}{\sqrt{2}}:\frac{2}{\sqrt{3}}$

For BCC : $d_1:d_2:d_3 = 1:\frac{2}{\sqrt{2}}:\frac{1}{\sqrt{3}}$

## Polymorphism and Allotropy

Polymorphism is the ability of a substance to crystallize in several solid phases that possess different lattice structures at different temperatures.

Many metals have different structures without any change in chemical composition when the temperature or pressure is varied, or when they are subjected to unusual thermal or mechanical treatments. This phenomenon is known as polymorphism.

The melting point of pure iron is $1535^0$C. Iron may exit in several allotropic forms example α, γ and δ in solid state. The existence of one form to the other depends on temperature to which the iron is heated.

OR

Allotropy is the properties by virtue of which an element can have more than one type of structure all of which have identical chemical properties but their physical property differ. For examples; Diamond and graphite

OR

Many elements or compounds exist in more than one crystalline form under different conditions of temperature and pressure. This phenomenon he is termed polymorphism and if the material is an elemental solid is called allotropy.

Example: Iron (Fe – Z = 26)

Liquid above the 1539C. δ-iron (BCC) between 1394 and 1539 °C.

γ-iron (FCC) between 912 and 1394 °C

α-iron (BCC) between -273 and 912 °C.

α iron→ (912) γ iron→ (1400)δ iron → (1539)liquid iron

BCC FCC BCC

Another example of allotropy is carbon. Pure, solid carbon occurs in three crystalline forms – diamond, graphite; and large, hollow fullerenes.

**Crystal structure of Diamond:**

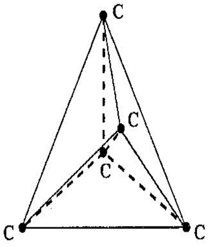
The diamond lattice can be considered as the superposition of 2 fcc sublattice one of which is displaced from the other along the body diagonal of the unit cell by $(1/4)^{th}$ the length of the diagonal. Thus a carbon atom will be present at the center of tetrahedron, with four carbon atoms of the other sublattice as its nearest neighbors located at four corners of the same tetrahedron. Thus the co-ordination number of diamond is 4 and there will be 8 carbon atoms present per unit cell**.** That is each carbon atom is at the center of a tetrahedron,4 carbon atoms are at diagonally opposite in the planes. The lattice constant is $3.5A^o$ and the bond length is $6.56A^o$.

The semiconductors like Si and Ge are having diamond structure.

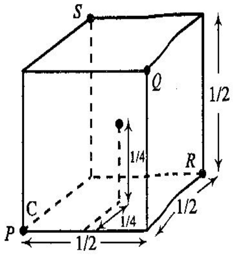
An FCC lattice has 4 atoms/unit cell. But the diamond lattice comprises of two interpenetrating FCC sub-lattice.

Therefore, Number of atoms per unit cell in the diamond lattice is 2x4 = 8.

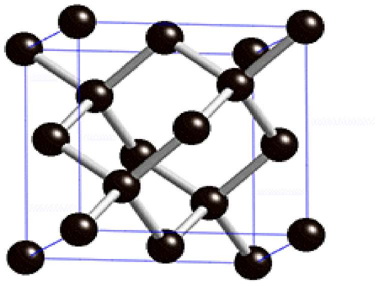
And Atomic Packing Factor = $\frac{8}{a^3}\times\frac{4}{3}\pi r^3 = \frac{8}{\left(\frac{8}{\sqrt{3}}r\right)^3}\times\frac{4}{3}\pi r^3 = \frac{\sqrt{3}}{16}\pi = 34\%$

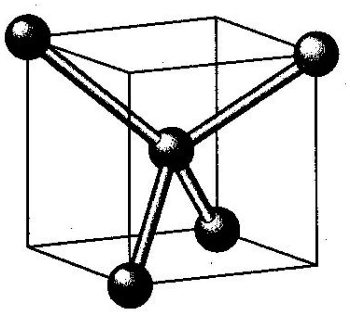


TETRAHEDRON FORMATION
BY C ATOMS



CO-ORDINATES OF
C ATOMS



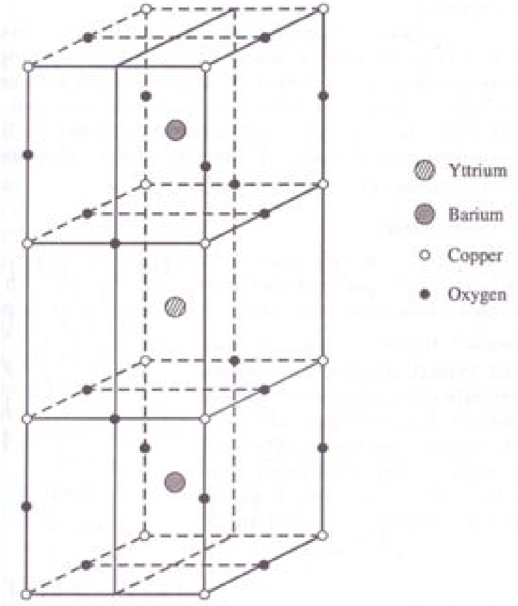


**Perovskites:**

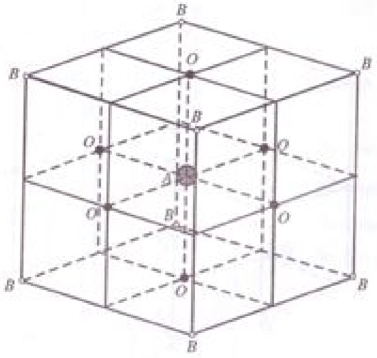
The compounds with the formula $AB\mathrm{O}_3$, where A & B are transition metals (ex:$\mathrm{CaTiO_3}$) Table provides a brief list of some well-studied $AB\mathrm{O}_3$perovskites. Many of the perovskites are cubic or nearly cubic, but they often undergo one or more structural phase transitions, particularly at low temperatures. The perovskites oxides are extremely interesting because of the enormous variety of solid-state phenomena they exhibit. Many of the perovskites are magnetically ordered and a large variety of magnetic structures can be found.

