LECTURE NOTES

ON

ENGINEERING PHYSICS

I B. Tech I semester

Dr. Rizwana
Professor

FRESHMAN ENGINEERING
INSTITUTE OF AERONAUTICAL ENGINEERING
(Autonomous)
Dundigal, Hyderabad - 500 043

ENGINEERING PHYSICS
(Common for CSE / ECE / EEE / IT)

Semester: I

Course Code	IA16-A1804	Hours / Week			Credits	Maximum Marks		
Category	**Foundation**	**L**	**T**	**P**	**C**	**CIE**	**SEE**	**Total**
		3	-	-	3	30	70	100

Contact Classes: 45	Tutorial Classes: Nil	Practical Classes: Nil	Total Classes: 45

Objectives:

The course should enable the students to:

I.   Develop strong fundamentals of nanomaterials.
II. Meliorate the knowledge of theoretical and technological aspects of lasers.
III. Correlate principles with applications of the quantum mechanics, dielectric and magnetic materials.
IV. Enrich knowledge in modern engineering materials like semiconductors.

UNIT-I	DIELECTRIC AND MAGNETIC PROPERTIES	Hours: 09

Dielectric Properties: Basic definitions, electronic, ionic and orientation polarizations-qualitative; Internal field in solids.
Magnetic Properties: Basic definitions, origin of magnetic moment, Bohr magneton, classification of dia, para and ferro magnetic materials on the basis of magnetic moment, domain theory of ferro magnetism on the basis of hysteresis curve.

UNIT-II	LASERS	Hours: 09

Lasers: Characteristics of lasers, spontaneous and stimulated emission of radiation, metastable state, population inversion, lasing action, Einstein's coefficients, ruby laser, He-Ne laser, semiconductor diode laser and applications of lasers.

UNIT-III	NANOMATERIAL	Hours: 09

Nanomaterial: Origin of nanomaterial, nano scale, surface to volume ratio, quantum confinement, properties of nanomaterials: physical, chemical, electrical, optical, magnetic and mechanical;

Bottom-up fabrication: sol-gel; top-down fabrication: chemical vapour deposition; applications of nanomaterials, characterization by XRD, TEM.

UNIT-IV	QUANTUM MECHANICS	Hours: 09

Quantum mechanics: Waves and particles, De Broglie hypothesis, matter waves, Heisenberg's uncertainty principle, Davisson and Germer experiment, Schrodinger's time independent wave equation, physical significance of the wave function, infinite potential well and its extension to three dimensions.

UNIT-V	SEMICONDUCTOR PHYSICS	Hours: 09

Semiconductor physics: Fermi Level in intrinsic and extrinsic semiconductors, calculation of carrier concentration in intrinsic and extrinsic semiconductors, energy gap, direct and indirect band gap semiconductors, Hall Effect.

Text Books:

1. Dr. K. Vijaya Kumar, Dr. S. Chandralingam, "Modern Engineering Physics", S. Chand & Co. New Delhi, 1st Edition, 2010.
2. P. K. Palanisamy, "Engineering Physics", Scitech Publishers, 4th Edition, 2014.

Reference Books:

1. V. Rajendran, "Engineering Physics", Tata Mc Graw Hill Book Publishers, 1st Edition, 2010.
2. R. K. Gaur, S. L. Gupta, "Engineering Physics", Dhanpat Rai Publications, 8th Edition, 2001.
3. A. J. Dekker, "Solid State Physics", Macmillan India ltd, 1st Edition, 2000.
4. Hitendra K. Malik, A. K. Singh, "Engineering Physics", Mc Graw Hill Education, 1st Edition, 2009.

Web References:

1. http://link.springer.com/book
2. http://www.thphys.physics.ox.ac.uk
3. http://www.sciencedirect.com/science
4. http://www.e-booksdirectory.com

E-Text Books:

1. http://www.peaceone.net/basic/Feynman
2. http://physicsdatabase.com/free-physics-books
3. http://www.damtp.cam.ac.uk/user/tong/statphys/sp.pdf
4. http://www.freebookcentre.net/Physics/Solid-State-Physics-Books.html

INDEX

| Unit	Contents	Page
I	**DIELECTRIC AND MAGNETIC PROPERTIES**	**4**
II	**LASERS**	**24**
III	**NANOTECHNOLOGY**	**39**
IV	**QUANTUM MECHANICS**	**58**
V	**SEMICONDUCTOR PHYSICS**	**79**

UNIT-I
DIELECTRIC PROPERTIES

1.1 Introduction

- Dielectrics are insulating materials. In dielectrics, all electrons are bound to their parent molecules and there are no free charges.
- Even with normal voltage or thermal energy electrons are not released.
- Dielectrics are non metallic materials of high specific resistance and have negative temperature coefficient of resistance.
- Dielectrics are electrical insulators. They possess high resistivity values within the range 10^6 Ωm to 10^{16} Ωm. Under high voltage bias, they allow very little current. They with stand for very high voltages. The conduction is mostly associated with ionic motion through defects or hopping of charges. They have no free charges. The electrical properties of a dielectric are associated with inherent property of possessing electric dipoles.
- Dielectrics are the materials having electric dipole moment permanently or temporarily by applying electric field. These are mainly used to store electrical energy and as electrical insulators. All dielectrics are electrical insulators. But all electrical insulators need not be dielectrics. For example the vacuum is a perfect insulator. But it is not a dielectric. The study of dielectrics is essentially study of insulators.

1,2 Basic Definitions

Electric dipole

$$\mu = qr$$
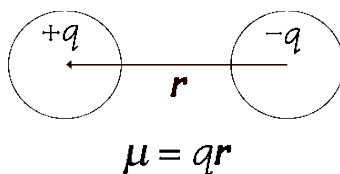
Fig. 1.1 Electric dipole

Two equal and opposite charges separated by a distance 'r' constitute a dipole.

Electric dipole moment (μ)

The product of charge and distance between two charges is called electric dipole moment.

$\mu = q \times r$

Units: coulomb - meter or Debye.

1 Debye = 3.33×10^{-30} coulomb - meter

4

Non-polar dielectrics

Mono atomic materials are made up of atoms. The centre of gravity of negative charge and the centre of gravity of positive charge of an atom coincide. That means even though there are two equal and opposite charges are not separated. Their dipole moment is zero.

$\because \mu = q \times r = q \times 0 = 0$

Such dielectrics are called Non- polar dielectrics.

Non-Polar Molecule

- Consider an atom. The positive charge of nucleus may be concentrated at a single point called as centre of gravity of the positive charge.
- The negative charge of electrons may be supposed to be concentrated at a single point called as Center of gravity of the positive charge.
- When the two centre of gravity coincide, the molecule is known as Non-polar molecule. The Non-polar molecules have symmetrical structure and zero electric dipole moment.
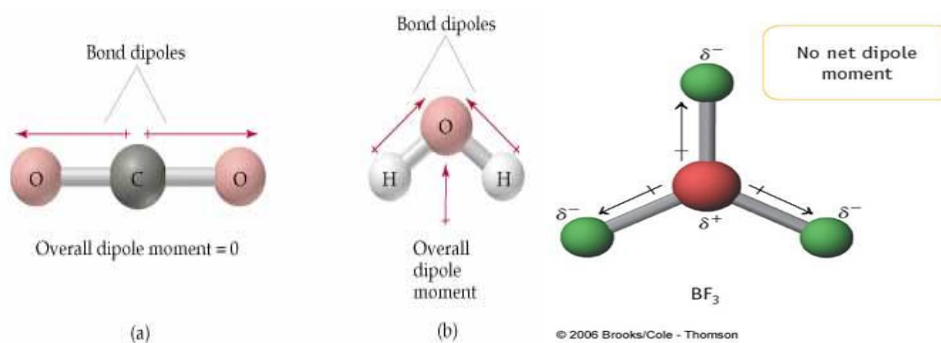- Examples: H_2, N_2, O_2, CO_2, Benzene.

Fig. 1.2 Non polar molecules with zero dipole moment ($\mu=0$)

- The electric dipole moment has a direction from positive charge to negative charge.

Polar dielectrics

- In polyatomic molecules, the center of gravity of negative charge distribution may not coincide with the center of positive charge distributions.
- There is an effective separation between centers of negative and positive charge distributions.
- The molecule has a net dipole moment. Such dielectrics are called Polar dielectrics.

Polar Molecules

They have unsymmetrical structure and have a permanent electric dipole moment.
The Center of gravity of positive and negative charges do not coincide, the
molecule is called as polar molecule.

e.g.:- H_2O, HCl, CO, N_2, NH_3 etc.

Fig.1.3 Polar molecules with net dipole moment ($\mu \neq 0$)

Dielectric constant ϵ_r (or) Relative permittivity of the medium

- It is the ratio between the permittivity of the medium and the permittivity of free
  space.

$\epsilon_r = \dfrac{\epsilon}{\epsilon_0}$. It has no units.

- Єr is also called as relative permittivity of the medium. It is a measure of
  polarization in the dielectric material.

$\epsilon_r = \epsilon_0 \epsilon_r$ where Є = absolute permittivity of the medium
Where Єo = permittivity of free space=8.854 x 10^{-12} F/m

Electric Polarization

When a dielectric substance is placed in an electric field, then positive and negative
charges are displaced in opposite direction.

- The displacement of charges produces local dipoles.
- This process of producing dipoles by the influence of electric field is called
  electric polarization.

$$\text{dielectric Polarization} = P = \frac{electric\ dipolemoment}{volume}$$

$$P = \frac{\mu}{V}$$

$$P = \frac{q \times l}{A \times l} = \frac{q}{A}$$

$$P = \frac{\text{charge}}{\text{area}} = \text{surface charge density 'σ'}$$

Polarizability (α)

The average dipole moment $\bar{\mu}$ is directly proportional to the electric field (E) applied.

$$\mu \; \alpha \; E$$
$$\mu \; = \; \propto \; E$$

$\propto$ = Polarizability = $\dfrac{\mu}{E}$ Farad/m^2

Polarization Vector (P)

It is defined as the average dipole moment per unit volume of a dielectric. If 'N' molecules are present per unit volume,

Then polarization vector $\vec{P} = \dfrac{N\bar{\mu}}{volume}$

$$\vec{P} = N \; \bar{\mu} \quad coulomb/m^2$$

Electric flux density (or) Electric displacement (D)

The number of electric lines of forces received by unit area is called Electric flux density.

$$D \; \alpha \; E$$
$$D = \epsilon E$$
$$\text{But } \epsilon = \epsilon_0 \; \epsilon_r$$
$$D = \epsilon_0 \; \epsilon_r \, E$$

Relation between Polarization (P), Electric field (E) & Dielectric constant ϵ_r

We know that electric flux density 'D' is written as

$$D = \epsilon \, E \qquad\qquad\qquad \rightarrow (1)$$

Where ϵ = absolute permittivity of medium

E = electric field

$$\text{Where} \quad E = \epsilon_0 \; \epsilon_r \qquad\qquad\qquad \rightarrow (2)$$

Hence substitute (2) in (1)

$$D = \epsilon_0 \; \epsilon_r \qquad\qquad\qquad \rightarrow (3)$$

Where $\quad \epsilon_0$ = permittivity of free space = 8.854 x10^{-12} F/m

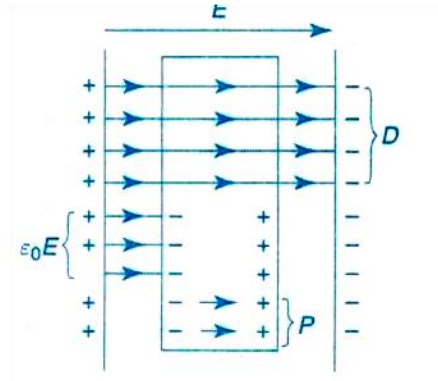ϵ_r = Dielectric constant or relative permittivity of the medium.

Fig. 1.4 Electric lines of forces in a polar dielectric

If 'P' is the polarization of the dielectric material due to the applied electric field (E), then the flux density 'D' is equal to the flux density in vacuum plus polarization of the material

$$\therefore D = \epsilon_0 E + P \qquad \rightarrow (4)$$

equating equations (3) & (4)

$$\epsilon_0 \epsilon_r E = \epsilon_0 E + P$$

$$P = \epsilon_0 E [\epsilon_r - 1]$$

$$P = \epsilon_0 \epsilon_r E - \epsilon_0 E \qquad \rightarrow (5)$$

Put $\qquad [\epsilon_r - 1] = \chi \qquad \rightarrow (6)$

Where χ = electric susceptibility

From equation (5) & (6)

$$\Rightarrow P = \epsilon_0 E \chi$$

$$\chi = \frac{P}{\epsilon_0 E} \qquad \rightarrow (7)$$

Conclusion:

$$\Rightarrow P = E [\epsilon_r - 1]$$

$$\chi = \epsilon_r - 1$$

$$\chi = \frac{P}{\epsilon_0 E}$$

Electric Susceptibility (χ)

The electric susceptibility 'χ' is defined as the ratio of polarization vector to the applied electric field 'E'.

$$\chi = P/\epsilon_0 E$$

χ has no units.

$$\Rightarrow P = \chi \epsilon_0 E$$

Where $\chi = \epsilon_r - 1$

8

Dielectric strength

It is defined as the minimum voltage required producing dielectric break down. Dielectric strength decreases with rising of temperature, humidity and age of the material.

1.3 Non-Polar Dielectric in an electric field

When a dielectric is placed in an electric field, say between the plates of a charged Condenser; the positive and negative charges are re oriented i.e. the center of gravity of positive charges is pulled towards the negative plate of the condenser and vice versa. Thus the net effect of the applied field is to separate the positive charges from the negative charges. This is known as Polarization of dielectric. The dielectrics which are polarized only when they are placed in an Electric field are called Non-polar dielectrics.
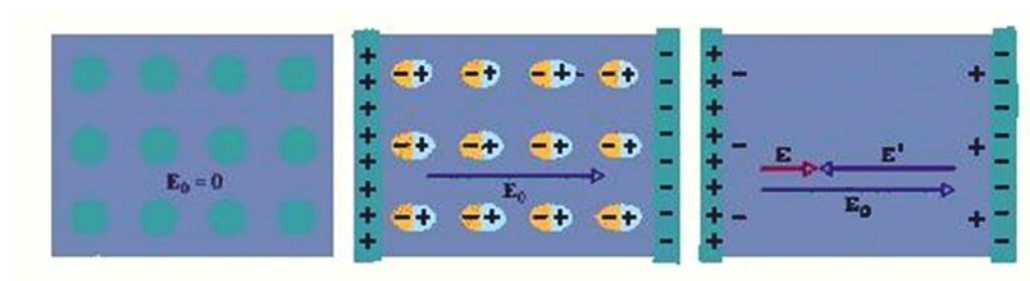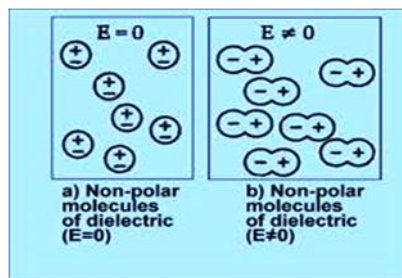

Fig. 1.5 (a) non polar dielectric in E=0 (b) Non polar dielectric when 'E' is applied
(c) Totally polarized non polar dielectric with net field

Thus if the dielectric is placed in an electric field, induced surface charges appear which tend to weaken the original field with in the dielectric. That means E^1 opposes the original field E_o.

1.4 Polar dielectric in electric field

We know that polar dielectric have permanent dipole moments with their random orientations. In the presence of an electric field, the partial alignment of dipoles takes place.
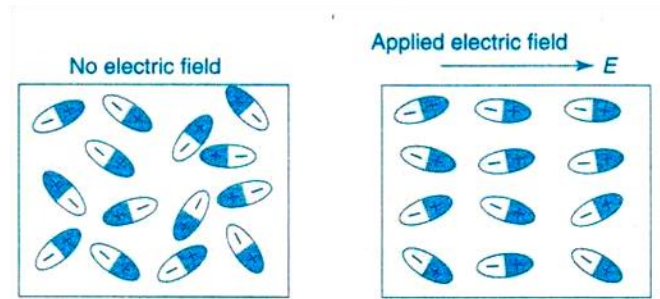
Fig. 1.6 Polar dielectric orientation without field and with field.

Polar dielectrics already possess some dipole moment inside due to the presence of permanent atomic dipoles. But these are randomly oriented when no field is applied. Their dipole moment and polarization increases since dipoles align along the field direction gives some extra polarization. Hence

P= { Polarization already Existing due to permanent dipoles } + { Polarization induced due to electric field }

$$P = P_p + P_i$$

1.5. The Local field (or) Internal field E_i (or) E_{local}

Definition: In dielectric solids, the atoms or molecules experienced not only the external applied electric field but also the electric field produced by the dipoles. Thus the resultant electric field acting on the atoms or molecules of dielectric substance is called the "Local field or an internal field."

Derivation:

Consider a dielectric material placed in an External field 'E_1', placed between the parallel plates of a capacitor. As a result opposite type of charges are induced on the surface of dielectric.
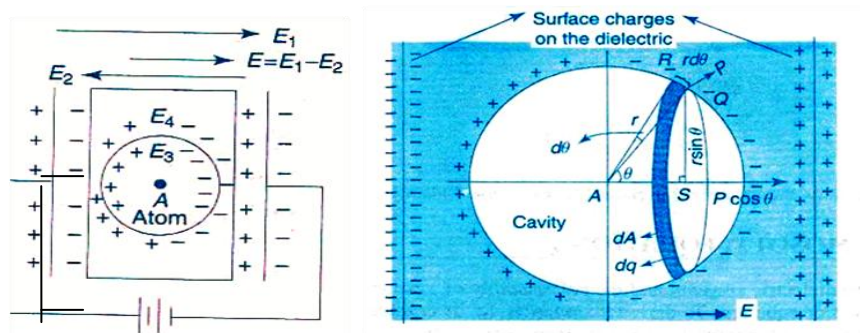

Fig.1.7 (a) Polar dielectric in electric field (b) Enlarged view of spherical cavity

Imagine a small spherical cavity of radius 'r'. In this sphere inside dipoles are present. Consider a dipole at the center of spherical cavity. This dipole experiences

10

the following fields, in addition to the externally applied field 'E_1'.
The total internal field experienced by the dipole

$$\text{E}_{\text{local}} = \text{E}_i = E_1 + E_2 + E_3 + E_4 \qquad \rightarrow (1)$$

Where E_1 = External applied field. Here,
   (a) The field 'E_2' produced by induced charges on the dielectric sample near the surface.
   (b) The field E_3 arising from dipoles inside the sphere. E_3depends on crystal symmetry. [For isotropic materials E_3=0]
   (c) The field E_4 is due to polarization of charges on the surface of spherical cavity. It is called the Lorentz cavity field.