The electronic properties of the perovskites can be altered in a controlled manner by substitution of ions into the *A* or *B* sites, or by departures from ideal stoichiometry.

The electronic energy bands of the perovskites are very unusual in that they exhibit two-dimensional behaviour that leads to unique structure in properties such as the density of states, Fermi surface, dielectric function, phonon spectra and the photoemission spectra.



UNIT CELL STRUCTURE OF YBa$_2$Cu$_3$O$_7$



CRYSTAL STRUCTURE OF PEROVSKITE

# Module–5

## Shock waves, Acoustics and Science of Nano Materials

Definition of Mach number, distinctions between- acoustic, ultrasonic,subsonic and supersonic waves. Description of a shock wave and itsapplications. Basics of conservation of mass, momentum and energy -derivation of normal shock relationships using simple basic conservationequations (Rankine-Hugoniot equations). Methods of creating shock wavesin the laboratory using a shock tube, description of hand operated Reddyshock tube and its characteristics.

.Introduction to Nano Science, Density of states in 1D, 2D and 3D structures.Synthesis: Top–down and Bottom–up approach, Ball Milling and Sol–Gelmethods.CNT – Properties, synthesis: Arc discharge, Pyrolysis methods, Applications.Scanning Electron microscope: Principle, working and applications.

**10 Hours**

# Content:

- **Shock waves**
- **Reddy shock tube**
- **CNT – Properties**
- **Electron microscope**
- **Mach number**
- **Mach angle**
- **SEM**
- **Arc discharge tube**

**Mach number:**

In Aerodynamics, the speeds of bodies moving in a fluid medium are classified in to different categories on the basis of Mach number. It is defined as the ratio of the speed of the object to the speed of the sound in the given medium, i.e.,

Mach * number $=\frac{object\ speed}{speed\ of\ sound\ in\ the\ medium}$

It is denoted as M. thus v is the object speed and the speed of sound in the medium is a, then, $M = \frac{v}{a}$.

Since it is a ratio of speeds, it doesn't have a unit as the name itself indicates, it is apure number.

**Speed of sound:**

The speed of sound 'a' in air or any gas medium at a temperature T (in Kelvin) is given by, $a=\sqrt{\gamma RT},$ where □ is the ratio of specific heats and R is the specific gas constant.

**Distinction between acoustic, ultrasonic, subsonic and supersonic waves:**

An acoustic wave is simply a sound wave. it moves with the speed 333 m/sin air at STP. Sound waves have frequencies between 20 Hz to20,000Hz.Amplitude of acoustic wave is very small.

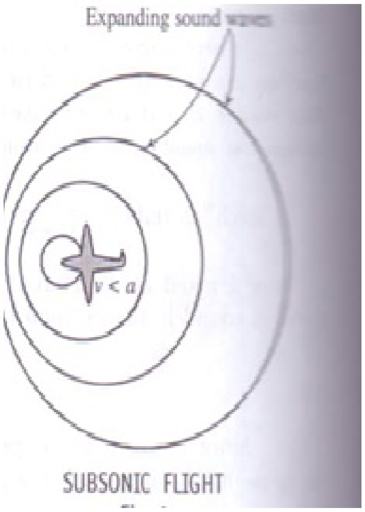
**Ultrasonic waves:**

Ultrasonic waves are pressure waves having frequencies beyond 20.000 Hz. but they travel with the same speed as that of sound. Amplitude of the ultrasonic wave is also small.

**Subsonic waves:**

If the speed of the mechanical wave or body moving in the fluid is lesser than that of sound then such a speed is referred to as subsonic and the wave is a subsonic wave. All subsonic waves have mach no<1.

The speeds of almost all the vehicles such as motor cars or trains that we see moving on the road fall in the subsonic category. The speeds of flight of birds is also subsonic.



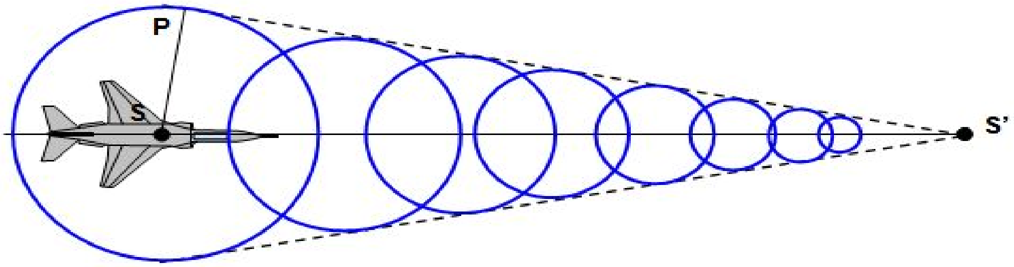
**Subsonic flight**

For a body moving with subsonic speed, the sound emitted by it manages to move ahead &away from the body since it is faster than the body

**Supersonicwaves:** Supersonic waves are mechanical waves which travels with speeds greater than that of sound, i.e. , with speeds for which, Mach number >1.

A body with supersonic speed. Zooms ahead by piercing its own sound curtain leaving behind a series of 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.



**Supersonic flight**

**Mach angle:**

A number of common tangents drawn to expanding sound waves mitted from a body a supersonic speed formulate a cone called mach cone. the angle made by tangent with the axis of the cone (half angle of the cone) is called mach angle μ. μ is related to the Mach number ‘M ʾ through the equation,

$$\mu = \sin{-}^{1}\left(\frac{1}{M}\right)$$

in supersonic waves ,we have a special class of waves called hypersonic waves. They travel with speeds for which Mach number$\geq 5$.

Research is being carried out in a half a dozen countries including India, to develop engines named “scram jets” which can empower vehicles fly at speeds of Mach number $\geq 5$

**Transonic waves:**

There is a speed range which overlaps on the subsonic & supersonic ranges. This is actually in the domain in which, there is a change of phase from subsonic to supersonic. Since it becomes very difficult to precisely categorize certain parameter at speeds near (or at) M=1. This range is brought into picture. We Say it is transonic range for speeds $0.8 < M > 1.2$ it is what we call as grey area where there is overlapping of some of the characteristics of both the subsonic &supersonic speeds.

**Shock waves**

**Description of a shock wave:**

Any flood that propagates at supersonic speeds, gives rise to a shock wave. Shockwaves are produced in nature during the earthquakes and when lightning strikes. when velocity of a body increases from subsonic to supersonic ,we can hear the booming sound of shockwaves .It is called “Sonic boom “ Shockwaves can be can be produced by sudden dissipation of mechanical energy in medium enclosed in small space .Shockwave is 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 and density of gas through which it propagates.Shockwaves are identified as strong or weak depending on the magnitude of instantaneous changes in pressure and temperature in the medium of space bound within the thickness of the shock front is of the order of few micrometres.

For example, the shockwaves created by nuclear explosion of crackers are weak characterized by low Mach number.

**Basics of conservation of Mass, Momentum and Energy:**

We know that conservation means the maintenance of certain quantities unchanged with physical process.

**Law of conservation of mass:**The total mass of any isolated system remains unchanged or constant and is independent of any chemical and physical changes that could occur within the system.

That is $\frac{dm}{dt}=\dot{m}=\text{const}$ in a physical system.

**Law of conservation of momentum:**In a closed or isolated system, the total moment remains constant. Or when two bodies collide with an isolated system, the total momentum of objects before collision equal to the after collision.

$$\dot{P}_1 = \frac{dmv_1}{dt}=0 \quad \text{ie,} mv_1=\text{const}$$

$$\dot{P}_2 = \frac{dmv_2}{dt}=0 \text{ie, } mv_2=\text{const}$$

$p_1$ →Momentum before collision

$p_2$ →Momentum after collision

**Law of conservation of energy:**The total energy of the isolated system or closed system is constant and it is independent of any changes occurring within the system.

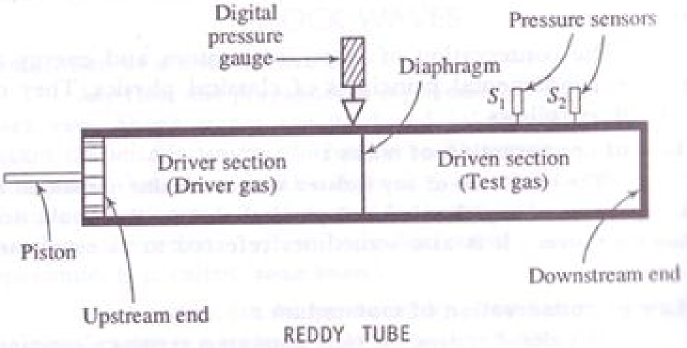
Let total energy of the system per unit mass consist of the internal energy U, kinetic energy is K , potential energy is V and work done by the pressure P,

Then conservation of energy can be written as

$$h_1+u_1{}^2=h_2+u_2{}^2 --(3)$$

## Reddy shock tube :

Reddy shock tube consist is hand operated shock tube capable of producing shockwaves by using human energy. Its long cylindrical tube with two sections areseparated by diaphragm. It’s one end is fitted with piston and other end is closed or open to the surroundings.



REDDY TUBE

## Construction:

Reddy shock tube consists of cylindrical stainless steel tube of about 30mm diameter and length 1m .It is divided into two section each of length 50cm ,one is driver tube and other one is driven tube separated by 0.1mm thick of diaphragm.

1. The Reddy tube has a piston fitted at far end of the driver section and far end of the driver section is closed.
2. 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 the filling the test gas to the required pressure.
3. The driver section is filled with a gas termed as driver gas ,which is held at relatively high pressure due to compressing action of the piston .the gas driven section is termed as driven gas.

## Working:

The driver gas is compressed by pushing the piston hard into driver tube until diaphragm ruptures .Then driver gas rushes into the driven section and pushes driven gas towards the far downstream end. This generate moving shock wave instantaneously raises the temperature and pressure of the driven gas as the shock move over it .

The propagating primary shock waves are reflected from the downstream end. After the reflection, the test gas undergoes further compression which boosts it temperature and pressure to still higher values by reflected shock waves.

This state of high values of pressure and temperature is sustained or continuous (it takes time of the order milliseconds) at the downstream end until an expansion wave reflected from the upstream end of the driver tube arrives there and neutralizes compression partially .these expansion waves are created at the instant the diaphragm is ruptured and they travel in the direction of shock waves.

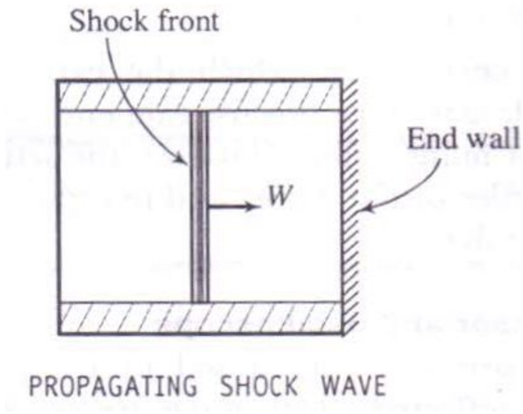
Actual creation of shock waves are is depends on the properties of driver and test gases and dimension of the shock tube .pressure rise caused by primary shock waves and reflected shock waves are sensed by sensors $s_1$ and $s_2$ respectively and they are recorded in digital cathode ray(CRO).the pressure sensors are piezoelectric transducers.