The surface charge density on the surface of the spherical cavity is Pcosθ.
If 'ds' is the area of the surface element shaded in figure shown.
Then charge on the surface element (q_1) is
= (normal component of polarization) x (area of the surface element)
$$q_1 = (\text{Pcos }θ)\,(ds) \qquad \rightarrow (2)$$

Let a test charge q_2 = q placed at the center of cavity.
From coulombs' law, the force experienced between the surface charges.
$$dF = \frac{1}{4\pi}\frac{q_1 q_2}{r^2} dF = \frac{1}{4\pi\epsilon_0}\frac{(Pcosθds).q}{r^2}$$
$$\frac{dF}{q} = \left[\frac{1}{4\pi\epsilon o}\right]\left[\frac{Pcosθds}{r^2}\right] \qquad \rightarrow (3)$$

The resulting electric field $\qquad E_4 = \frac{dF}{q} = \left[\frac{1}{4\pi\epsilon o}\right]\left[\frac{Pcosθds}{r^2}\right] \qquad \rightarrow (4)$

The electric field is resolved into two components:
One component is along the direction of 'P' & other perpendicular to it.
The Perpendicular components cancel themselves out leaving only the horizontal components. Hence the sum of all such horizontal components of electric field for the whole Surface is:
$$E_4 = \int dE_4 cosθ = \int \frac{1}{4\pi\epsilon o}\frac{(Pcosθ)(cosθds)}{r^2} \qquad \rightarrow (5)$$
The surface area of the ring $\quad ds = 2\pi r^2 sinθdθ \qquad \rightarrow (6)$
Substitute (6) in (5)
$$E_4 = \frac{1}{4\pi\epsilon o}\int \frac{Pcos^2θ\,2\pi r^2 sinθdθ}{r^2}$$
Limits are θ = 0 to π
$$E_4 = \frac{P}{2\epsilon o}\int_0^\pi cos^2θdθ \qquad \rightarrow (7)$$
Let cosθ = z
-sindθ = dz & Limits are z = 1 to z = -1
Equation (7) becomes $E_4 = \frac{P}{2\epsilon o}\int_1^{-1} z^2\,(-dz)$

$$E_4 = \frac{-P}{2\epsilon_0} \int_{+1}^{-1} z^2 \, dz$$

$$= \frac{-P}{2\epsilon_o} \left[\frac{z^3}{3} \right]_{1}^{-1} = \frac{+P}{3\epsilon_o}$$

$$E_4 = \frac{P}{3\epsilon_o} \qquad\qquad \rightarrow (8)$$

Substitute the value of E_4 in equation (1)

Total internal field (or) local field

$$E_i = E_{loc} = E_1 + E_2 + E_3 + E_4$$

$$\text{Here } E_3 = 0$$

$$\therefore E_i = E_1 + E_2 + E_4$$

$$\text{Let } E_1 + E_2 = E$$

$$\implies \quad E_i = E + E_4$$

$$E_i = E + \frac{P}{3\epsilon_o}$$

1.7 Types of Polarization

Polarization is the process of inducing dipole moment in a molecule. There are four types of polarization. They are:

(1) Electronic Polarization

(2) Ionic Polarization

(3) Orientation (or) Dipolar Polarization

(4) Space charge polarization

1.7.1 Electronic Polarization:

Definition:

When an electric field is applied on a dielectric material then all the positive nuclei of atoms move in the field direction and all the negative electron cloud of atoms move in opposite directions, hence dipoles are formed to produce dipole moment.

- The electron cloud readily shifts towards the positive end of the field. The extent of shift by electrons is proportional to field strength.
- Hence dipole moment is the product of charge and shift distance.
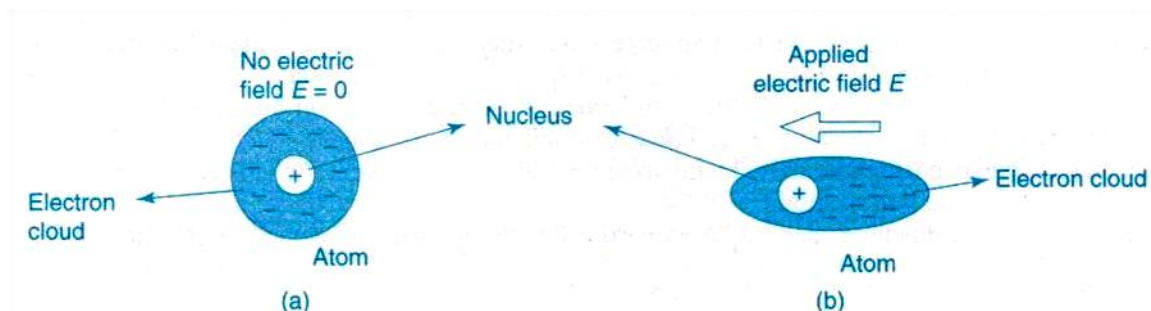
Expression for Electronic Polarizability α_e

12

- Consider an atom of dielectric material such that its atomic radius is 'R' & atomic number 'Z'. When no field is applied the charge centers of electron cloud and positive nucleus are at the same point & hence there is no dipole moment.
- Suppose an atom is placed in an electric field of strength E, due to Lorentz force the positive nucleus move towards the field direction and electron cloud will move in opposite direction of the field.
- When nucleus and electron cloud are displaced from their equilibrium positions, an attractive Coulomb force act between them to maintain original position. But Lorentz force will tend to separate them from them equilibrium position.
- When these forces are equal and opposite produces a net dipole moment.

Let the displacement between centers of nucleus and electron could be 'X'.
Let 'ze' is charge of nucleus.
'-ze' is charge of electron cloud in a sphere of radius 'R'.
$\Rightarrow$ The charge density due to negative electron cloud of radius R (E=0) is

$$\rho = \frac{(-ze)}{(\frac{4}{3}\pi r^3)}$$

$$\rho = \frac{-3}{4}\frac{ze}{\pi R^3} \qquad \rightarrow (1)$$

Lorentz force which tends to separate positive nucleus from negative electron cloud is

$$= (-ze)\ E \qquad \rightarrow (2)$$

Coulomb force which tends force of attraction between them is

$$\Rightarrow (ze)\ \frac{[\ charged\ enclosed\ in\ sphere\ of\ radius\ x]}{4\pi\epsilon_0 x^2} \qquad \rightarrow (3)$$

But the charge enclosed in the sphere of radius 'x' due to electrons of radius 'x'

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

$$= \frac{4}{3}\pi x^3 \left[\frac{-3}{4}\frac{ze}{\pi R^3}\right]\{from\ equation\ (1)\}$$

$$= \frac{-zex^3}{R^3} \qquad \rightarrow (4)$$

Substitute equation (4) in (3) we get

$$Coulomb\ force = \frac{(ze)\left[\frac{-zex^3}{R^3}\right]}{4\pi\epsilon_0 x^2}$$

$$Coulomb\ force = \frac{-z^2 e^2 x}{4\pi\epsilon_0 R^3} \qquad \rightarrow (5)$$

In equilibrium position coulomb & Lorentz forces are equal.

$\therefore$ Comparing equations (5) & (2) we get

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

Hence electron cloud displacement 'X' $= \left[\frac{4\pi\epsilon_0 R^3}{ze}\right]E \qquad \rightarrow (6)$

The two charges (+ze) of nucleus & (-ze) of electron cloud are displaced through 'X'.
Hence electric dipole moment is $\mu_e = |$ charge $| \times$(displacement)

13

$$= \lvert ze \rvert (X)$$
$$= (ze)\left(\frac{4\pi \epsilon_0 R^3}{ze}\right)E \quad [i.e \; from \; equation \; (6)]$$
$$\mu_e = (4\pi \epsilon_0 R^3)\, E \qquad\qquad\qquad \to (7)$$

We know that electronic polarizability

$$\alpha_e = \frac{dipole \; electric \; moment}{electric \; field}$$

$$\alpha_e = \frac{(4\pi R^3\,)E}{E} \quad [i.e \; from \; equation \; (7)]$$

$\Longrightarrow$ Electronic Polarisability $\quad \alpha_e = 4\pi \epsilon_0 R^3$

Where R= radius of an atom.

1.7.2 Ionic Polarization

Ionic polarization takes place in ionic dielectrics due to displacement of positive and negative ions by the influence of external electric field.

Expression for Ionic Polarisability

When an electron field is applied on an ionic dielectric then positive ions move in the field direction & negative ions move in opposite direction, hence dipoles will be formed. This phenomenon is known as ionic polarization.
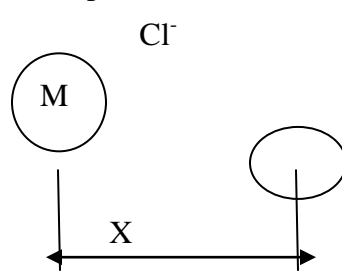
Fig. 1.9 (a) In the absence of field   *Fig. 5.9(b) when   field is applied*
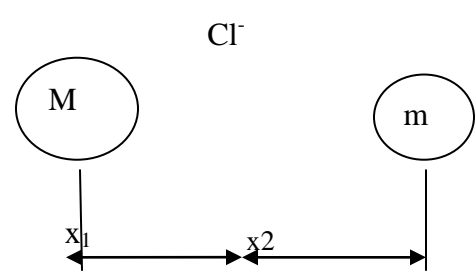
Let 'e' the charge of ions and M and m be the masses of negative and positive ions respectively. When an electric field 'E' is applied on an ionic dielectric then positive ions displaces in the field direction through x_1 distance and negative ion displaces in opposite direction through x_2 distance.

The induced dipole moment

$$\mu = \lvert charge \rvert \times displacement$$
$$\mu = \lvert e \rvert \, (x_1 + x_2) \qquad\qquad \to (1)$$

But against to the displacement of positive and negative ions, restoring force acts and opposes the displacements of cation and anion.

Under equilibrium conditions, the restoring force

$$F = k_1 x_1 \quad [\text{for negative ion}]$$
$$F = k_2 x_2 \quad [\text{for positive ion}]$$

$$\Rightarrow x_1 = \frac{F}{k_1}$$

$$x_2 = \frac{F}{k_2}$$

$$\rightarrow (2)$$

where k_1 k_2 are force constants

But

$$k_1 = M\omega_0^2$$
$$k_2 = m\omega_0^2$$

$$\rightarrow (3)$$

where ω_0= angular velocity of the ions

Substituting (3) in (2) we get

Hence $x_1 = \frac{F}{M\omega_0^2}$ & $x_2 = \frac{F}{m\omega_0^2}$

But F = e E

$$\Rightarrow x_1 = \frac{eE}{M\omega_0^2}$$

$$x_2 = \frac{eE}{m\omega_0^2}$$

$$\rightarrow (4)$$

Substituting equation (4) in equation (1)

$\Rightarrow$ Electric dipole moment

$$\mu = e[x_1 + x_2]$$

$$\mu = e\left[\frac{eE}{M\omega_0^2} + \frac{eE}{m\omega_0^2}\right]$$

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

$$\rightarrow (5)$$

We know that the Ionic Polarizability

$$\alpha_i = \frac{dipole\ moment}{electric\ field} = \frac{\mu}{E}$$

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

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

Here ω_0 = natural frequency of the ionic molecule.

1.7.3 Orientational Polarization

Definition:

When Electric field is applied on a polar dielectric then all the dipoles tend to rotate
In the field direction, hence dipole moment increases gradually. This phenomenon is
known as dipolar (or) orientational polarization.

Expression for Orientational (or) dipolar Polarisability

Orientation Polarisation takes place only in polar dielectrics in which dipoles orient in
random manner such that the net dipole moment is zero. When Electric field is
applied, all the dipoles try to rotate in the field direction as shown in the figure 5.10.

15
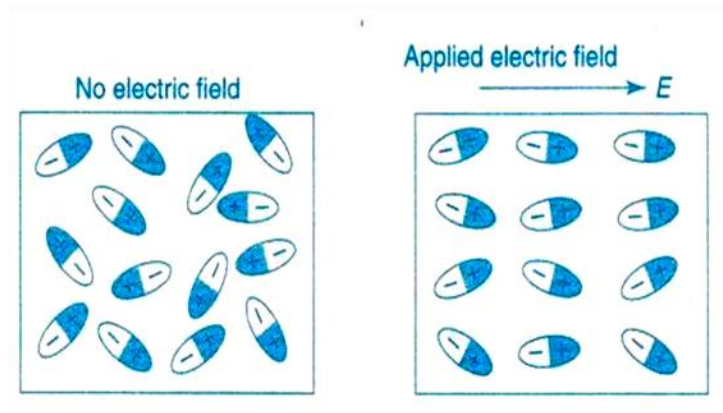
Fig. 1.10: Orientational polarization

To derive an expression for dipolar Polarisability of a system, we have to know the total dipole moment and total number of dipoles present in the system since

Average dipole moment $\mu = \dfrac{Total\ dipole\ moment}{Total\ number\ of\ dipoles}$

$$\alpha_0 E = \frac{\mu^2}{3K_B T}\, E$$

$$\alpha_d = \alpha_0 = \frac{\mu^2}{3K_B T}$$

α_0 = Orientational (or) dipolar polarisability

μ = dipole moment

K_B = Boltzmann constant

T = absolute temperature.

Note:

The total polarizability, $\alpha = \alpha_e + \alpha_i + \alpha_0$

$\alpha = \{4\pi \epsilon_0 R^3\} + \left\{\dfrac{e^2}{\omega_0^2}\left[\dfrac{1}{M} + \dfrac{1}{M}\right]\right\} + \left\{\dfrac{\mu^2}{3K_B T}\right\}$

MAGNETIC PROPERTIES

1.8 Introduction

- The magnetic effects in magnetic materials are due to atomic magnetic dipoles in the materials. These dipoles result from effective current loops of electrons in atomic orbits, from effects of electron spin & from the magnetic moments of atomic nuclei.

- The electric currents in an atom are caused by orbital and spin motions of electrons and those of its nucleus. Since all these motions of charged particles form closed electric currents, they are equivalent to "magnetic dipoles". When such dipoles are subjected to an external electric field, they experience a torque which tends to align their magnetic moments in the direction of the externally applied field.

1.9. Definitions

Magnetic dipole

Each tiny dimension of a magnetic material (or) atoms in magnetic materials is called magnetic dipole. This magnetic dipole produces magnetic moment depending on the alignment with respect to the applied magnetic field.

Magnetic flux (Φ)

It is defined as the amount of magnetic lines of forces passing perpendicularly through unit area of a given material. It is denoted by '**Φ**'

$$\Phi = AB$$

Where   A= Area of cross section of the material in m^2

B = magnetic Induction in Wb/ m^2

Units: Weber (Wb)

Intensity of Magnetization (M)

When a material is magnetized, it develops a net magnetic moment. The magnetic moment per unit volume is called Intensity of magnetization

$$\text{Magnetization (M)} = \frac{\text{Magnetic moment}}{\text{Volume}}$$

Units: Amp/m

Magnetic Induction (B)

Magnetic induction at a point is defined as the force experienced by a unit North Pole Placed at that point. It is denoted by 'B'

$$\text{i.e. B} = \frac{\Phi}{A} \text{ weber / } m^2$$

Magnetizing field strength (H)

When a medium is exposed to a magnetic field of intensity 'H', it causes an induction 'B' in the medium.

$$\text{i.e. } B \propto H$$
$$B = \mu H$$

17

Where μ = absolute permeability of the medium.
If the medium is air or vacuum

$$B = \mu_0 H$$

μ_0 = permeability of free space i.e. air or vacuum
$\mu_0 = 4\pi \times 10^{-7}$ H/m
Units for H: Amp /m.

Permeability (μ)

It indicates, with which the material allows magnetic lines of force to pass through it.

Or

It is the ability of the medium to pass magnetic lines of forces through it.
There are three Permeabilities i.e. μ_1, μ_0, μ_r

$$\mu = \mu_0 \, \mu_r$$

Where μ = Absolute permeability of the medium
μ_0 = Permeability of free space i.e. air or vaccum
μ_r = Relative permeability of the medium

Magnetic moment

Magnetic moment μ_m = (current) $\times$ (area of circulating orbit)

$$\mu_m = (I) \times (\pi r^2)$$

Units: Amp-m^2
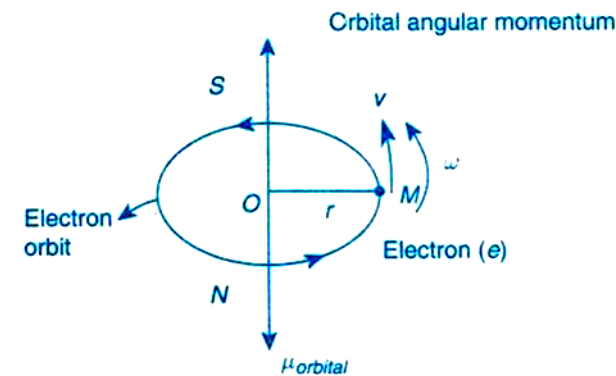
Fig.1.12 Revolving electron in an atom produces magnetic moment

When the magnetic dipoles (atoms consisting of charged particles like protons & neutrons) undergo orbital motion (or) spin motion produces a magnetic moment. Since motion of charged particles is considered as closed electric current loops which inturn produces a magnetic moment.