Since the experiment involves 1millisecond duration measurement, rise time of oscilloscope should be few microseconds with bandwidth of 1 MHz or more is required. From the recording the CRO, shock wave arrival time is calculated and also Mach number, pressure and temperature can be calculated.

## Rankine and Hugoniot equations (Shock relations):

Consider a shock wave propagating with a speed W in a shock tube. The condition 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 and Hugoniot relations.

Consider two regions with reference to the shock front, one which is ahead of shock front and other behind it .Both the regions are at far enough distances from the shock front so that equilibrium conditions attained in two regions where physical conditions such as pressure, density, temperature etc. are uniform.



Let $p_1$,$T_1$,$\rho_1$ and $h_1$ be the values of pressure ,temperature ,density and enthalpy before creation of the shock wave .Hence, these conditions attained in the region ahead of the shock wave.

Similarly,$p_2$,$T_2$,$\rho_2$ and $h_2$ be the corresponding values after the diaphragm ruptures. Hence they are applicable in the region behind the wave. Then the three conservation relations which corresponds to the conservation laws are as stated in the following taking shock stationary frame of reference.

$$\rho_1 u_1 = \rho_2 u_2 \quad \text{………………………. (1)}$$

(Conservation of mass)

Where, $u_1$→ velocity of the fluid ahead of the shock.

$u_2$→ Velocity of the fluid following the shock.

$$p_1 + \rho_1 {u_1}^2 = p_2 + \rho_2 {u_2}^2 \text{………………… (3)}$$

(Concerning conservation of momentum)

$$h_1 + \frac{{u_1}^2}{2} = h_2 + \frac{{u_2}^2}{2} \quad \text{………………………... (4)}$$

(Concerning conservation of energy)

These 3 equations along with the equation of state

i.e PV =RT …………………………..(5)

Using the above equations ,the following normal shock relations called Rankine –hugoniot equations can be derived in which $p_5$&$T_5$ represent pressure and temperature at the downstream end behind the reflected shock wave.

1. $\frac{p_2}{p_1}=[1+\frac{2\gamma}{\gamma+1}(M^2-1)]$

**2.** $\frac{T_2}{T_1}=\frac{p_2}{p_1}\left[\frac{\frac{\gamma+1}{\gamma-1}+\frac{p_2}{p_1}}{1+\left(\frac{\gamma+1}{\gamma-1}\right)\frac{p_2}{p_1}}\right]$

**3.** $\frac{P_5}{P_2}=\frac{(3\gamma-1)\frac{p_2}{p_1}-(\gamma-1)}{(\gamma-1)\frac{p_2}{p_1}+(\gamma+1)}$

**4.** $\frac{T_5}{T_2}=\frac{p_5}{p_2}\left[\frac{\frac{\gamma+1}{\gamma-1}+\frac{p_5}{p_2}}{1+\left(\frac{\gamma+1}{\gamma-1}\right)\frac{p_5}{p_2}}\right]$

These are Rankine –Hugoniot equations.

**Methods of creating shock waves in the laboratory using a shock tube :**

Shock waves can be created in the laboratory by

1. Using a reddy tube

2. Detonation (A violent release of energy or explosion)

3. Very high pressure gas cylinder

4. Combustion

5. Using small charge explosives

## Introduction to Nano Science:

Matter arranged by exercising control over lengths of 1 to 100 nano meter and the formulating structures exhibit characteristics that are specific to their size and dimensions, the resulting materials are called Nano materials. Inorganic and organic Nano materials are the two types.

## INORGANIC NANO MARETIALS:

Nano structured inorganic materials such as Fullerene's, Carbon nano tubes and Nano wires are of this category. Fullerene's full form is Buckminster fullerene. It is also called Bucky ball, because of its soccer ball shaped structure. Each fullerene molecule comprises of 60 carbon atoms arranged in globular shape. Nano wires are arrangements in one dimension made of silicon, zinc oxide and various metals. They are having diameter in nano meter range but lens in micrometre range. Nano wires can act like an optical fiber and their conductance can be tuned by binding it to different molecules.

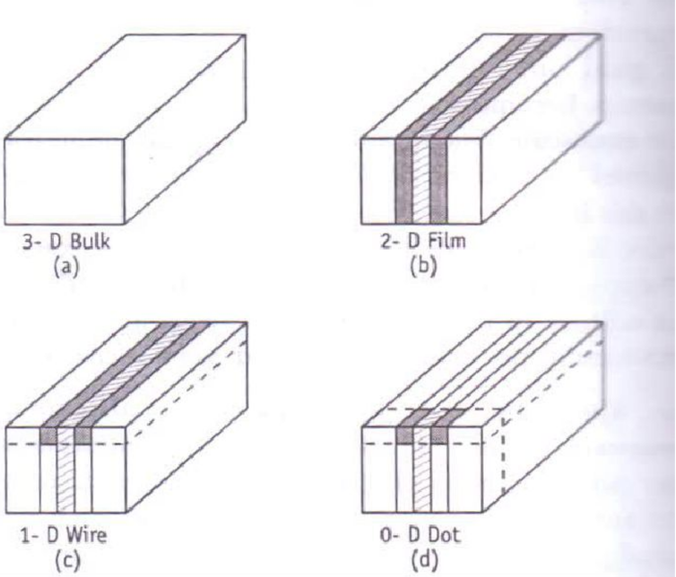
## ORGANIC NANO MATERIALS

Carbon compounds having nano structures are called organic nano materials. A DNA molecule is relatively rigid. Several strands taken from a DNA molecule when combined, from structures with higher stiffness. Artificially synthesized DNA structures possess the repeatable capacity, show promise as self-assembly into geometrical structure. It is repeated that an 8-sided structure is a good candidate for cloning. By manipulating the DNA of cells, the cells could be induced to produce the type of proteins. Protein based nanostructures could be then made which even conduct electricity.