Relation between B, H, M

We know that

$$B = \mu H \qquad\qquad \rightarrow (1)$$

But $\quad \mu = \mu_0 \, \mu_r$

$$B = \mu_0\,\mu_r\,H$$

$$\rightarrow (2)$$

Adding &subtracting with $\mu_0 H$ on right hand side of equation (2)

$$B = [\mu_0\,\mu_r\,H] + \mu_0\,H - \mu_0\,H$$

$$= [\mu_0\,\mu_r\,H - \mu_0\,H] + \mu_0\,H$$

$$= \mu_0\,H\,[\mu_r - 1] + \mu_0 H$$

But $\quad\quad M = H\,[\mu_r\text{-}1]$ $\quad\quad\quad\quad \rightarrow (3)$

Now eq(3) becomes $\quad B = \mu_0 M + \mu_0 H$

$$B = \mu_0\,[H + M] \quad\quad\quad\quad \rightarrow (4)$$

Consider equation (3), $\quad\quad M = H\,[\mu_r\text{-}1]$

$$\frac{M}{H} = \mu_r - 1 \quad\quad\quad\quad \rightarrow (5)$$

But magnetic susceptibility $\quad \chi = \dfrac{M}{H}$

From equations (5) and (6)

$$\chi = \frac{M}{H} = \mu_r - 1$$

$$\mu_r = 1 + \chi$$

Magnetic susceptibility (χ)

If H is the applied magnetizing field intensity and M is the amount of magnetization of the material, Then $\chi = \dfrac{M}{H}$

$\chi = 0$ in vacuum

$\chi = $ +ve for paramagnetic and Ferro magnetic materials

$\chi = $ -ve for diamagnetic materials

Units:It has no units.

1.10. Origin of magnetic moment (Or) Sources of magnetic moment

In atoms, the permanent magnetic moment arises due to

a) Orbital motion of electrons and its magnetic moment is called orbit magnetic moment of electrons (μ_l)

b) The spin of electrons and its magnetic moment is called spin magnetic moment of electrons (μ_s)

c) The spin of nucleus (due to protons) and its magnetic moment is called spin magnetic moment of the nucleus. ($\mu_n\ or\ \mu_p$).

Explanation

a) Magnetic moment due to orbital motion of the electrons (μ_l)

Let us consider an electron of charge 'e' revolving around a nucleus in time period 'T' in a circular orbit of radius 'r'. Then a magnitude of circular current 'I' is given by

$$I = \frac{Charge}{Time} = \frac{e}{T} \quad\quad\quad\quad \rightarrow (1)$$

But $\quad\quad T = \dfrac{2\pi}{\omega}$

19

Where ω = angular velocity of electron

$$I = \frac{e\omega}{2\pi}$$

But magnetic moment of electron is $\mu_l = I \times A$

μ_l = current area of circulating orbit

$$\mu_l = \frac{e\omega}{2\pi}(\pi r^2)$$

$$\mu_l = \frac{e\omega r^2}{2} \qquad\qquad \rightarrow (2)$$
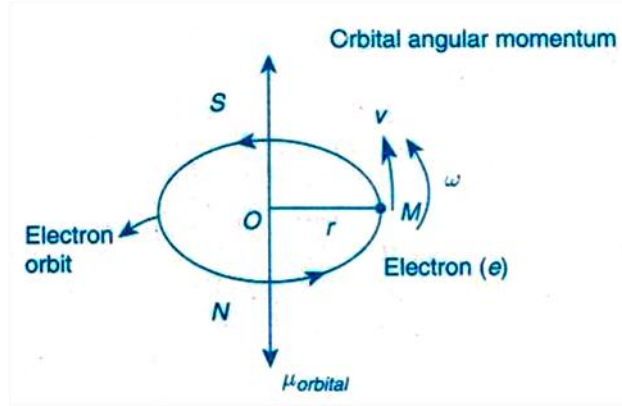
Fig. 1.13 Orbital magnetic moment of electrons

We know that angular momentum of any particle, $L = m\omega r^2$

Substituting eq.(4) in eq.(3) we get

Orbital magnetic moment, $\mu_l = (-\frac{e}{2m}).L \qquad\qquad \rightarrow (5)$

[-ve sign indicates μ_l and are in opposite directions]

$$\mu_l = (-\frac{e}{2m})\,L$$

But from Bohr's atomic model

$$mvr = \frac{nh}{2\pi}$$

$$L = \frac{lh}{2\pi} \qquad \text{Where } l = \text{orbital quantum number}$$

L = orbital angular momentum

The values of l = 0, 1, 2---------- (n-1)

$$\text{Hence } \mu_l = (-\frac{e}{2m})\,(\frac{lh}{2\pi})$$

$$\mu_l = -(\frac{eh}{4\pi m})\,l \qquad\qquad \rightarrow (6)$$

Where $\frac{eh}{4\pi m} = \mu_B$ is a constant called Bohr magneton and its value is 9.27×10^{-24} amp-m^2

Hence eq(6) becomes

$$\mu_l = l\,\mu_B \qquad\qquad \rightarrow (7)$$

Bohr magneton is the fundamental unit of magnetic moment.

It is clear from eq (7) that electron can take only certain specified values of magnetic moment depending on the value of 'l'.

Bohr suggested that both magnitude and direction of 'l' are quantified. It is known as "Spatial quantization".

The spatial quantization introduces a new set of quantum numbers.
(a) Orbital magnetic quantum number (m_l)
(b) Spin magnetic quantum number (m_s)

For example: If electron is in 'p' shell. Then n = 2, L= 0 to n-1, L = 0, 1,
If electron is placed in external magnetic field then eqn (6) can be written as

$$- \left(\frac{eh}{4\pi m}\right) m_l \qquad\qquad \rightarrow (8)$$

Hence for 'p' shell electron, m_l= 0 to ± L. The values are m_l = -1, 0, 1
Hence eqn (8) becomes

$$- \left(\frac{eh}{4\pi m}\right), 0, \left(\frac{eh}{4\pi m}\right)$$

Therefore we have "Three" possible orientations for electron in d-shell which is shown in the figure 6.3.

$m_l = -2$ A
$m_l = 1$ B
$m_l = 0$ C
$m_l = -1$ φ
$m_l = -2$ E
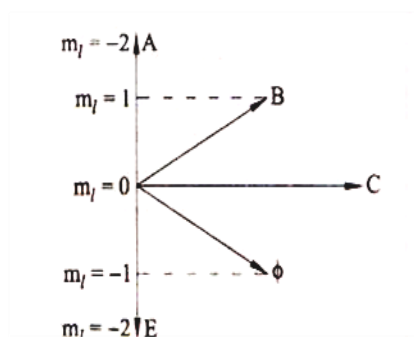
Fig. 1.13 The three possible orientations of electron

'OC' represents the orientation of electron if $m_l = 0$
'OB' represents the orientation of electron if $m_l = +1$
'OD' represents the orientation of electron if $m_l = -1$

b) Magnetic moment of electrons due to spin of electrons (μ_s)
According to quantum theory; electrons should have intrinsic angular momemtum due to spin. Spin is also quantized both in magnitude and direction spin can take only one value i.e ½ or - ½. The magnetic moment produced due to spin of electrons is called spin magnetic moment (μ_s).
It is given by

$$\text{Spin magnetic moment } \mu_s = -2\left(\frac{e}{2m}\right) S \qquad\qquad \rightarrow (9)$$

Where S=spin angular momentum, e = charge of electron, m = mass of electron

$$S = \frac{sh}{2\pi}$$

where S = spin quantum number
    h = Planck's constant.
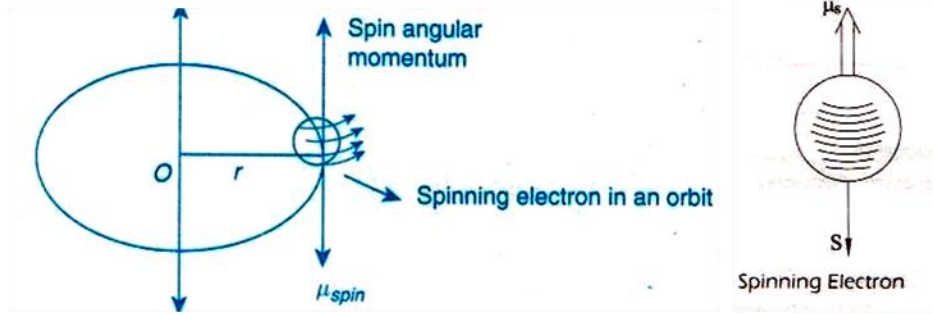
Fig. 1.14 Spin magnetic moment of electrons

From equation (9), $\mu_s = -2(\frac{e}{2m})$ S

Since $S = \frac{sh}{2\pi}$

$\mu_s = -2(\frac{e}{2m})(\frac{sh}{2\pi})$

$s = \pm\frac{1}{2}$, $\mu_s = \pm \frac{eh}{4\pi m}$

$\mu_s = \frac{eh}{4\pi m}, -\frac{eh}{4\pi m}$

$\mu_s = +\mu_B, -\mu_B$

Hence spin magnetic moment of electron is equal to μ_B. That is one Bohr magneton

Hence there are two possible orientations of electron.

Conclusion: Para magnetism, Ferro magnetism is due to spin magnetic moment.

Diamagnetism is due to orbital magnetic moment.

(c) Magnetic moment due to Nuclear spin or spin of all protons (μ_n)

The magnetic moment of the nucleus is given by $\mu_n = \frac{eh}{4\pi m_p}$ $\rightarrow$ (10)

Where m_p= mass of proton

The constant $\frac{eh}{4\pi m_p}$ is called nuclear magneton.

The value of nuclear magneton $\frac{eh}{4\pi m_p} = 5 \times 10^{-27}$ A-m^2
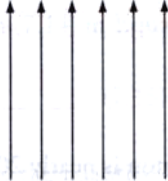
This is small when compared to Bohr magneton.

1.11. Classification of Magnetic Materials

Magnetic materials are classified as follows:

a) Diamagnetic
b) Paramagnetic
c) Ferro magnetic

Diamagnetic materials	Paramagnetic materials	Ferromagnetic materials
1.Diamagnetism: It is the property of the material which has repulsive nature (or) opposing magnetization	*1.Paramagnetism:* It is the property of the material which has weak attractive force.	*1.Ferromagnetism* It is property of the material which has strong attractive force
2.The property is due to orbital motion of electrons	2.The property is due to spin of electrons	2.The property is due to spin of electrons
3.There is no spin	3.Spin is random	3.Spin is parallel
4. These materials are lack of magnetic dipoles	4.These materials have permanent dipoles	4.They have permanent magnetic dipoles
5. They do not possess permanent dipole magnetic moment (it is zero). Hence spontaneous magnetization is zero.	5. They possess permanent magnetic dipole moment. But there is no spontaneous magnetization in the absence of external field. Due to random spin.	5. They possess permanent magnetic dipole moment. Also in the absence of field they have spontaneous magnetization even in the absence of external field due to parallel

UNIT - II

LASERS

2.1 Introduction

LASER stands for light amplification by stimulated emission of radiation. It is different from conventional light (such as tube light or electric bulb), there is no coordination among different atoms emitting radiation. Laser is a device that emits light (electromagnetic radiation) through a process is called stimulated emission.

2.2 Spontaneous and stimulated emission

In lasers, the interaction between matter and light is of three different types. They are: absorption, spontaneous emission and stimulates emission .Let E_1 and E_2 be ground and excited states of an atom. The dot represents an atom. Transition between these states involves absorption and emission of a photon of energy $E_2-E_1=h\nu_{12}$. Where 'h' is Planck's constant.

(a) Absorption: As shown in fig8.1(a), if a photon of energy $h\nu_{12}(E_2-E_1)$ collides with an atom present in the ground state of energy E_1 then the atom completely absorbs the incident photon and makes transition to excited state E_2.

(b) Spontaneous emission: As shown in fig8. 1. (b), an atom initially present in the excited state makes transition voluntarily on its own. Without any aid of external stimulus or an   agency to the ground. State and emits a photon of energy h ν_{12}(=E_2-E_1).this is called spontaneous emission. These are incoherent.

(c) Stimulated emission: As shown in fig8.1.(c), a photon having energy $h\nu_{12}(E_2-E_1)$impinges on an atom present in the excited state and the atom is stimulated to make transition to the ground state and gives off a photon of energy $h\nu_{12}$. The emitted photon is in phase with the incident photon. These are coherent. This type of emission is known as stimulated emission.
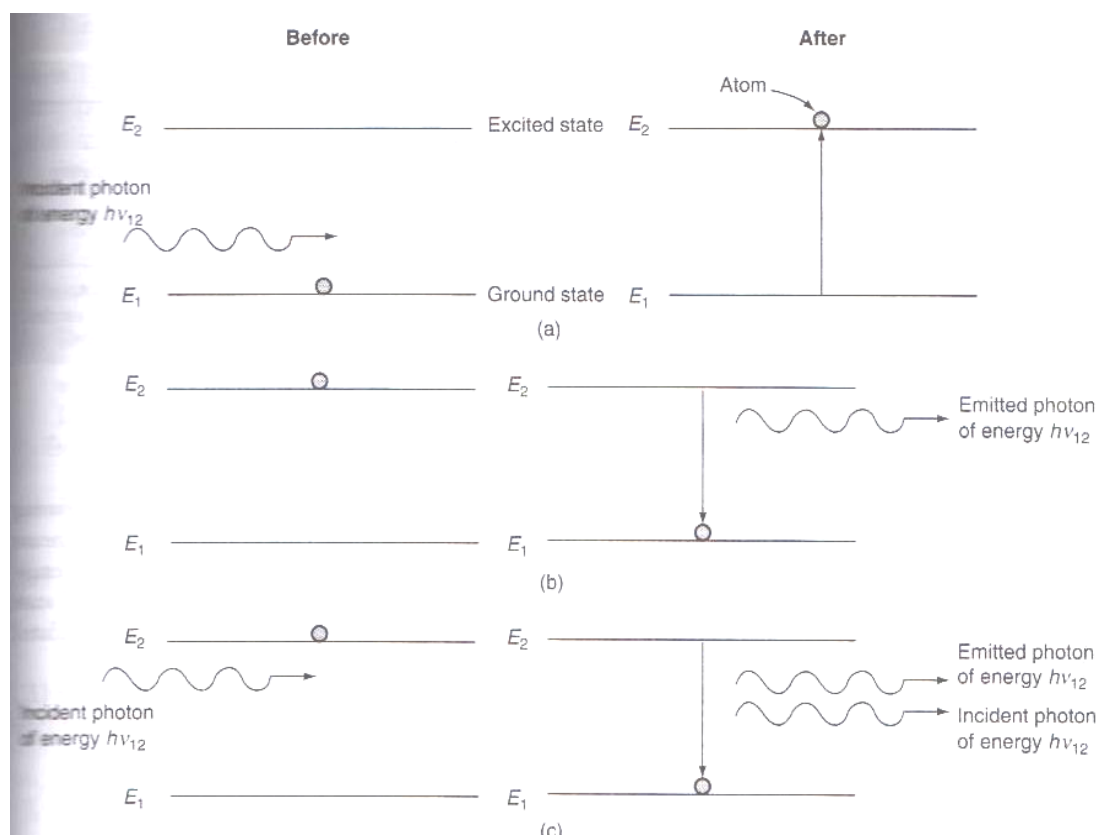
Fig.2.1 (a) Absorption ;(b) Spontaneous emission;(c) Stimulated emission

Differences between Spontaneous emission and stimulated emission of radiation

Spontaneous emission	Stimulated emission
1. Polychromatic radiation	1. Monochromatic radiation
2. Less intensity	2. High intensity
3. Less directionality, more angular spread during propagation	3. High directionality, so less angular spread during propagation.
4. Spatially and temporally in coherent radiation	4. Specially and temporally coherent radiation.
5. Spontaneous emission takes place when excited atoms make a transition to lower energy level voluntarily without any external stimulation.	5. Stimulated emission takes place when a photon of energy equal to h v_{12} (=E_2-E_1) stimulates an excited atom to make transition to lower energy level.

2.3 Characteristics of Laser Light

(i). Coherence: Coherence is one of the unique properties of laser light. It arises from the stimulated emission process. Since a common stimulus triggers the emission events which provide the amplified light, the emitted photons are in step and have a definite

25

phase relation to each other. This coherence is described in terms of temporal and spatial coherence.

(ii). Monochromaticity: A laser beam is more or less in single wave length. I.e. the line width of laser beams is extremely narrow. The wavelengths spread of conventional light sources is usually 1 in 10^6, where as in case of laser light it will be 1 in 10^5.I.e. if the frequency of radiation is 10^{15} Hz., then the width of line will be 1 Hz. So, laser radiation is said to be highly monochromatic. The degree of non-monochromaticity has been expressed as

$\xi = (d\lambda/\lambda) = d\nu/\nu$, where $d\lambda$ or $d\nu$ is the variation in wavelength or variation in frequency of radiation.

(iii) Directionality: Laser beam is highly directional because laser emits light only in one direction. It can travel very long distances without divergence. The directionality of a laser beam has been expressed in terms of divergence. Suppose r_1 and r_2 are the radii of laser beam at distances D_1 and D_2 from a laser, and then we have.

Then the divergence, $\Delta\theta = (r_1 - r_2)/ D_2 - D_1$

The divergence for a laser beam is 0.01 mille radian where as incase of search light it is 0.5 radian.

(iv) High intensity: In a laser beam lot of energy is concentrated in a small region. This concentration of energy exists both spatially and spectrally, hence there is enormous intensity for laser beam. The power range of laser is about 10^{-13} w for gas laser and is about 10^9 w for pulsed solid state laser and the diameter of the laser beam is about 1 mm. then the number of photons coming out from a laser per second per unit area is given by

$$N_1 = P/ h\nu\pi r^2 \approx 1022 \text{ to } 1034 \text{ photons/m}^{-2}\text{-sec}$$

By assuming $h\nu = 10^{-19}$ Joule, Power $P = 10^{-3}$ to 10^9 watt $\quad$ r=0.5×10^{-3} meter

Based on Planck's black body radiation, the number of photons emitted per second per unit area by a body with temperature T is given by

$$N_{th} = (2h\pi C/ \lambda^4) (1/e^{(h\nu/k T)}-1) \, d\lambda \approx 10^{16} \text{photons/m}^2.\text{sec}$$
$$\text{By assuming } T=1000k, \lambda=6000A^0$$

This comparison shows that laser is a highly intensive beam.

2.4. Einstein's Coefficients

Let N_1 be the number of atoms per unit volume with energy E_1 and N_2 the number of atoms per unit volume with energy E_2. Let 'n' be the number of photons per unit volume at frequency ν such that $h\nu = E_2 - E_1$. Then the energy density of interacting photons $\rho(\nu)$ is given by

$$\rho(\nu) = n \, h \, \nu \qquad\qquad\qquad \rightarrow(1)$$

When these photons interact with atoms, both upward (absorption) and downward (emission) transitions occur. At equilibrium these transition rates must be equal.

Upward Transition

Stimulated absorption rate depends on the number of atoms available in the lower energy state for absorption of these photons as well as the energy density of interacting radiation. I.e. stimulated absorption rate $\alpha \, N_1$

$$\alpha \, \rho(\nu)$$
$$= B_{12} N_1 \, \rho(\nu) \qquad\qquad\qquad \rightarrow (2)$$

Where the constant of proportionality B_{12} is the Einstein coefficient of stimulated absorption

Downward transition

Once the atoms are excited by stimulated absorption, they stay in the excited state for a short duration of time called the lifetime of the excited state. After their life time they move to their lower energy level spontaneous by emitting photons. This spontaneous emission rate depends on the number of atoms in the excited energy state.

i.e., spontaneous emission rate α N_2

$$= N_2 A_{21} \qquad \rightarrow (3)$$

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

Stimulated emission

Before excited atoms de excites to their lower energy states by spontaneous emission they may interact with photons resulting in stimulated emission of photons. Therefore stimulated emission rate depends on the number of atoms available in the excited state as well as energy density of interacting photons

I.e. stimulated emission rate α N_2

$$\alpha \, \rho(v)$$
$$= N_2 \rho(v) B_{21} \qquad \rightarrow (4)$$

Where the constant of proportionality B_{21} is the Einstein coefficient of stimulated emission.

During stimulated emission, the interacting photon called the stimulating photon and the photon due to stimulated emission are in phase with each other. Please note that during stimulated absorption, the photon density decreases where as during stimulated emission it increases.

For a system in equilibrium, the upward and down word transition rates must be equal and hence we have

$$N_1 \rho(v) B_{12} = N_2 \rho(v) B_{21} + N_2 A_{21} \qquad \rightarrow (5)$$

Hence
$$\rho(v) = \frac{N_2 A_{21}}{N_1 B_{12} - N_1 B_{21}} \rightarrow (6)$$

$$\rho(v) = \frac{A_{21}/B_{21}}{\left(B_{12}/B_{21}\right)\left(N_1/N_2\right) - 1}$$

The population of various energy levels in thermal equilibrium is given by Boltzmann distribution law.
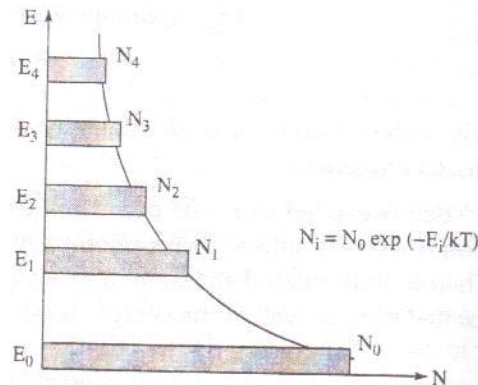

Fig.2.2 Boltzmann distribution for several energy levels

27

$$N_i = g_i N_o \exp(-E_i/KT)$$

Where N_i is the population density of the energy level E_i, N_0 is the population density of the ground state at temperature T_1, g_i is the degeneracy of the ith level and k is the Boltzmann constant $(=1.38 \times 10^{-23}$ joule/k). The concept of degeneracy occurs since more than one level has the same energy.

$$\text{Hence } N_1 = g_1 N_o \exp(-E_1/kT)$$

$$\frac{N_1}{N_2} = \frac{g_1}{g_2} \exp\left[\frac{(E_2 - E_1)}{kT}\right]$$

$$= \frac{g_1}{g_2} \exp\left[\frac{h\nu}{kT}\right] \qquad \rightarrow (7)$$

Substituting e q (6) in e q (4) $\rho(\nu) = \dfrac{[A_{21}/B_{21}]}{\left[\frac{B_{12}}{B_{21}}\frac{g_1}{g_2}\exp[\frac{h\nu}{kT}]\right]}$ $\qquad \rightarrow (8)$

From Planck's law of blackbody radiation, the radiation density is given by

$$\rho(\nu) = \frac{8\pi h\nu^3}{C^3} \frac{1}{\exp\left[\frac{h\nu}{kT}\right] - 1} \qquad \rightarrow (9)$$

Comparing equations (8) and (9), we get

$$\frac{B_{12}}{B_{21}} \frac{g_1}{g_2} = 1$$

$$g_1 B_{12} = g_2 B_{21}$$

$$\rightarrow (10)$$

And $\quad \dfrac{A_{21}}{B_{21}} = \dfrac{8\pi h\nu^3}{C^3}$ $\qquad \rightarrow (11)$

Equation's (10) and (11) are referred to as the Einstein relations.

The ratio of spontaneous emission rate to the stimulated emission rate is given by

$$R = \frac{N_2 A_{21}}{N_2 \rho(\nu) B_{21}} = \frac{A_{21}}{\rho(\nu) B_{21}}$$

From equation (9)

$$R = \frac{A_{21}}{\rho(\nu) B_{21}} = \left[exp^{\left[\frac{h\nu}{kT}\right]} - 1\right] \qquad \rightarrow (12)$$

In practice, the absorption and emission phase occur simultaneously. Let us calculate the rates of spontaneous emission and stimulating emission for a tungsten filament lamp operating at a temperature of 2000k. Taking the average frequency to be 5×10^{14} Hz, this ratio is

$$R = e^{\frac{(6.6 \times 10^{-34}) \times (5 \times 10^{14})}{(1.38 \times 10^{-23} \times 2000)}} - 1 \qquad \rightarrow (13)$$

This confirms that under conditions of thermal equilibrium, even for sources operating at higher temperatures and lower frequencies, spontaneous emission predominates.

From equation (12), we understand that to make R smaller $\rho(\nu)$ the energy density of interacting radiation has to be made larger. Let us consider the relation of stimulated emission rate to stimulated absorption rate

Thus at thermal equilibrium stimulated absorption predominates over stimulated emission. Instead if we create a situation that $N_2 > N_1$. Stimulated emission will predominate over stimulated absorption. If stimulated emission predominates the photon density increases and light amplifies the photon density increases and light amplification by stimulated emission of radiation (LASER) occurs. Therefore, in order to achieve more

28

stimulated emission, population of the excited state (N_2) should be made larger than the population of the lower state (N_1) and this condition is called population inversion. Hence if we wish to amplify a beam of light by stimulated emission, then we must create population inversion and increase the energy density of interacting radiation.

2.4.1 Population inversion

Usually in a system the number of atoms (N_1) present in the ground state (E_1) is larger than the number of atoms (N_2) present in the higher energy state. The process of making $N_2 > N_1$ called population inversion. Conditions for population inversion are:

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

Population inversion can be achieved by a number of ways. Some of them are (i) optical pumping (ii) electrical discharge (iii) inelastic collision of atoms (iv) chemical reaction and (v) direct conversion

2.5 Helium-Neon gas laser

Helium-Neon gas laser is a continuous four level gas laser. It consists of a long, narrow cylindrical tube made up of fused quartz. The diameter of the tube will vary from 2 to 8 mm and length will vary from 10 to 100 cm. The tube is filled with helium and neon gases in the ratio of 10:1. The partial pressure of helium gas is 1mm of Hg and neon gas is 0.1mm of Hg so that the pressure of the mixture of gases inside the tube is nearly 1 mm of Hg.

Laser action is due to the neon atoms. Helium is used for selective pumping of neon atoms to upper energy levels. Two electrodes are fixed near the ends of the tube to pass electric discharge through the gas. Two optically plane mirrors are fixed at the two ends of the tube at Brewster angle normal to its axis. One of the mirrors is fully silvered so that nearly 100% reflection takes place and the other is partially silvered so that 1% of the light incident on it will be transmitted. Optical resources column is formed between these mirrors.

Fig.2.3 Helium-Neon gas laser

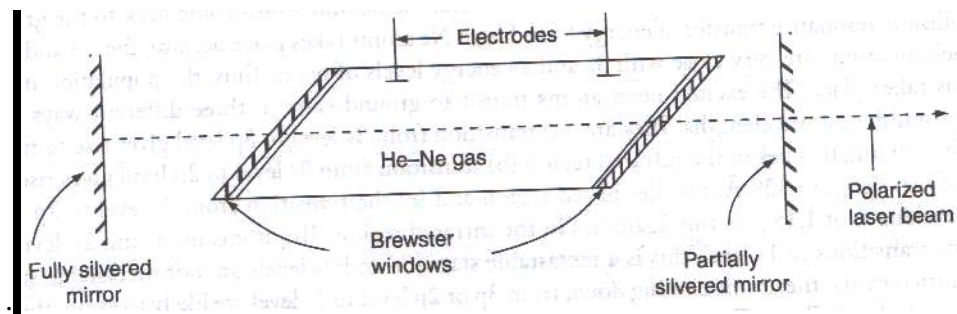**Working**

When a discharge is passed through the gaseous mixture, electrons are accelerated down the tube. These accelerated electrons collide with the helium atoms and excite them to higher energy levels. The different energy levels of Helium atoms and Neon atoms is shown in fig.2.3 the helium atoms are excited to the levels F_2 and F_3 these levels happen to be meta stable energy states.

Energy levels and hence Helium atoms exited levels spend sufficiently large amount of time before getting de excited. As shown in the fig 2.5(a), some of the excited states of neon can correspond approximately to the same energy of excited levels F_2 and F_3. Thus, when Helium atoms in level F_2 and F_3 collide with Neon atoms in the ground level E_1, an energy exchange takes place. This results in the excitation of Neon atoms to the levels E_4 and E_6 and de excitation of Helium atoms to the ground level (F_1). Because of long life times of the atoms in levels F_2 and F_3, this process of energy transfer has a high probability. Thus the discharge through the gas mixture continuously populates the neon atoms in the excited energy levels E_4 and E_6. This helps to create a state of population inversion between the levels E_4 (E_6) to the lower energy level (E_3 and E_5). The various transitions $E_6 \rightarrow E_5$, $E4 \rightarrow E_3$, $E_6 \rightarrow E_3$ leads to the emission of wave lengths 3.39mm, 1.15 um and 6328 A^0. Specific frequency selection may be obtained by employing mirrors

The excited Neon atoms drop down from the level E_3 to the E_2 by spontaneously emitting a photon around wavelength 6000A^0. The pressures of the two gases in the mixture are so chosen that there is an effective transfer of energy from the Helium to the Neon atoms. Since the level E_2 is a meta stable state, there is a finite probability of the excitation of Neon, atoms from E_2 to E_3 leading to population inversion, when a narrow tube is used, the neon atoms in the level E_2 collide with the walls of the tube and get excited to the level E_1. The transition from E_5 to E_3 may be non radioactive. The typical power outputs of He-Ne laser lie between 1 and 50 mw of continuous wave for inputs of 5-10W.
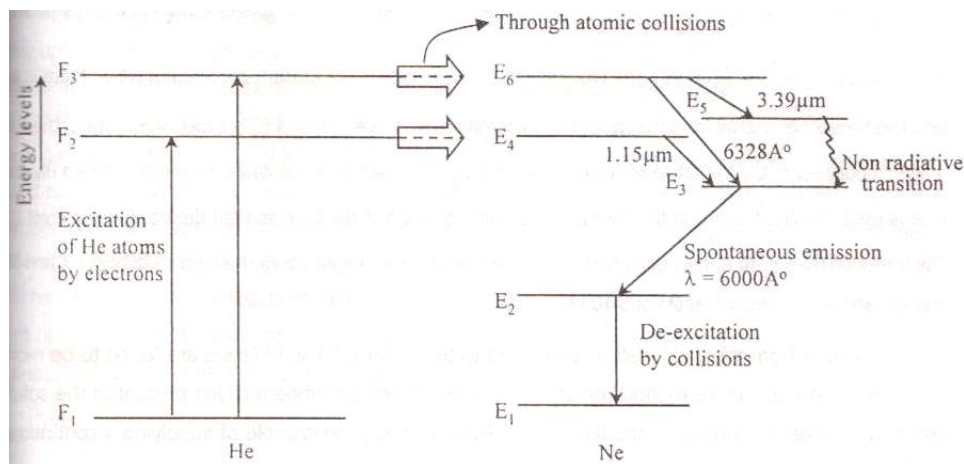
Fig.2.4. Energy level diagram of He-Ne atoms.

2.6 Ruby Laser

Ruby Laser is a solid state pulsed, three level lasers. It consists of a cylindrical shaped ruby crystal rod of length varying from 2 to 20cms and diameter varying 0.1 to 2cms. This end faces of the rod are highly flat and parallel. One of the faces is highly silvered and the other face is partially silvered so that it transmits 10 to 25% of incident light and reflects the rest so as to make the rod-resonant cavity. Basically, ruby crystal is aluminum oxide [Al_2O_3] doped with 0.05 to 0.5% of chromium atom. These chromium atoms serve as activators. Due to presence of 0.05% of chromium, the ruby crystal

appears in pink color. The ruby crystal is placed along the axis of a helical xenon or krypton flash lamp of high intensity.
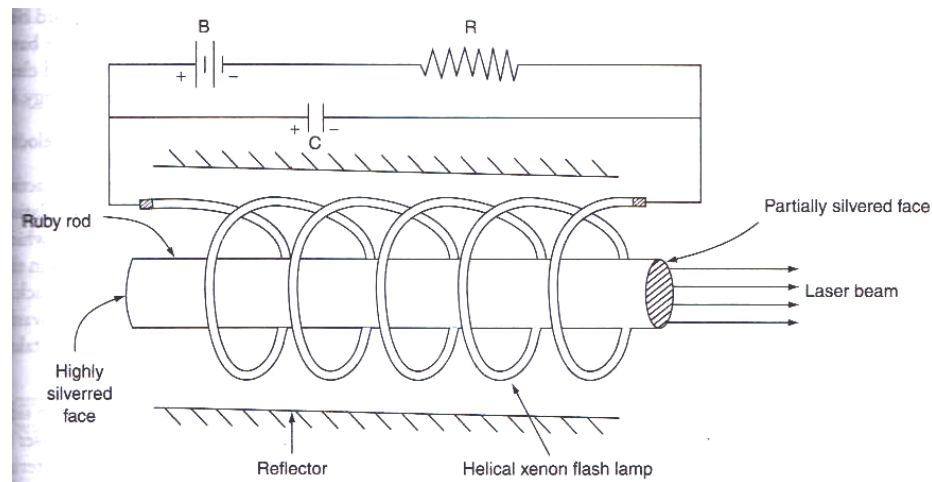
Fig.2.5 Ruby laser
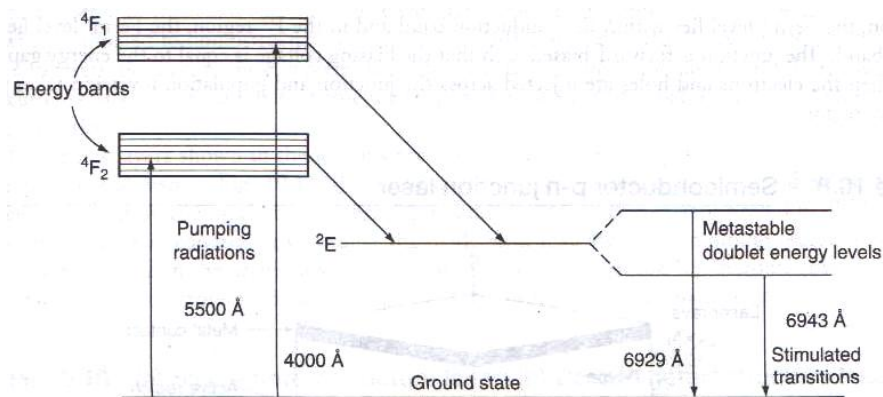
Fig.2.6 Energy level diagram of chromium ions in a ruby crystal

Construction:

Ruby ($Al_2O_3+Cr_2O_3$) is a crystal of Aluminum oxide in which some of Al^{+3} ions are replaced by Cr^{+3} ions. When the doping concentration of Cr^{+3} is about 0.05%, the color of the rod becomes pink. The active medium in ruby rod is Cr^{+3} ions. In ruby laser a rod of 4cm long and 5mm diameter is used and the ends of the rod are highly polished. Both ends are silvered such that one end is fully reflecting and the other end is partially reflecting.