Quantum structures:

As we go down from bulk scale Nanomaterials,we visualize the materials of lower dimensions in the Nano scale as follows.

When the reduction from the bulk material (in 3-dimentions)is in one direction, it results in a structure in 2- dimensions and is called *2D-film* (fig .1).



Schematic diagram of quantum structures

If the reduction is in two directions, obviously the resultant structure will be in one dimension which is called quantum wire. if the reduction is in all the three directions, the material reduces to a point which is well known as a quantum dot. It is also called a nanoparticle or cluster.

**Density of states (Dos) for various quantum structures:**

Treating the free electrons as electron gas in one, two & three dimensions, we can arrive at expression for density of states for the respective cases.

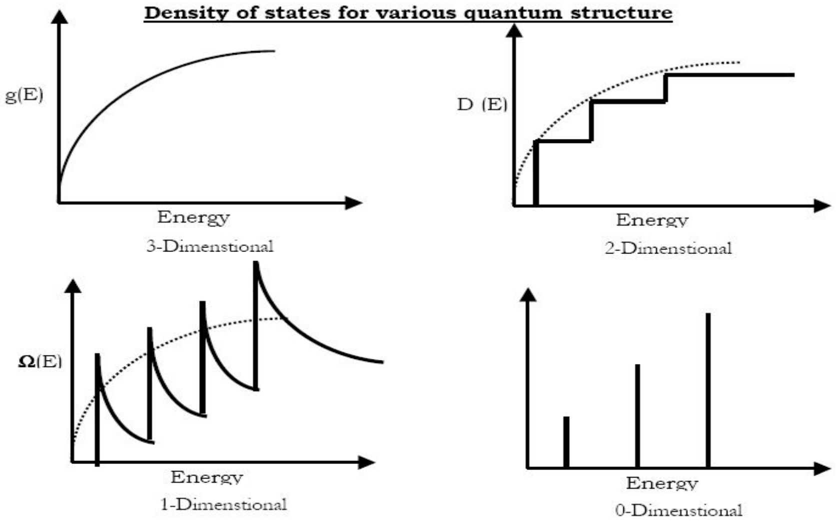
The density of states (Dos) for the various quantum structures as function of energy are shown in fig.

The DOS denoted as g(E) for 3D materials, various continuously. The density will be typically of the order of the order of $10^{26}/ m^3$ev. for a 2 -D structure,

The DOS subbands in a 2-D structure is given by

D(E)=$\frac{m^*}{\pi\hbar^2}$

the dos denoted as D (E) varies as a step-function i.e., there will be sudden rise in D (E) at certain energy values such as $E_{1,}E_2$,,, (fig .2b).it happens because the energy progress ( in terms of energy states) of the first sub band continues even when the second subband starts.



Density of states for various quantum structure

So. In the second subband, apart from to its own energy states, there will be additional contribution from the continuation of energy states of firstsubband. Hence the dos rises at once at the beginning of second subband .henceDOS rises at once at the beginning of second subband. Again, the combined the energy progress of first & second subbands enter into the third subband ,& DOS rises further at the commencement of third subband. Thus the overall variation takes a stair case shape. however, the locus of all the corners of the will be a parabola. If the thickness of the 2-D material is increased, more subbands will be created which results increase of the step width. If thickness increase continues, then it is limit ,the material reaches 3-dimensions at which time, the innumerable steps would be seen merged into an envelope of parabolic variation for DOS (as it should be for a 3-D material).the density is typically of the order of$10^{18}/m^2$eV for 2-D structure.)

D (E) dE $=\frac{m*}{\square h^2}\sum H(E-E_i)$ dE,Where m* is the effective mass of electron in the structure, and H (E-$E_i$) is a step function called Heaviside function.its values are zero for E <$E_i$ and, 1 for E ≥ $E_i$

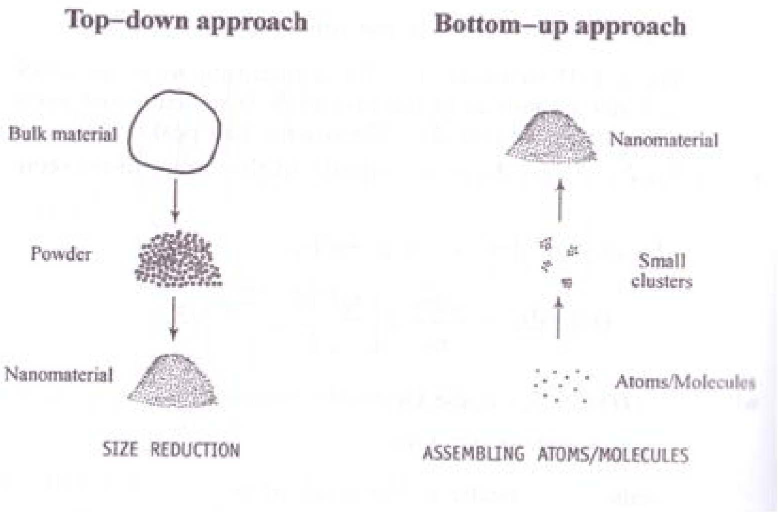
$E_i$is the $i^{th}$energy level in the subband.For a 1- D structure, i.e., for a Quantum wire, the DOS variation is not smooth as in the case of 3-D structure not even constant over the sub band also. The density hits peaks at energy values e$E_1$, $E_2$…, and decreases rapidly in the range in between

The DOS in this case is given by,electrons are confined in one or more directions by reducing the dimensions of the material in those directions, the density of the state's changes due to quantization if energy,
Which is a material reduced in 1-dimention to nano scale, there is Quantization of energy due to confinement of electrons in one direction the density of states for a quantum well o r2-D film is given by $\Omega(E)\,dE = \frac{\sqrt{2m}}{\pi h^2}\sum \frac{n_i\, H(E-E_i)}{\sqrt{(E-E_i}}\,dE$

Where H(H-$E_i$) is the Heaviside function.$n_i$ is the degenerate function.