The ruby rod is surrounded by helical xenon flash lamp tube which provides the optical pumping to raise the Chromium ions to upper energy level (rather energy band). The xenon flash lamp tube which emits intense pulses lasts only few milliseconds and the tube consumes several thousands of joules of energy. Only a part of this energy is used in pumping Chromium ions while the rest goes as heat to the apparatus which should be cooled with cooling arrangements as shown in fig.2.5. The energy level diagram of ruby laser is shown in fig.2.6

Working:

   Ruby crystal is made up of aluminum oxide as host lattice with small percentage of Chromium ions replacing aluminum ions in the crystal chromium acts as do pant. A do pant actually produces lasing action while the host material sustains this action. The pumping source for ruby material is xenon flash lamp which will be operated by some external power supply. Chromium ions will respond to this flash light having wavelength of $5600A^0$. When the Cr^{+3} ions are excited to energy level E_3 from E_1 the population in E_3 increases. Chromium ions stay here for a very short time of the order of 10-8 seconds then they drop to the level E_2 which is mat stable state of life time 10^{-3}s. Here the level E_3 is rather a band, which helps the pumping to be more effective. The transitions from E_3 to E_2 are non-radioactive in nature. During this process heat is given to crystal lattice. Hence cooling the rod is an essential feature in this method. The life time in mete stable state is 10^5 times greater than the lifetime in E_3. As the life of the state E_2 is much longer, the number of ions in this state goes on increasing while ions. In this state goes on increasing while in the ground state (E_1) goes on decreasing. By this process population inversion is achieved between the exited Meta stable state E_2 and the ground state E_1. When an excited ion passes spontaneously from the metastable state E_2 to the ground state E_1, it emits a photon of wave length $6943A^0$. This photon travels through the rod and if it is moving parallel to the axis of the crystal, is reflected back and forth by the silvered ends until it stimulates an excited ion in E_2 and causes it to emit fresh photon in phase with the earlier photon. This stimulated transition triggers the laser transition. This process is repeated again and again because the photons repeatedly move along the crystal being reflected from its ends. The photons thus get multiplied. When the photon beam becomes   sufficiently intense, such that part of it emerges through the partially silvered end of the crystal.

Drawbacks of ruby laser:
1. The laser requires high pumping power to achieve population inversion.
2. It is a pulsed laser.
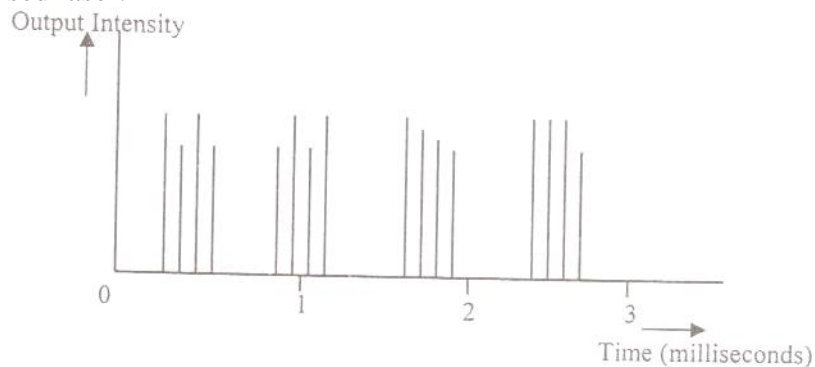
.   *Fig.2.7 the output pulses with time.*

2.7 Semi conductor laser

   The semiconductor laser is also called diode laser. Among the different semiconductors there are direct band gap semiconductors and indirect band gap semiconductors. In the case of direct band gap semiconductors, there is a large possibility for direct recombination of holes and electrons which emit photons. But in indirect band gap semi conductors like silicon and germanium, direct recombination

of holes and electrons is less possible and hence there is no effective emission of photons. A well know example of a direct band gap semiconductor is GaAs. Let E g be the energy gap of a material, then it emits a photon of wavelength (λ) is given the relation

$$\lambda = \frac{Ch}{E_g} \qquad \qquad \rightarrow (1)$$

Where C is the velocity of light and h is the Planck's constant
The equation (1) is reduced to

$$\lambda = \frac{1.24}{E_g}\ \mu m \qquad \qquad \rightarrow (2)$$

Where E_g is expressed in eV

As E_g increases, it emits shorter wavelengths. Diode lasers are always operated in forward bias. If p and n type materials are prepared from the same material then the p-n junction, is called as Homo junction semiconductor laser source. If p and n type materials are prepared from different materials then they are called as Hetero junction semi conductor laser source.

Construction of GaAs Semiconductor diode laser

The basic mechanism responsible for light emission from a semi conductor is the recombination of electrons and holes at p-n junction when a current is passed through the diode. The active medium is a p-n junction diode made from crystalline Gallium Arsenide . The p-region and n-region in the diode are obtained by heavily doping with suitable do pants. At the junction the sides through which emitted light is coming out are well polished and parallel to each other. Since the refractive index of GaAs is high, the reflectance at the material air interface is sufficiently large so that the external mirrors are not necessary to produce multiple reflections. When a current is passed through a p-n junction p region being positively biased, holes are injected from p-region into n-region and n-region being negatively biased electrons are injected from n-region into p-region and is shown in fig8.9.
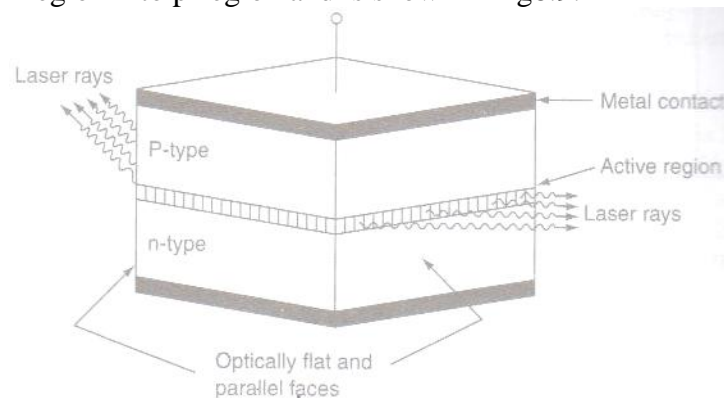
Fig.2.8 GaAs semiconductor diode laser

The connections in this p-n junction circuit are called forward bias. The electrons and holes recombine and release of light energy takes place in or near the junction. In the case of GaAs homo junction which has an energy gap of 1.44ev gives a laser beam of wavelength around $8600A^0$ the electron-hole recombination takes place in the active region of the device. When the junction is forward biased, a large amount of the order of 104 amp/cm^2 is passed through the narrow junction. Thus the electrons (holes) are

injected from n side to p side (p side to n side) respectively.
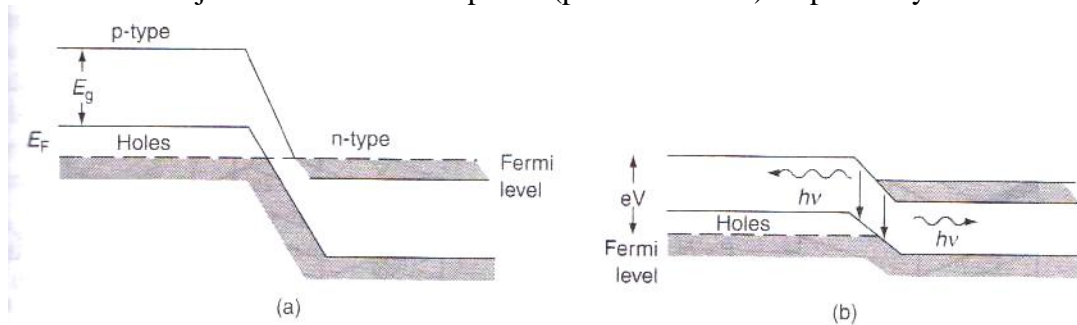
Fi2.9 (a) Band diagram of heavily doped p-n junction in equilibrium.
(b) Band diagram of heavily doped p-n junction with forward bias

The electrons are minority charge carriers in p-side and holes are the minority charge carriers in n-side. The continuous injection of charge carriers creates the population inversion of minority carriers is n and p side respectively. The excess minority charge carries diffuse away from the region recombining with majority carriers of the n and p type material, resulting in the release of photons. Further, the emitted photons increase the recombination of injected electrons from the n-region and holes in p-region by inducing more recombinations thus the stimulated emission takes place more effectively. The efficiency of a laser emission increases when the device is cooled.

The drawbacks of homojunction lasers
1. Only output is obtained
2. The threshold current density is very large(400amps/mm^2)
3. Electromagnetic confinement is poor.
4. Output has more beam divergence, poor coherence.

To overcome these deficiencies, scientists have developed heterojunction laser sources like GaAs/GaAlAs structures. The advantages of heterojunction laser structures are:
1. Low threshold current density(5-10amp/mm^2)
2. The output is continuous
3. Carrier confinement is more effective there by less beam divergence.
4. High output power.
5. Narrow beam, high coherence, high mono chromaticity is achieved.
6. Long lifetime of the device
7. Very stable. Hence hetero junction laser diode used extensively in optical fiber communication

2.8. Applications of Lasers
Lasers find applications in various fields. They are described below.

 a) **In Communications :**
   Lasers are used in optical fiber communications. In optical fiber communications, lasers are used as light source to transmit audio, video signals and data to long distances without attention and distortion.

34

b) The narrow angular spread of laser beam can be used for communication between earth and moon or to satellites.

c) As laser radiation is not absorbed by water, so laser beam can be used in under water (inside sea) communication networks.

2. Industrial Applications

a) Lasers are used in metal cutting, welding, surface treatment and hole drilling. Using lasers cutting can be obtained to any desired shape and the curved surface is very smooth.

b) Welding has been carried by using laser beam.

c) Dissimilar metals can be welded and micro welding is done with great case.

d) Lasers beam is used in selective heat treatment for tempering the desired parts in automobile industry

e) Lasers are widely used in electronic industry in trimming the components of ICs

3. Medical Applications

1. Lasers are used in medicine to improve precision work like surgery. Brain surgery is an example of precision surgery Birthmarks, warts and discoloring of the skin can easily be removed with an unfocussed laser. The operations are quick and heal quickly and, best of all, they are less painful than ordinary surgery performed with a scalpel.

2. Cosmetic surgery (removing tattoos, scars, stretch marks, sun spots, wrinkles, birthmarks and hairs) see lasers hair removal.

3. Laser types used in dermatology include ruby(694nm),alexandrite(755nm),pulsed diode array(810nm), Nd:YAG(1064nm), HO:YAG(2090nm), and Er:YAG(2940nm)

4. Eye surgery and refracting surgery.

5. Soft tissue surgery: Co_2 Er :YAG laser.

6. Laser scalpel (general surgery, gynecological, urology, laparoscopic).

7.   Dental procedures.

8. Photo bio modulation (i.e. laser therapy)

9. "No-touch" removal of tumors, especially of the brain and spinal cord.

10. In dentistry for caries removal, endodontic/periodontic, procedures, tooth whitening, and oral surgery.

4. Military Applications

The various military applications are:

a) **Death rays**: By focusing high energetic laser beam for few seconds to aircraft, missile, etc can be destroyed. So, these rays are called death rays or war weapons.

b) **Laser gun:** The vital part of energy body can be evaporated at short range by focusing highly convergent beam from a laser gun.

c) **LIDAR (Light detecting and ranging)**: In place of RADAR, we can use LIDAR to estimate the size and shape of distant objects or war weapons. The differences between RADAR and LIDAR are that, in case of RADAR, Radio waves are used where as incase of LIDAR light is used.

5. In Computers: By using lasers a large amount of information or data can be stored in CD-ROM or their storage capacity can be increased. Lasers are also used in computer printers.

6. In Thermonuclear fusion: To initiate nuclear fusion reaction, very high temperature and pressure is required. This can be created by concentrating large amount of laser energy in a small volume. In the fusion of deuterium and tritium, irradiation with a high energy laser beam pulse of 1 nano second duration develops a temperature of 10^{17} ^{0}c, this temperature is sufficient to initiate nuclear fusion reaction.

7. In Scientific Research: In scientific, lasers are used in many ways including
  a) A wide variety of interferometrie techniques.
  b) Raman spectroscopy.
  c) Laser induced breakdown spectroscopy.
  d) Atmospheric remote sensing.
  e) Investigating non linear optics phenomena
  f) Holographic techniques employing lasers also contribute to a number of measurement techniques.
  g) Laser (LADAR) technology has application in geology, seismology, remote sensing and atmospheric physics.
  h) Lasers have been used abroad spacecraft such as in the cassini-huygens mission.
  i) In astronomy lasers have been used to create artificial laser guide stars, used as reference objects for adaptive optics telescope.

Multiple Choice Questions

1. Laser action is found in _____ semiconductor   ( )
   (a) Direct band gap   (b) indirect band gap
   (c) Germanium   (d) silicon
2. In computer _____ laser is used   ( )
    (a) He-Ne gas   (b) ruby
    (c) Semi conductor   (d) CO_2
3. Laser radiation is _____   ( )
   (a) Highly monochromatic   (b) partially monochromatic
   (c) White light   (d) none
4. Under population inversion, the number of atoms in the higher energy state is _____
   Than in the lower energy state   ( )
   (a) Laser   (b) larger   (c) both a and b   (d) none
5. Laser radiation is ____   ( )
   (a) Highly directional   (b) monochromatic
   (c) Coherent and stimulated   (d) all
6. In conventional light sources   ( )
   (a) Different atoms emit radiation at different times
   (b) There is no phase relation between the emitted photons
   (c) Different atoms emit photons in different directions
   (d) all
7. In laser source   ( )
   (a) Photons emitted by different atoms are in phase or maintain constant phase relationship
 (b) Different atoms emit photons in the same direction

(c) Both a and b   (d) none
8. In spontaneous emissions   ( )
   (a) Atoms are initially in the excited state
   (b) Transitions are without   any aid of an external agency
   (c) Both a and b   (d) none
9. In conventional light sources, the ratio of spontaneous emission rate to stimulated emission rate is nearly   ( )
   (a)10^{10} (b)10^{20} (c)10^5 (d)10^3
10. In excited states, the atoms will remain for a time of   ( )
   (a)10^8 s   (b)10^{-8} s   (c) 10^{-3} s   (d)10^{-5} s
11. He-Ne gas laser is a_____   ( )
   (a) Continuous laser   (b) pulsed laser
   (c) Both a and b   (d) none
12. The ratio of the helium and neon gaseous atoms are   ( )
   (a) 1:10   (b)10:1   (c)1:1   (d)1:20
13. Ruby laser is a solid state: ( )
   (a)   Pulsed, three level laser   (b) pulsed, four level laser
    (c)   Continuous, three level laser (d) continuous four level lasers
14. if the ruby rod contains 0.005% of chromium atoms then it appears in ___ color ( )
   (a) Read   (b) yellow   (c) pink   (d) green
15. At room temperatures, the threshold current density in hetero structure is of the order of _____ A/m^2 ( )
    (a) 10^5 (b) 10^3 (c) 10^2 (d) 10^4

16.   In hetero structure strip geometry semiconductor lasers, the strip width will vary from ( )

(a) 5 to 30 µm   (b) 50 to 100 µm   (c) 5 to 150 µm   (d) 1 to 5 µm

ANSWERS
1.a 2.c 3.a 4.b 5.d   6.d   7.c   8.c   9.a   10.b 11.a 12.b 13.a 14.c 15.b 16.a

SOLVED PROBLEMS
1. A semi conductor laser diode laser has a peak emission wavelength of 1.55 µm. find its energy gap in e V.
(2009)
Solution.   Energy gap of a semiconductor,
                Energy of emitted photon, $E_g= h\nu = \frac{hC}{\lambda}$
                            Where C= velocity of light=3×10^8m/s
            Wavelength, λ=1.55 µm=1.55×10^{-6}m
            Energy gap, E_g=?
            $E_g= \frac{hC}{\lambda} = \frac{(6.63\times10^{-34}\times3\times10^8)}{1.55\times10^{-6}}J$

            $= \frac{6.63\times10^{-34}\times3\times10^8}{1.55\times10^{-6}\times1.6\times10^{-19}} eV = 0.8eV$

2. Calculate the wavelength of emitted radiation from GaAs which has a band gap of 1.44eV   (2010)

Solution: Energy gap of a semiconductor, $E_g = h\nu$

Where h is Planck's constant$=6.63 \times 10^{-34}$J.S

$E_g = h\nu = \dfrac{hC}{\lambda}$ or $\lambda = \dfrac{hC}{Eg}$

$E_g = 1.44eV = 1.44 \times 1.6 \times 10^{-19}$J

$E_g = \dfrac{hC}{\lambda} = \dfrac{6.63 \times 10^{-34} \times 3 \times 10^8}{1.44 \times 1.6 \times 10^{-19}} = 8633 \times 10^{-10}m=8633$A^0

3. Calculate the ratio of the stimulation rate to spontaneous emission rate for an in candescent lamp operating at a temperature of 1100k. Assume average operating length $\lambda = 0.55$ µm.

(Model problem)

Solution: We know that $C = \nu\lambda$

$\nu = \dfrac{C}{\lambda}$ $= \dfrac{3 \times 10^8}{0.55 \times 10^{-6}}$

$= 5.455 \times 10^{14}$Hz.

$\dfrac{Stimulated\ emission\ rate}{spontaneous\ emission\ rate} = \dfrac{1}{exp^{(\frac{h\nu}{kT})} - 1} = 4.5 \times 10^{-11}$

Where $h = 6.63 \times 10^{-34}$J.S, $\nu = 5.455 \times 10^{14}$Hz $K_B = 1.38 \times 10^{-23}$J/K, T$=1100$K.

NANOTECHNOLOGY

3.1 Introduction

- Nanotechnology is the study of the control of matter on an atomic scale. Generally, Nanotechnology deals with structures of the size 100 nanometers or smaller, and involves developing materials or devices within that size. These are known as Nanostructures.

- Nanotechnology deals with the design, manufacturing and applications of nanostructures in useful nanoscale devices such as electronic circuits and mechanical devices at the molecular level.

- In Nanotechnology, the fundamental properties of materials and machines depend on their size.