**Synthesis of nanomaterial's:**There are two different approaches of material fabrication. One is the top-down approach and the other is the bottom-up approach.

**Top-down technique:**In top-down technique, generally a bulk material is taken and machined it to modify into the desired shape and product. In this method the macro or micro size particles are milled till we get the nanosize particles. Examples of this type of technique are themanufacturing of integrated circuits using a sequence of steps such as, lithography, etching, ion implantation, etc. For nanomaterial synthesis, ball milling is an important top-down approach, where microcrystalline structures are broken down to nanocrystalline structures, but original integrity of the material is retained.

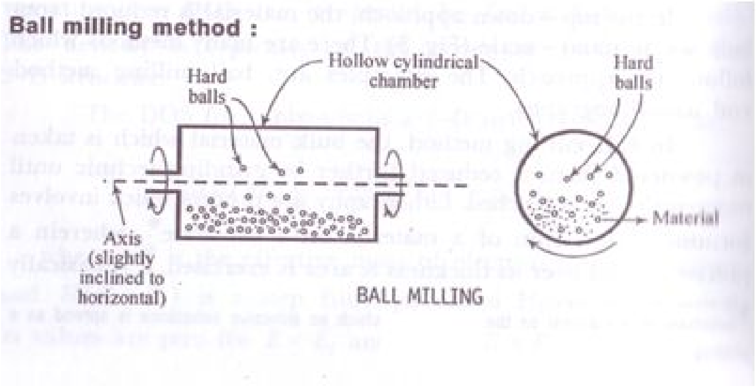


**Bottom-up technique:**

Bottom-up technique is used to build something from the basic materials, for example, assembling materials from the atoms/molecules up till we get the nanosize particles and, therefore very important for nano-fabrication. Unlike lithographic technique of top-down approach, which is extensively used in silicon industry, this bottom-up nonlithographic approach of nanomaterial synthesis is not completely proven in manufacturing yet, but has great potential to become important alternative to lithographic process. Examples of bottom-up technique are self-assembly of nanomaterials, sol-gel technology, electro deposition, physical and chemical vapour deposition (PVD, CVD), epitaxial growth, laser ablation, etc.

**Ball-milling:** Ballmilling method is topdown approach, that is bulk material is broken down into nanosize particle.

**Construction:**A ball mill consists of a hollow cylindrical chamber rotating about its axis. The axis of the shell may be either horizontal or at a small angle to the horizontal.



Inside the chamber there are hard & heavy balls made up of tungsten carbide /steel, these produce smaller size particles .the chamber is mounted, such that its axis is inclined to the horizontal to enable material inside ti slide and accumulate in one region.

**Working**

The given material made into small grain size & fed into the chamber is start rotate about its own axis, the balls are gets carried upwards. Due to gravity balls are comes down &hits to the sample with a high speed. This procedure repeated until the material to get reduced to nanosize particle.

**Sol-Gel technique:**The sol is a name of a colloidal solution made of solid particles few hundred nm in diameter, suspended in a liquid phase and the gel can be considered as a solid macromolecule immersed in a solvent.

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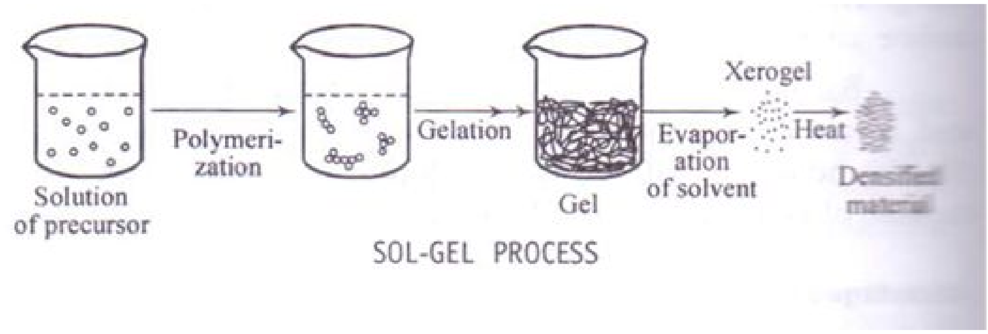
The sol-gel process is a wet-chemical based self-assembly process for nanomaterial formation. (Also known as Chemical Solution Deposition) widely used recently in the fields of materials science and ceramic engineering. Such methods are used primarily for the fabrication of materials (typically a metal oxide) starting from a chemical solution (sol, short for solution) which acts as the precursor for an integrated network (or gel) of either discrete particles or network polymers.