- Nanotechnology deals with the fabrication of devices or materials which lie in the sizes of 1 to 100nm. Nanotechnology produces materials that are built up atom-by-atom.

  Ex: With carbon atoms, tubular molecules called Carbon nanotubes are made. Spherical molecules with 60 carbon atoms having a diameter slightly less than 1nm, called Bucky balls or Fullerenes are also made with carbon.

3.2 Nano scale

- Nano scale means 10^{-9}. A nanometer (nm) is one thousand millionth of a meter (10^{-9}).

- The diameter of a single atom can vary from 0.1 to 0.5nm, depending on the type of the element.

- For example, one carbon atom is approximately 0.15nm in diameter. A red blood cell is approximately 7000nm wide and a water molecule is almost 0.3nm across. The diameter of a human hair is about 60,000 to 80,000 nms. 1nm would approximately be equal to the length of ten hydrogen atoms in a line.

- A material is called a nanomaterial if the size of the material is below 100nm. This is because, many physical and chemical properties of a material start changing significantly when the size of the grains is below 100nm. The length that is of interest in nanoscience is from 100nm down to the atom scale i.e., 0.2nm.

3.3 Origin of Nanotechnology

- The existence of nanostructures and nanodevices is not new, while the word nanotechnology is relatively new.

- Richard Feynman, in 1960, presented a visionary lecture at a meeting of the American physical society entitled "There is plenty of room at the bottom." In his lecture, he speculated on the potential and possibility of nanosized materials.
- He envisioned etching lines of few atoms wide with beams of electrons-today's electron beam lithography, used for making silicon chips. He envisioned building circuits of nanometer scale for use in computer-today's nanoelectronics. He recognized the existence of nanostructures in biological systems- biological nanoparticles.
- He proposed manipulating individual atoms to make new small structures having very different properties.
- Ralph landaner, from IBM, proposed nanoscale electronics in 1957. Magnetic fluids consisting of nanosized magnetic particles were developed in 1960s. In the early 1970s, Bell laboratories and IBM fabricated the first 2 dimensional quantum wells. Laser vapour deposition method resulted in development of metal nanoclusters in 1981. Later, this method was used to synthesize the fullerene.
- The inventions of Scanning Tunneling Microscope (STM) in 1981 and Atomic Force Microscope (AFM) in 1986 provided new important tools for viewing, characterizing and atomic manipulation of new structures.
- Ijima made Carbon nanotubes in 1991. Super conductivity and Ferro magnetism were found in C_{60} structures.
- In 1994, stable gold nanoparticles were made in solution.
- In 1996, scientists at IBM succeeded in moving and precisely positioning individual molecules at room temperature. In 1999, molecular logic gates were created.
- From 2000, quite a lot of research and development activities are in progress.

3.4 Nanomaterials

- All materials are composed of grains, which in turn comprise of many atoms. Conventional materials have grains of size varying from hundreds of microns to centimeters.
- *Nanomaterials could be defined as those materials which have structural components with size less than 100nm at least in one dimension.*
- Materials that are Nano scale in one dimension (and are extended in the other two dimensions) are layers, such as thin films or surface coatings.
- Materials that are Nano scale in two dimensions (and are extended in one dimension) include nanowires and nanotubes.
- Materials that are nanoscale in three dimensions are particles, for example, precipitates, colloids and quantum dots (tiny particles of semi conductor devices)

3.5 Factors that differentiate Nano materials from Bulk materials

- The factors that differentiate Nano materials from bulk materials are the increase in surface area to volume ratio and quantum confinement effects.

(i) **Surface area to Volume ratio**

- This value is very large for nanomaterials. Consider a spherical material of radius 'r.' Then,

$$\frac{\text{Surface area of the sphere}}{\text{Volume of the sphere}} = \frac{4\pi r^2}{\left(\frac{4}{3}\right)\pi r^3} = \frac{12\pi r^2}{4\pi r^3} = \frac{3}{r}$$

- As the size of the sphere decreases, the above ratio increases. Alternatively, if the material is cubic, as it is divided into small cubes, then also, the surface to volume ratio increases. Hence, the nanomaterials possess large value of surface area to volume ratio as compared to the bulk materials.

(ii) **Quantum Confinement Effects**

- According to band theory, solid materials have energy bands and isolated atoms possess discrete energy levels. Nanomaterials are in intermediate to the above two cases.
- For nanomaterials, if the dimensions of potential wells or potential boxes are of the order of the de Broglie wavelength of electrons (mean free path of electrons), then the energy levels of electrons change, and the electron will remain confined to a small region of the material. This is called quantum confinement. Energy is discrete, not continuous in a quantum system.
- The electronic properties of solids are altered with the reductions in the particle size. This effect does not come into play by going from macro to micro dimensions. However, it becomes dominant when the nanometer size range is reached.
- Materials reduced to nanoscale can suddenly show very different properties compared to what they exhibit on a macro scale.
  Ex: Opaque substances become transparent (Copper)
  Inert materials become catalysts (Platinum)
  Stable materials become combustible (Aluminium)
  Solids turn into liquids at room temperature (Gold)
  Insulators become conductor

3.6 Properties of Nanomaterials

3.6.1 Physical Properties

At the macro scale, the physical and chemical properties are not dependent on the size of the material, but at the nanoscale, everything, including colour, melting point and chemical properties will change, compared to what they exhibit on a macro scale. The various physical properties are explained below.

(i)Geometric structure

- Large nanoparticles have the same crystal structure as that of the bulk material, but different lattice parameters.
- In nanomaterials, the surface area to volume ratio increases. Similarly, the interatomic distance decreases by reducing the size of nanoparticles.

(ii) Optical properties

- Different sized nanoparticles scatter different wavelengths of light incident on it and hence, they appear with different colours.

For ex., nanoscale gold particles can be orange, purple, red or greenish in colour, depending on their grain size. The bulk copper is opaque whereas nanoparticle copper is transparent. Porous silicon exhibits red photoluminescence, but bulk silicon does not show this effect.

(iii)Thermal properties

- The melting point of nanogold decreases from 1200k to 800k as the size of the particles decreases from $300A^o$ to $200A^o$.
- The Debye temperature and ferro electric phase transition temperature are lower *for Nano materials.*
- Super plasticity of nanomaterial occurs at lower temperatures by reducing the grain size.
- Stable Aluminium becomes combustible in nano phase. Solid Gold changes to liquid as it goes from bulk to nanomaterial at room temperature.

(iv) Magnetic properties

The magnetic properties of nanomaterials are different from that of bulk materials.
- In nanomaterials single domains are used, unlike large no of domains in bulk materials. The co-ercivity of single domain is very large.
- Fe, Co, Ni and Gd are ferro magnetic in bulk but they exhibit super paramagnetism in the nanophase. Na, K and Rh are Paramagnetic in bulk but in nanophase, they are ferromagnetic.

42

- Small clusters (containing less than 80 atoms) of non-magnetic substances show spontaneous magnetic moment where as in the case of magnetic nanoparticles, the magnetic moment is reduced.
- Clusters of non-magnetic element, supported on metal substrates also show magnetism. This shows that small particles possess more magnetism than the bulk material. Nanoparticles of even non-magnetic solids are found to be magnetic.

(v)Electronic properties

- The electrical conductivity and energy band width of some materials change when they pass from bulk phase to nanoparticle phase. **For Ex.,** bulk silicon is an insulator; it becomes a conductor in the nano phase. Nanomaterial semi-conductors such as Ge and Si do not show semi-conducting property.
- In nanoceramics and in nanomagnetic composites, electrical conductivity increases with reducing particle size. In metals, electrical conductivity decreases with reducing particle size.
- By reducing the size of metal particles from bulk top nano, the energy bands become narrower and hence the ionization potential energy increases.

(vi)Mechanical properties

- Mechanical properties such as hardness, toughness, elastic modulus, scratch resistance, fatigue strength, crack initiation and propagation are significantly different for nanostructures than bulk materials.
- In metals and alloys, the hardness and toughness are increased by reducing the size of nanoparticles. In ceramics, the ductility and super plasticity are increased on reducing particle size. Hardness increases 4 to 6 times as one goes from coarse grain Cu to nanocrystalline Cu and it is 7 to 8 times for Ni. The hardness increases 2 to 7 times by decreasing the size of nanocrystalline metals from 1μm to $10\,\mu$m.
- Materials with smaller grain size are stronger because crack propagation can be delayed or reduced in nanostructures than in bulk materials. Brittle materials (ceramics, inter metallic) can become ductile by reducing their grain size.
- The transition from bulk to nano phase reduces elastic strength and increases plastic behavior. Creep involves atomic transport along grain boundaries. This leads to super plasticity. The creep rate can be increased by 6 to 8 times by reducing the grain size from microns to nanometers.

3.6.2 Chemical Properties

- The nanostructures in chemistry are colloids and these are formed in a condensed phase having sizes in the range of 1-100nm.

- The ionization potential increases as the cluster size drops below the bulk limit and it has limited applicability.
- Clusters of Platinum, Iridium or Osmium reduced to the size of 1nm, and supported on Aluminium or silica exhibits electronic properties similar to those found for large crystallites of the metal.
- The reactivity of a cluster depends on the cluster size. This is useful in preparation of catalytic agents.
- Some chemically inert bulk materials become good chemical catalysts in the nano phase.
  Ex: Gold, Platinum.

Hydrogen storage in metals

- Most of the metals do not absorb hydrogen; those that absorb have a metal to hydrogen atom ratio of 1. The small positively charged clusters of Ni, Pd and Pt, containing atoms in between 2 to 60, can absorb hydrogen atoms up to 8 per metal atom.
- The hydrogen absorption increases with the decrease in the cluster size. Thus, small particles may be very useful in hydrogen storage in metals.

3.7 Production of Nanomaterials

- Nanomaterials can be produced by a number of ways. Nanomaterials can be synthesized by **"top down"** techniques, producing very small structures from large pieces of the material. One way of doing this is, mechanically crushing of the solid into fine nanopowder (ball milling).
- Nanomaterials may also be synthesized by **"bottom up"** techniques, atom by atom or molecule by molecule. One way of doing this is to allow the atoms or molecules, arrange themselves into a structure, due to their natural properties. **Ex:** crystal growth.
- There are many known methods to produce nanomaterials. They are:

Sol-Gel method
- In solutions, nanosized molecules are dispersed randomly whereas in colloids, the molecules have diameters in the range of 20μm-100μm and are suspended in the solvent. So, the colloid appears cloudy.
- A colloid that is suspended in a liquid is called a **Sol**. The gelation of the sol in the liquid to form a network is called **gel**. Gel is the suspension that keeps its shape.
- Sol-gel formation occurs in different stages.
  (a) Hydrolysis
  (b) Condensation and polymerization of monomers to form particles.
  (c) Agglomeration of particles.

This is followed by the formation of networks which extends throughout the liquid medium and forms a gel.

- Using sol-gel method, silica gels, zirconia and yttrium gels and aluminosilicate gels are formed. Nanostructured surfaces are formed using the sol-gel method.
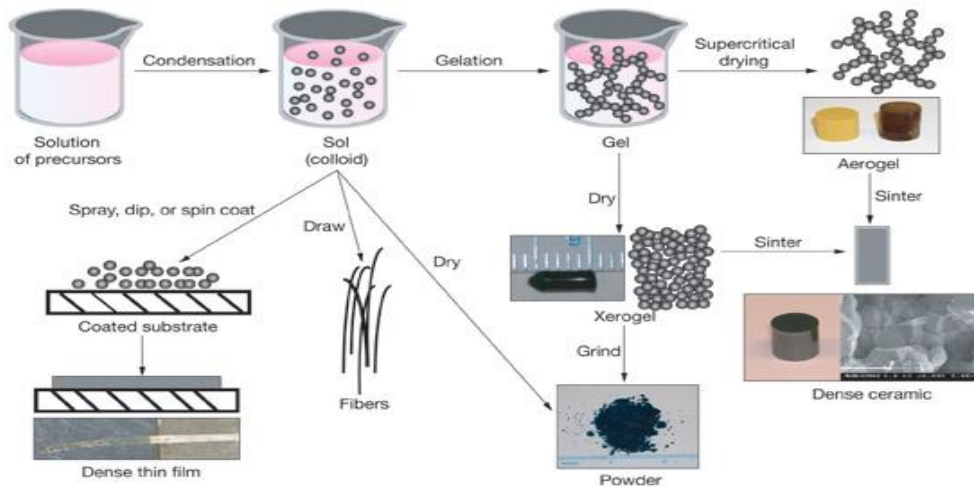

Fig. 3.1 Schematic of Sol-Gel method

3.7.3 Chemical Vapour Deposition (CVD)

- In this method, the material is heated to gaseous phase and allowed to condense on a solid surface in vacuum.
- Nanomaterials of metallic oxides or metallic carbides can be formed by heating metal and carbon or metal and oxygen, in a vacuum chamber to gaseous phase, and allowed to deposit on the surface of a solid.
- Pure metal powders (nanoparticles) are formed by this method. The metal is melted, excited with microwave frequency and vaporized to produce plasma at 1500°c. By cooling this plasma with water in a reaction column, nanoparticles are produced.
- The grain size of the nanoparticles depends on the concentration of the metal vapour, its rate of flow in the reaction column and temperature. This method can also be used to grow surfaces.

45

Fig3.2 Schematic of Chemical Vapour Deposition
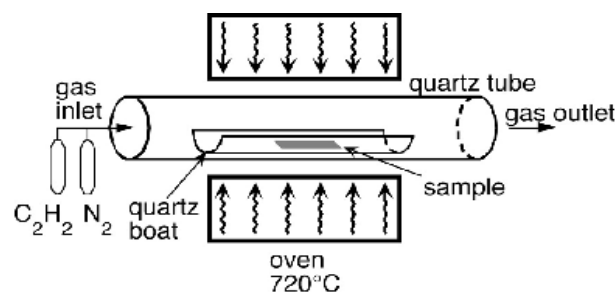
3.8 Characterization of Nanomaterials

The characterization technique that is employed for the characterization of Nanomaterial depends on the type and application of the nanomaterial. For all Nanomaterials, particle size determination is essential and this can be done using X-ray diffraction and Electron microscopy.

3.8.1. X-ray Diffraction Method

- Phase identification using X-ray diffraction lies mainly on the position of the peaks in the diffraction profile and to some extent on the relative intensities of these peaks.
- The shape, particularly the width of the peak is a measure of the amplitude of thermal vibrations of the atoms at their regular lattice sites.
- It can also be a measure of any deviations from the normal structure.
  Ex: Plastic deformation, impurity doping, second phase addition to the host phase. When X-ray powder pattern is taken on poly crystalline powders, the crystallite size causes peak broadening. The crystallite size is easily calculated as a function of peak width, specified as Full Width at Half Maximum (FWHM), peak position and wavelength. The average crystallite size 'L' is given by,

$$\langle L \rangle_{\text{Vol}} = \frac{K\lambda}{B_{1/2}\cos\theta_B}$$

Where, θ_B is the Bragg's angle $B_{1/2}$ is FWHM of the diffraction peak; K is a constant and λ is the wavelength of X-rays used.
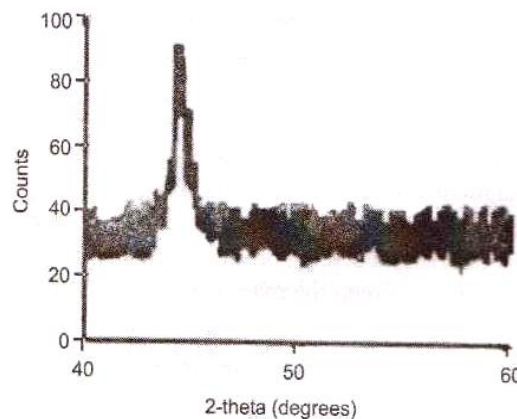

Fig. 3.3 *X-ray diffraction of Ag nanoparticles*

46

3.8.2. Electron Microscopy

Electron microscopes are a beam of highly energetic electrons to examine objects on a very fine scale. The examination gives information about,

a) **Topography:** The surface features of the object or "how it looks," its texture, relation between them and the material properties (hardness, reflectivity etc.,)

b) **Morphology:** The shape and size of the particles making up the object, direct relation between these structures and material properties (ductility, strength, reactivity etc.,)

c) **Composition:** The elements and compounds that the object is composed of, direct relation between composition and material properties (melting point, reactivity, hardness etc.,)

d) **Crystallographic information:** Atomic arrangement in the object, relation between them and the material properties (conductivity, electrical properties, strength etc.,)
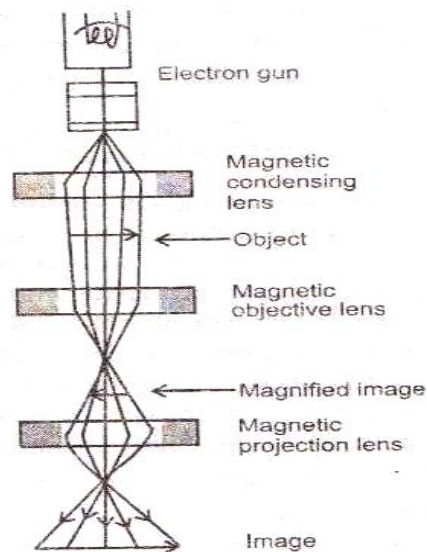
Fig.3.4 Electron Microscope

3.8.3.Scanning Electron Microscopy (SEM)

The image in scanning electron microscope is produced by scanning the sample with a focused electron beam and detecting the secondary and back scattered electrons. Electrons and photons are emitted at each beam location and subsequently detected.
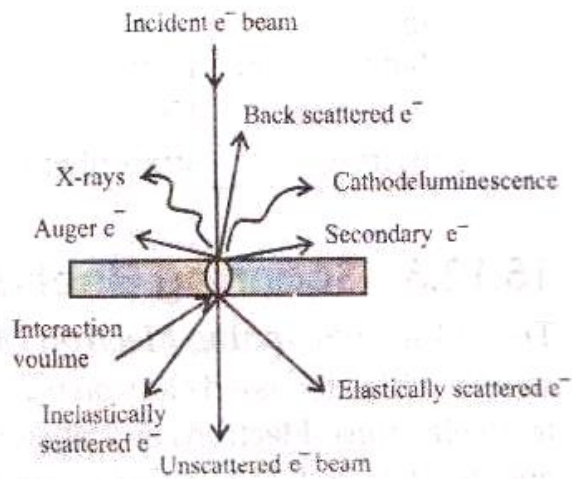
Fig.3,5 Specimen interactions in SEM

Schematic representation of SEM

1) The electron gun produces a stream of monochromatic electrons.
2) The electron stream is condensed by the first condenser lens. It works in conjunction with the condenser aperture to eliminate the high angle electrons from the beam.
3) The second condenser lens forms the electrons into a thin, light coherent beam.
4) Objective aperture further eliminates high angle electrons from the beam.
5) A set of coils acting as electrostatic lens scans and sweeps the beam in a grid fashion (as in television)
6) The objective lens focuses the scanning beam onto the part of the specimen.
7) When the beam strikes the sample, interaction occurs. The intensity of display is determined by the interaction number. More interactions give a brighter pixel.
8) This process is repeated until the grid scan is finished and then repeated. The entire pattern can be scanned 30 times per second.
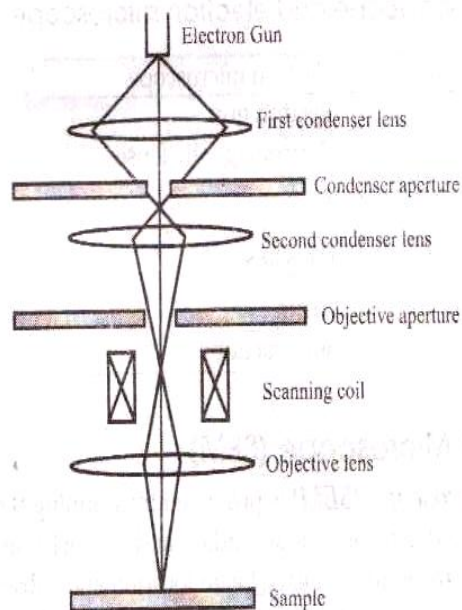
Fig.3.6 Schematic representation of SEM

SEM gives useful information on

1) **Topography:** The surface features of an object or "how it looks," its texture, detectable features, limited to a few nanometers.
2) **Morphology:** The shape, size and arrangement of particles making up the object that are lying on the surface of the sample or have been exposed by grinding or chemical etching, detectable features limited to a few nanometers.
3) **Composition:** The elements and compounds the sample is composed of and their relative ratios, in areas approximately 1 micrometer in diameter.
4) **Crystallographic Information:** The arrangement of atoms in the specimen and their degree of order, only useful on single-crystal particles >20 μms.

3.8.4. Transmission Electron Microscopy (TEM)

- When transmitted electrons are utilized for imaging, it results in Transmission Electron Microscopy (TEM).
- In the TEM analysis, a thin or diluted sample is bombarded under high vacuum with a focused beam of electrons. Electrons that are transmitted through the material, form contrast patterns that reproduce the image of the sample. This pattern arises from the scattering of the electrons. In addition, diffracted electrons give information about the lattice structure of the material. The shape of the sample can also be determined from the image.
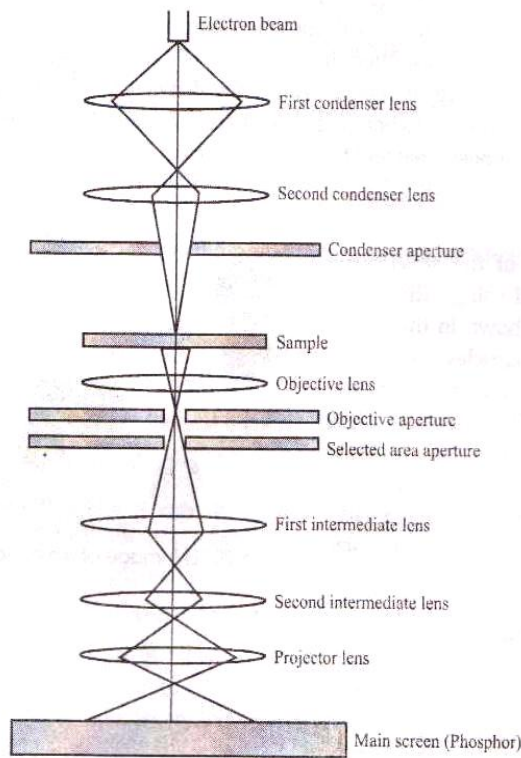
Schematic representation of TEM

1. The electron gun produces a stream of monochromatic electrons.
2. This stream is focused to a small coherent beam by the first and second condenser lenses.
3. The condenser aperture knocks off high angle electrons.
4. The beam strikes the specimen.
5. The transmitted portion is focused by the objective lens into an image.
6. Objective aperture enhances the contract by blocking out high angle diffracted electrons.
7. Selected area aperture enables to examine the periodic diffraction of electrons by an ordered arrangement of atoms in the sample.
8. Intermediate and projector lenses enlarge the image.

The beam strikes the phosphor screen and image is formed on the screen. The darker areas of the image represent thicker sample areas since these areas transmit lesser electrons. The brighter areas of the image represent thinner sample areas since these areas transmit more electrons.

TEM gives the information about

1) Morphology: The size, Shape and arrangement of particles as well as their relationship to one another on the scale of atomic diameters.
2) Crystallographic information: The arrangement of atoms in the specimen and their degree of order, detection of atomic scale defects, a few nanometers in diameter.
3) Compositional information: The elements and compounds, the sample is composed of and their relative ratios.

Fig. 3.7 Schematic representation of TEM.

Applications of Nanotechnology

1) Electronics industry

- Reduction in size of electronic components leads to faster switching times.
- Nanotechnology includes fabrication of nanowires used in semiconductors.
- Porous silicon emits visible light. So, it finds application in optoelectronics.
- Quantum dot laser emits good quality laser beam compared to semiconductor laser diodes. They are cheaper and the emitted wavelength depends on the diameter of the dot.
- Materials like nanocrystalline selenide, zinc sulphide, lead telluride and cadmium sulphide synthesized by sol-gel method improve the resolution of the image in television or in a monitor. The resolution depends on the size of the pixel made of phosphors. The resolution increases as the size of the pixel reduces.
- Batteries made of nanocrystalline nickel and metal hydrides are long lasting and require minimal recharging.

2) Industry

- Nanocrystalline materials such as tungsten carbide, titanium carbide are harder than conventional materials. They are more wear resistant and erosion resistant. So, they can be used in cutting tools and drilling bits.

51

- Nanocrystalline silicon nitride and silicon carbide are used in the manufacturing of high strength springs, ball bearings and valve lifters.
- Nanocrystalline ceramics such as zirconia are easily pressed and sintered into various shapes at lower temperatures, because they are softer than conventional materials.

3) High power magnets
- The magnetic strength of a material is directly proportional to the surface area per unit volume.
- The magnetic nanocrystalline yttrium-samarium-cobalt possesses very high magnetic properties due to large surface area.
- The high power rare earth magnets are used in submarines, generators, electric motors, automobile alternators, magnetic resonance imaging (MRI) instruments and in ultrasensitive analytical instruments.

4) Motor vehicles and air craft
    The wastage of thermal energy generated in engines is reduced by coating the cylinders with nanocrystalline ceramics such as zirconia and alumina.
- In air craft, by decreasing the grain size of the materials, the fatigue strength increases as much as 300 %. The components made of nanomaterials are stronger and operate at higher temperatures. So, air craft can fly faster using the same amount of aviation fuel.

5) Aero gels
- Aero gels are nanocrystalline and porous. Hence, air is trapped at the interstices. These materials can be used in offices and homes to reduce cooling and heating bills by saving power. These are also used for smart windows so that the materials become darkened when the sun is too bright and lightened when the sun is not shining brightly.

6) Energy efficiency
- Energy consumption can be greatly reduced by using quantum edged atoms or LEDs instead of ordinary filament bulbs.
- Nanostructures have increased solar energy conversion efficiency as compared to ordinary semiconductor solar cells.
- In hydrogen fuel cells, nanostructured catalyst material is used on carbon supported noble metal particles, with diameters between 1 & 5nm.
- For hydrogen storage, CNTs, zeolites etc., are used.

7) Medical field
- Nanomaterials are used in the development of diagnostic devices, drug delivery vehicles, and analytical tools and in physical therapy applications.

- The genetic sequence of a sample can be detected by tagging gold nanoparticles with short segments of DNA.
- Magnetic nanoparticles are used to label molecules, structures or micro organisms of an antibody.
- Iron nanoparticles are used in cancer treatment. Nanotechnology is used to repair or to reproduce damaged tissue.

8) Textile industry
Clothes made of nanofibers are water and stain repellent and wrinkle free. They can be washed less frequently at low temperatures.

9) Information technology
Nanoscale fabricated magnetic materials are used in data storage. Quantum computers use fast quantum algorithms and have quantum bit memory space (qubit). So, it involves several computations at the same time.

10) Cosmetics
- Sunscreens based on mineral nanoparticles such as titanium-di-oxide offer several advantages. They have high UV protection compared to the bulk material. In addition to these, there are quantum dots, suntan lotion, nanotubes, and protective coatings.
- Fullerenes (C_{60}) are used as lubricants (molecular ball bearings), diamond seeding, diamond protection, xerographic materials, photo chronic goggles etc.

QUESTIONS

1. Write a detailed note on Nanoscience and Nanotechnology.
2. Write the important applications of Nanomaterials in medicine.
3. What are Nanomaterials? Explain.
4. Describe the various types of carbon Nanotubes.
5. Explain the fabrication of carbon Nanotubes.
6. Write a detailed note on Nano science.
7. Why Nanomaterials exhibit different properties? Explain.
8. Describe any three processes by which Nanomaterials are fabricated.
9. Describe the important applications of nanotechnology.
10. What is the meaning of nanotechnology? Explain.
11. Describe the process of sol-gel and precipitation in the fabrication of nanostructures.
12. Write the applications of nanotechnology in the electronic industry.

13. Describe the top-down methods by which Nanomaterials are fabricated.

14. Explain how x-ray diffraction can be used to characterize nanoparticles.

15. Describe any three processes by which Nanomaterials are fabricated.

16. Describe the important applications of nanotechnology.

17. Write about (i) origin of nanotechnology (ii) nanoscale.

18. Discuss quantum confinement effect on nanoparticles.

19. Explain how TEM can be used to characterize nanoparticlesset.

20. Write notes on (i) origin of nanotechnology (ii) nanoscale.

21. Describe the combustion method and PVD method for fabrication of nanostructures.

22. Give the applications of nanotechnology in the electronic industry.

23. Give three methods of fabrication of Nanomaterials.

24. Give the important applications of nanotechnology.

25. Describe the top-down methods of fabrication of Nanomaterials.

26. Explain X-ray diffraction method for characterization of Nanomaterials.

27. Write notes on (i) nanoscale (ii) origin of nanotechnology

28. How the physical and chemical properties of Nanomaterials vary with their size?

1. Diameter of one carbon atom is <u>0.15nm</u>.
2. In Nano materials with decrease of size the interatomic spacing <u>decreases.</u>
3. In Nano materials with decrease of size the melting point <u>decreases.</u>
4. In Nano materials the ionization potential <u>is higher</u> when compared with that of the bulk.
5. Gold Nano spheres of 100nm appear <u>in orange</u> in color while 50nm appear <u>green</u> in color.
6. With <u>decrease</u> of coordination number, the magnetic moment <u>increases.</u>
7. Young's modulus value of single walled Nanotubes is about <u>1 Terapascal</u>.
8. Nanotechnology is the engineering of functional systems at the <u>molecular scale</u>.
9. Nanomaterials are having <u>domain size about 100nm</u>.
10. Properties of Nano materials differ from bulk materials due to <u>the presence of less no. of </u><u>atoms.</u>

11. When a metal particle having bulk properties, is reduced in size , the density of states <u>decreases.</u>

12. Nano sized particles are chemically very active <u>because the no. of surface molecules of a</u><u>toms is more.</u>

13. In the fabrication of nanoparticles, macro crystalline structures are broken down to Nano crystalline structures in <u>ball milling.</u>

14. The advantages of <u>sol-gel technique</u> in the fabrication a low temperature process, the product can be obtained in any form and polished to optical quality.

15. <u>An electrochromic device</u> is display device which displays information by changing color when a voltage is applied.

16. <u>Fullerene</u> is carbon molecule with carbon atoms arranged in a spherical shape.

17. Carbon Nanotubes are <u>sheets of graphite rolled into a tube.</u>

18. The approach used to construct Nanomaterials by merging smaller components into more complex assemblies is <u>bottom-up approach</u>.

19. The approach used to construct Nanomaterials by deforming large complex molecules in to small ones is <u>top-down approach</u>.

20. Lithographic method of preparing the Nanomaterials falls under <u>top-down approach</u>.

21. Epitaxial growth falls under <u>top-down approach</u>.

22. STM, AFM and SFM fall under <u>top-down approach</u>.

23. A nanometer is <u>one thousand of a meter (i.e. 10^{-9})</u> .

24. Photographic film is an emulsion consisting of <u>silver nanoparticles</u> in gelatin.

25. <u>Nano materials</u> are defined as those materials which have structured components with size less than 100nm at least in dimension.

26. Materials that are nanoscale in one dimension are <u>layers, such as thin films or surface </u><u>c</u><u>oatings.</u>

27. Materials that are nanoscale in two dimensions are <u>nanotubes and nanowires.</u>

28. Materials that are nanoscale in three dimensions are <u>particles like precipitates, colloids, quantum dots, grains.</u>

29. <u>Nanoscience </u>is the study of phenomena and manipulation of materials at atomic, molecular and macromolecular scales where properties differ significantly from those at a larger scale .

30. <u>Nanotechnology</u> can be defined as the design, characterization, production and application of structures, devices and systems by controlling shape and size at the nanometer scale.

31. A <u>fullerene</u> is a molecule entirely of carbon, in the form of hallow sphere, called <u>bucky</u> balls.

32. Cylindrical fullerenes are called <u>nanotubes and bucky tubes</u>

33. Fullerenes are similar to <u>graphite</u> containing pentagonal rings.

34. Fullerene was discovered by <u>Buckminsterfullerene C_{60}.</u>

35. CNTS are two types <u>SWNTs and MWNTs</u>.

36. Properties of Nano materials changes due to <u>Increase in surface area to volume ratio and Quantum confinement effects.</u>

37. When the dimensions of potential wells, potential boxes are of the order of de Broglie wavelength of electrons, the energy levels of electrons changes. This effect is called <u>Quantum Confinement</u>.

38. The physical, electronic, magnetic, mechanical, chemical, thermal, optical properties of materials depend <u>on size.</u>

39. The interatomic spacing and melting point <u>decreases</u> with size.

40. Nano particles may emit or absorb specific wave lengths of light by <u>controlling size</u>.

41. Ionization potential and mechanical properties <u>are higher</u> in Nano materials.

42. CNTs are rolled graphite sheets which are mechanically <u>strong and flexible</u> and first observed by <u>Sumio Iijima</u>.

43. Nano particles are more magnetic than bulk materials.

44. <u>Plasma arcing</u> is used produce CNTs.

45. <u>Evaporative deposition</u> is the method where the material is heated and vaporized by electrically resistive heating under high vacuum.

46. <u>Electron beam physical vapor deposition</u> is the method where the material to be deposited is heated to a high vapor pressure by electron bombardment in high vacuum.

47. <u>Sputter deposition</u> is the method where the material to be deposited is vaporized by bombarding the material with aglow plasma discharge.

48. <u>Cathodic arc deposition</u> is a high power arc directed at the target material.

49. <u>Pulsed laser deposition</u> is a high power pulsed laser ablates the material from the target into a vapor.

50. <u>Chemical vapor deposition</u> is the method where the material is heated to form a gas and allowed to deposit on a solid surface under vacuum condition by chemical reaction.

51. Nano powders of oxides and carbides of metals are produced by <u>chemical vapor deposition</u>. It is also used to <u>grow</u> surfaces.

52. Sol-gels are <u>suspensions of colloids in liquids that keep their shape</u>.

53. Electron microscope consists <u>of electron gun, electromagnetic fields as lenses maintained under high vacuum.</u>

54. <u>SEM and TEM</u> gives information on topography, morphology, composition and crystallographic information.

55. Nano sized ball bearings are used as lubricants <u>to reduce friction</u>.

56. Nano particles in cosmetics <u>are harmful</u> to humans.

57. Nano materials in food and drinks for package materials, storages like additives are <u>harmful</u> to humans.

PRINCIPLES OF QUANTUM MECHANICS

4.1.1 Wave and particle duality

A particle has mass, it is located at some definite point, it can move from one place to another, it gives energy when slowed down or stopped. Thus, the particle is specified by

      (1)   Mass m

      (2)   Velocity v

      (3)   Momentum p and

      (4)   Energy E.

A wave is spread out over a relatively large region of space , it cannot be said to be located just here and there, it is hard to think of mass being associated with a wave. Actually a wave is nothing but a rather spread out disturbance. A wave is specified by its

      (1)   Frequency

      (2)   Wavelength,

      (3)   Phase of wave velocity,

      (4)   Amplitude and

      (5)   Intensity

Considering the above facts, it appears difficult to accept the conflicting ideas that radiation has a dual nature, i.e., radiation is a wave which is spread out over space and also a particle which is localized at a point in space. However, this acceptance is essential because radiation sometimes behaves as a wave and at other times as a particle as explained below:

(1) Radiations including visible light, infra-red, ultraviolet, X-rays, etc. behave as waves in experiments based on interference, diffraction, etc. This is due to the fact that these phenomena require the presence of two waves at the same position at the same time. Obviously, it is difficult for the two particles to occupy the same position at the same time. Thus, we conclude that radiations behave like wave..