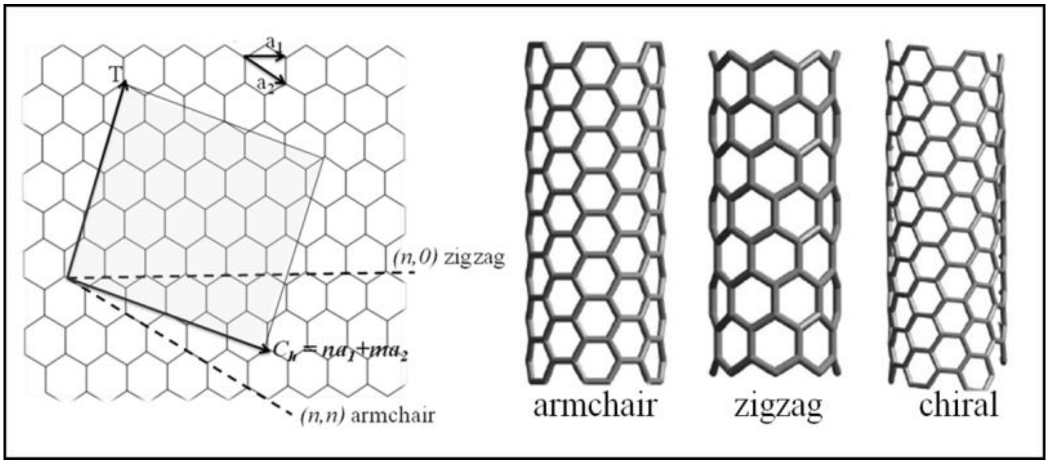


SOL-GEL PROCESS

## CARBON NANOTUBES:

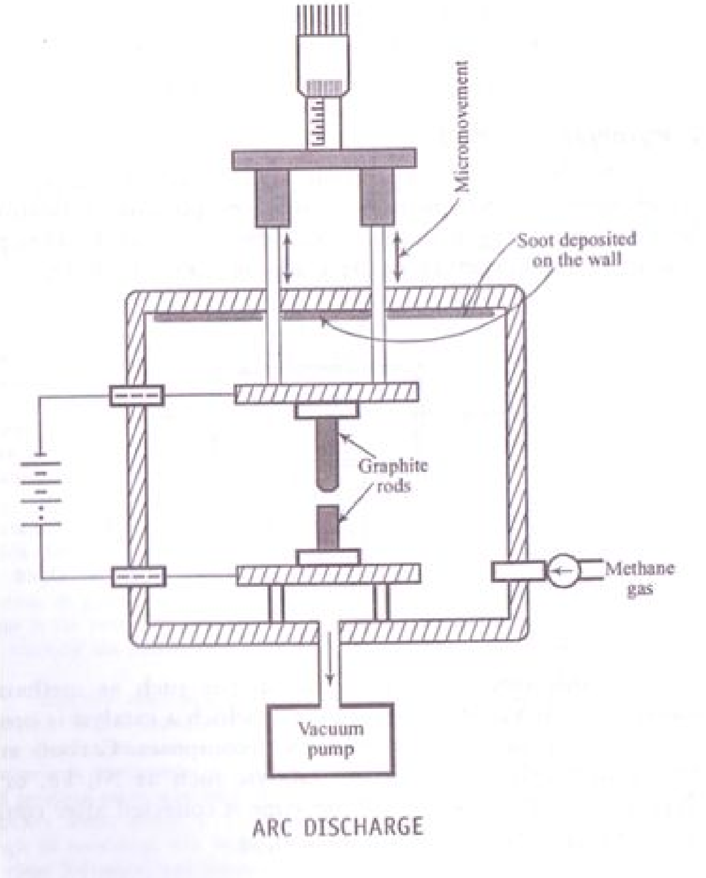
Carbon Nanotubes is a molecular tubes of about 10,000 times thinner than a human hair, consist of rolled up sheets of carbon hexagons as shown in the figure. These nanotubes are single molecules measuring a few nanometers in diameter and several microns in length.

The nano tubes conducting properties depend upon how the two ends of the sheet meet along. For a particular way of arrangement of atoms along the meeting line makes the entire tube conducting like a metal and for another type of arrangement, the tube behaves like a semiconductor. When one type nano tube is rolled inside another type we get multi walled nano type. Using semiconductor nano tubes transistors and logic gates are constructed. Nano wires are made using nano tubes.



Nano tubes non-reactive and with high temperatures .A transistor fabricated using nano tube at Holland can switched on and off with flow of a single electron. This reduces the size of the circuits in computers.Synthasis of carbon nano tubes

**Arc discharge:**



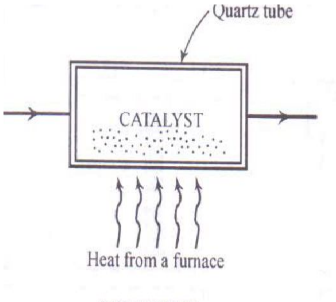
ARC DISCHARGE

The carbon arc discharge method, initially used for producing C60 fullerenes, is the most common and perhaps easiest way to produce CNTs, as it is rather simple. A method for the synthesis of carbon nanotubes where a dc arc voltage is applied across two graphite electrodes immersed in an inert gas such as He.

Nanotubes were observed in 1991 in the carbon soot of graphite electrodes during an arc discharge, by using a current of 100 amps,that was intended to produce fullerenes. This method creates CNTs through arc-vaporization of two carbon rods placed end to end, separated by approximately 1mm, in an enclosure that is usually filled with inert gas at low pressure. A direct current of 50 to 100A, driven by a potential difference of approximately 20 V, creates a high temperature discharge between the two electrodes. The discharge vaporizes the surface of one of the carbon electrodes, and forms a small rod-shaped deposit on the other electrode. Producing CNTs in high yield depends on the uniformity of the plasma arc, and the temperature of the deposit forming on the carbon electrode.

During this process, the carbon contained in the negative electrode sublimates because of the high-discharge temperatures (The arc –plasma evaporation of pure graphite rods led to the discovery of carbon nanotube (CNTs).)

**Pyrolysis**



PYROLYSIS

Pyrolysis is the decomposition of chemical compound of higher molecular weight into simpler compounds by heating in the absence oxygen so that no oxidation occurs ,its carried at $400^0$Cto $800^0$ C.The hydrocarbon gas such as methane is passed through a heated quartz tube in which catalyst is present due to pyrolysis the gas decomposes then carbon atoms are free. Bind with catalyst such as Ni,Fe, or Co.Carbon nanotubes grow on the catalyst and same is collected after cooling.

**Application of CNTs**

Nanomaterial's are of interest because at this scale distinctive optical, magnetic, electrical and other properties emerge due to this, these materials having wide range of potential application in magnetic information storage , catalysis , enhanced optical and magnetic imaging , as well as in targeted-specific therapy.

1.It has been used for wind turbines, marine paints and variety of sports gear such as skis, ice hockey sticks, baseball bats, hunting arrows, and surfboards.

2. It is used as tips for atomic force microscope probes.

3. In tissue engineering, carbon nanotubes can act as scaffolding for bone growth.

4. Because of the carbon nanotube's superior mechanical properties, many structures have been proposed ranging from everyday items like clothes and sports gear to combat jackets and space elevators.

5. Nanotube-based transistors, also known as carbon nanotube field-effect transistors (CNTFETs), have been made that operate at room temperature and that are capable of digital switching using a single electron. This reduces the size of the circuits in computers.

Notes:

1. Wires for carrying electrical current may be fabricated from pure nanotubes and nanotube-polymer composites. Recently small wires have been fabricated with specific conductivity exceeding copper and aluminium; these cables are the highest conductivity carbon nanotube and also highest conductivity non-metal cables.

2. The exceptional electrical and mechanical properties of carbon nanotubes have made them alternatives to the traditional electrical actuators for both microscopic and macroscopic applications.

3. One of the promising applications of single-walled carbon nanotubes (SWNTs) is their use in solar panels, due to their strong UV/Vis-NIR absorption characteristics.

4. Radars work in the microwave frequency range, which can be absorbed by MWNTs. Applying the MWNTs to the aircraft would cause the radar to be absorbed

and therefore seem to have a smaller signature. One such application could be to paint the nanotubes onto the plane.

5. Single-walled carbon nanotubes are inserted around cancerous cells, then excited with radio waves, which causes them to heat up and kill the surrounding cells.

## SEM:

**Principle**:The principle used in the working of SEM is the wave nature of the electrons.An electron accelerated under a potential difference of V volts behave like awave of wavelength

$$\lambda = \frac{h}{\sqrt{meV}} = \frac{h}{\sqrt{mE}}$$

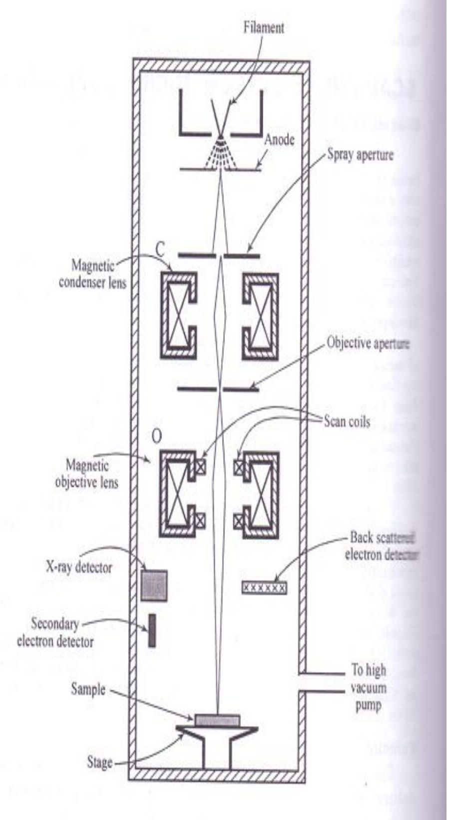
**Construction:** The apparatus consists of an highly evacuated chamber inside which there is an electron gun at the top which comprises of the filament and the anode. There are two magnetic lenses, one is the condensing lens ‘C’ and the other one is the objective lens ‘O’.with a coil. There is a spray aperture using which ,spherical aberration during focusing will be minimized, A flat surface called stage is provided at the bottom portion of the apparatus to place the specimen under study.

There are three types of detectors in the apparatus. They are ,back scattered electron detector, secondary emission electron detector, and X-ray detector which could be used selectively depending upon the particular application.

**Working:**

The sample to be investigated is placed on the specimen stage after which, inside of the chamber is evacuated by connecting it to a high vacuum pump.

Electrons are emitted by the filament by thermionic emission and are accelerated by a suitable positive potential is applied to the anode, with respect to the filament. Then accelerated electrons from the electron gun pass through the spray aperture from where the electron beam emerges. The condensing lens converges the beam and eliminates some high-angle electrons. The beam then passes through the objective aperture where the size of the beam can be controlled. a thinner beam then enters into the field of objective lens ‘o’ ,which focuses the beam on to the desired part of the specimen.



SCANNING ELECTRON MICROSCOPE (SEM)

A set of coils called scan coils placed along with the objective lens, enables the beam to scan the specimen in a particular way called raster.

Upon incidence, electrons are knocked out from the specimen due to the impact of the beam. Back scattered electrons, secondary electrons and the X-rays emitted are detected by the respective detectors and corresponding signal is produced. This signal is converted into a micro spot of corresponding brightness on a screen. The beam focus is shifted to the next adjacent spot in order, where it again dwells

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**Applications:**

SEM is used to study.

(1) External morphology of biological organisms in the sub microscope.
(2) Chemical composition
(3) Crystalline structure.SEM is also used in forensic investigation.
(4) Used to study the corroded layers on metal surfaces
(5) Used to study biological specimens like pollen grains.