(2) Planck's quantum theory was successful in explaining black body radiation, the photo electric effect, the Compton Effect, etc. and had clearly established that the radiant energy, in its interaction with matter, behaves as though it consists of corpuscles. Here radiation interacts with matter in the form of photon or quanta. Thus, we conclude that radiations behave like particle.

4.1.2 de–Broglie Hypothesis

In the Newton time, matter and radiation both were assumed to consist of particles. With the discovery of phenomena like interference, diffraction and polarization it was established that light is a kind of a wave motion.

In the beginning of 20th century some new phenomena (photoelectric effect, Compton effect, etc.) were discovered which could not be explained on the basis of wave theory. These phenomena were explained on the basis of quantum theory in which light quanta or photons are endowed corpuscular properties – mass ($h\nu/c^2$), velocity v and momentum $h\nu/c$. But, when the photon theory was applied to phenomenon such as

interference, diffraction, etc. (which have been fully explained on wave theory) it proved helpless to explain them. Thus, light has a dual nature, i.e., it possesses both particle and wave properties. In some phenomena corpuscular nature predominates while in others wave nature predominates. The manifest of properties depends upon the conditions under which the particular phenomena occur. But wave and particle never expected to appear together.

Louis de- Broglie in 1924 extended the wave particle parallelism of light radiations to all the fundamental entities of Physics such as electrons, protons, neutrons, atoms and molecules etc. He put a bold suggestion that the correspondence between wave and particle should not confine only to electromagnetic radiation, but it should also be valid for material practices, i.e. like radiation, matter also has a dual (i.e., particle like and wave like) character.

In his doctoral thesis de-Broglie wrote that there is an intimate connection between waves and corpuscles not only in the case of radiation but also in the case of matter. A moving particle is always associated with the wave and the particle is controlled by waves. This suggestion was based on the fact that nature loves symmetry, if radiation like light can act like wave some times and like a particle at other times, then the material particles (e.g., electron, neutron, etc.) should act as waves at some other times. These waves associated with particles are named de- Broglie waves or matter waves.

4.1.3 Expression for de- Broglie wavelength

The expression of the wavelength associated with a material particle can be derived on the analogy of radiation as follows:

Considering the plank's theory of radiation, the energy of photon (quantum) is

$$\text{E} \ = \ h\upsilon \ = \frac{hc}{\lambda} \qquad\qquad \rightarrow (1)$$

Where c is the velocity of light in vacuum and λ is its wave length.

According to Einstein energy – mass relation

$$\text{E} \ = \ \text{mc}^2 \qquad\qquad \rightarrow (2)$$

$$\lambda \ = \ \frac{h}{mc} \ = \frac{h}{p} \qquad\qquad \rightarrow (3)$$

Where mc = p is momentum associated with photon.

If we consider the case of material particle of mass m and moving with a velocity v , i.e momentum mv, then the wave length associated with this particle (in analogy to wave length associated with photon) is given by

$$\lambda \ = \ \frac{h}{mv} \ = \frac{h}{p} \qquad\qquad \rightarrow (4)$$

Different expressions for de-Broglie wavelength

(a) If E is the kinetic energy of the material particle then

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

$$\Rightarrow \quad p^2 \ = 2mE \text{ or } \quad p = \sqrt{2mE}$$

Therefore de- Broglie wave length $\quad \lambda \ = \ \frac{h}{\sqrt{2mE}} \qquad\qquad \rightarrow (5)$

(b) When a charged particle carrying a charge 'q' is accelerated by potential difference
v, then its kinetic energy K .E is given by

$$E \;=\; qV$$

Hence the de-Broglie wavelength associated with this particle is

$$\lambda \;=\; \frac{h}{\sqrt{2mqV}} \qquad\qquad \rightarrow (6)$$

For an electron $q = 1.602 \times 10^{-19}$

Mass $m = 9.1 \times 10^{-31}$ kg

$$\therefore \quad \lambda \;=\; \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.602 \times 10^{-19}V}}$$

$$=\; \sqrt{\frac{150}{V}} \quad=\; \frac{12.26}{\sqrt{V}} \; A^0 \qquad\qquad \rightarrow (7)$$

4.1.4 Properties of Matter Waves

Following are the properties of matter waves:
 (a) Lighter is the particle, greater is the wavelength associated with it.
 (b) Smaller is the velocity of the particle, greater is the wavelength associated with it.
 (c) When $v = 0$, then $\lambda = \infty$, i.e. wave becomes indeterminate and if $v = \infty$ then
    $\lambda = 0$. This shows that matter waves are generated only when material particles
    are in motion.
 (d) Matter waves are produced whether the particles are charged particles or not
    ($\lambda = \frac{h}{mv}$ is independent of charge). i.e., matter waves are not electromagnetic
    waves but they are a new kind of waves .
 (e) It can be shown that the matter waves can travel faster than light i.e. the velocity
    of matter waves can be greater than the velocity of light.
 (f) No single phenomenon exhibits both particle nature and wave nature
    simultaneously.

4.1.5 Distinction between matter waves and electromagnetic waves

S.No	Matter Waves	Electromagnetic Waves
1	Matter waves are associated with moving particles (charged or uncharged)	Electromagnetic waves are produced only by accelerated charged particles.
2	Wavelength depends on the mass of the particle and its velocity, $\lambda = \frac{h}{mv}$	Wavelength depends on the energy of photon
3	Matter waves can travel with a velocity greater than the velocity of light.	Travel with velocity of light $c = 3 \times 10^8$ m/s

4.	Matter wave is not electromagnetic wave.	Electric field and magnetic field oscillate perpendicular to each other.
5.	Matter wave require medium for propagation, i.e, they cannot travel through vacuum.	Electromagnetic waves do not require any medium for propagation, i.e., they can pass through vacuum.

4.2.1 Davisson and Germer's Experiment

The first experimental evidence of matter waves was given by two American physicists, Davisson and Germer in 1927. The experimental arrangement is shown in figure 3.1(a).

The apparatus consists of an electron gun G where the electrons are produced. When the filament of electron gun is heated to dull red electrons are emitted due to thermionic emissions. Now, the electrons are accelerated in the electric field of known potential difference. These electrons are collimated by suitable slits to obtain a fine beam which is then directed to fall on a large single crystal of nickel, known as target T which is rotated about an angle along the direction of the beam is detected by an electron detector (Faraday cylinder) which is connected to a galvanometer. The Faraday cylinder 'c' can move on a circular graduated scale s between 29^0c to 90^0 to receive the scattered electrons.
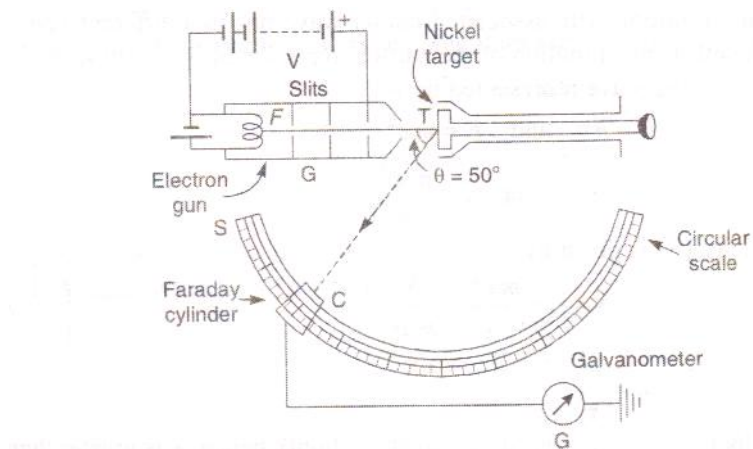

Fig 4.1(a) Davisson and Germer's experimental arrangement for verification of matter waves

First of all, the accelerating potential V is given a low value and the crystal is set at any orbital azimuth (θ). Now the Faraday cylinder is moved to various positions on the scale's' and galvanometer current is measured for each position. A graph is plotted between galvanometer current against angle θ between incident beam and beam entering the cylinder [Figure3.1(b)]. The observations are repeated for different acceleration potentials.
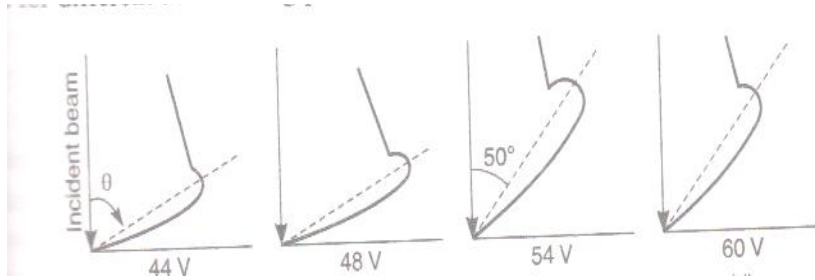
Fig. 4.1(b) Variation of Galvanometer current with variation of angle θ between incident beam and beam entering the cylinder

It is observed that a 'bump' begins to appear in the curve for 44 volts. Following points are observed.

(a) With increasing potential, the bump moves upwards.

(b) The bump becomes most prominent in the curve for 54 volts at $\theta = 50^0$.

(c) At higher potentials, the bumps gradually disappear.

The bump in its most prominent state verifies the existence of electron waves. According to de- Broglie, the wavelength associated with electron accelerated through a potential V is given by

$$\lambda = \frac{12.26}{\sqrt{V}} \ \text{A}^0.$$

Hence, the wavelength associated with an electron accelerated through 54 volt is

$$\lambda = \frac{12.26}{\sqrt{54}} = 1.67 \ \text{A}^0$$

From X-ray analysis, it is known that a nickel crystal acts as a plane diffraction grating with space $d = 0.91 \ \text{A}^0$ [see Figure 3.1(c)]. According to experiment, we have diffracted electron beam at $\theta = 50^0$. The corresponding angle of incidence relative to the family of Bragg plane

$$\theta^1 = \frac{180-50}{54} = 65^0$$

Using Bragg's equation (taking n=1), we have

$$\lambda = 2d\sin\theta$$
$$= 2(0.91\text{A}^0) \sin 65^0$$

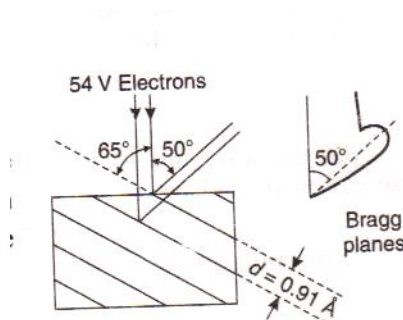This is in good agreement with the wavelength computed from de-Broglie hypothesis.

Fig. 4.1(c) Bragg planes in Nickel crystal

As the two values are in good agreement, hence, confirms the de-Broglie concept of matter waves.

4.2.2 G .P. Thomson′s Experiment

The experimental arrangement is as shown in Figure 3.2. High energy electron beam produced by the cathode 'C' is accelerated with a potential up to 50kV. A fine pencil of accelerated beam is obtained by allowing it to pass through a narrow slit S and is made to fall on a very thin metallic film F of gold (or silver or aluminum). The electron beam is scattered in different directions by the metallic film and incident on photographic plate P. The entire apparatus is exhausted to a high vacuum so that the electrons may not lose their energy in collision with the molecules of air.
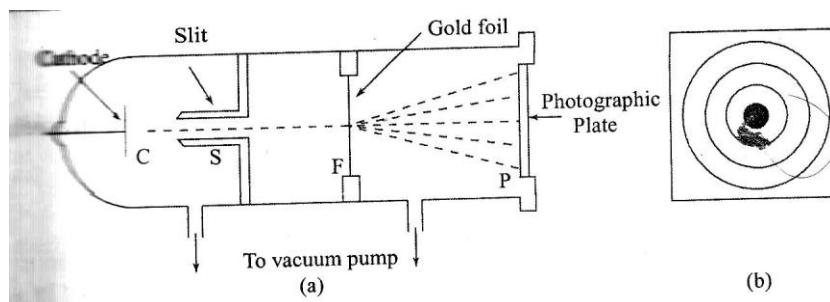

Fig 4.2: (a) G.P.Thomson's Apparatus, (b) pattern recorded on the photographic plate

Since ordinary metals like gold are micro crystalline in structure, the diffraction pattern produced by them are similar in appearance to the X- ray diffraction powered pattern and consist of a series of well-defined concentric rings about a central spot as shown in figure 4.2(b).

To make sure that this pattern is due to electrons and not due to any possible X - rays generated, the cathode rays in the discharge tube are deflected by magnetic field. It was observed that the diffraction pattern observed on the fluorescent screen placed instead of photographic plate also shifted. This confirmed that the pattern is due to the electrons.

Thomson calculated the wavelength of the de-Broglie waves associated with the cathode rays using the equation

$$\lambda = \frac{12.26}{\sqrt{V}} \text{ A}^0$$

and determined the spacing between the planes in the foils using Bragg's equation. The results obtained are in good agreement with those from X-ray studies.

4.3 Heisenberg′s Uncertainty Principle

As a direct consequence of the dual nature of matter, in 1927, Heisenberg proposed a very interesting principle known as uncertainty principle.

If a particle is moving, based on classical mechanics, at any instant we can find its momentum at any position. In wave mechanics, a moving particle can be regarded as a wave group. The particle that corresponds to this wave group may be located anywhere within the group at any given time.

In the middle of the group, the probability of finding the particle is more but the probability of finding the particle at any other point inside the wave group is not zero. Narrower the wave group higher will be the accuracy of locating the particle. At the

same time, one cannot define the wavelength λ of the wave accurately when the wave group is narrower. Since ($\lambda = \frac{h}{mv}$), measurement of particles momentum (mv $= \frac{h}{\lambda}$) also becomes less accurate.
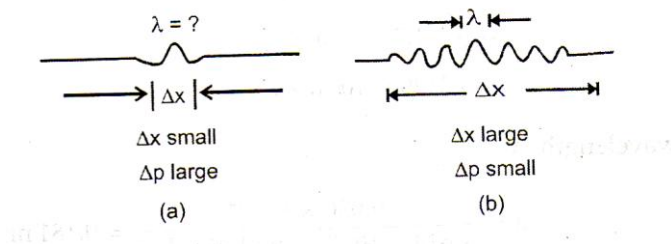

λ = ?   →λ←

Δx small   Δx large
Δp large   Δp small
(a)   (b)

Fig 4.3 (a) A narrow de – Broglie wave group. Since the position can be precisely determined, Δ x is small. As the measurement of is less accurate, Δ p is large. (b) A wide de –Broglie wave group. Measurement of λ is accurate and hence Δ p is small whereas, since wave group is wide, Δ x is large

On the other hand, when we consider a wide wave group, wavelength λ can be well defined hence measurement of momentum becomes more accurate. At the same time, since the width of the wave group is large, locating the position of the particle becomes less accurate.

Thus the uncertainty principle can be stated as *"it is impossible to know both exact position and exact momentum of an object at the same time".*

If Δx and Δp are the uncertainties in the position and momentum respectively when they are simultaneously measured, then

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

Another form of the uncertainty concerns energy and time. In an atomic process let energy 'E' be emitted during the time interval Δt, If the energy is emitted in the form of electromagnetic waves, we cannot measure frequency v of the waves accurately in the limited time available . Let the minimum uncertainty in the number of waves that we count in a wave group be one wave.

$$\text{Since frequency} = \frac{number \ of \ waves}{time \ interval}$$

$$\Delta v \ = \ \frac{1}{\Delta t}$$

Hence the corresponding uncertainty in energy

$$\Delta E \ = h \, \Delta v$$

$$\Delta E \geq \frac{h}{\Delta t} \ \text{ or } \ \Delta E \, \Delta t \geq h$$

A more precise calculation based on the nature of wave of wave groups modifies this result to

$$\Delta E \, \Delta t \geq \frac{h}{4\pi}$$

This gives uncertainty in the measurement of energy and time of a process.

Thus the more generalized statement of Heisenberg's uncertainty principle is

"It is impossible to specify precisely and simultaneously the values of both members of particular pair of physical variables that describe the behavior of an atomic system".

4.4.1 Schrodinger's time independent wave equation

Schrodinger developed a differential equation whose solutions yield the possible wave functions that can be associated with a particle in a given situation. This equation is popularly known as Schrodinger equation. The equation tells us how the wave function changes as a result of forces acting on the particle. One of its forms can be derived by simply incorporating the de-Broglie wavelength expression into the classical wave equation.

If a particle of mass 'm' moving with velocity v is associated with a group of waves, let ψ be the wave function of the particle. Also let us consider a simple form of progressing wave represented by the equation

$$\psi = \psi_0 \sin(\omega t - kx) \qquad \rightarrow (1)$$

Where $\quad \psi \;=\; \psi (x, t)$

ψ_0 is amplitude

Differentiating eq (1) partially with respect to 'x', we get

$$\frac{\partial \psi}{\partial x} = -K \psi_0 \cos(\omega t - kx)$$

Again differentiating equation (1) with respect to 'x'

$$\frac{\partial^2 \psi}{\partial x^2} = -K^2 \psi_0 \sin(\omega t - kx)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi$$

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \qquad \rightarrow (2)$$

Since $k = \frac{2\pi}{\lambda}$, $\qquad \frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2}{\lambda^2} \psi = 0 \qquad \rightarrow (3)$

Eq (2) or Eq (3) is the differential form of the classical wave equation. Now, incorporating de- Broglie wavelength expression $\lambda = \frac{h}{mv}$ in to eq (3), we get

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2 m^2 v^2}{h^2} \psi = 0 \qquad \rightarrow (4)$$

The total energy E of the particle is the sum of its kinetic energy k and potential energy V

i.e., $E = K + V$

But $K = \frac{1}{2} mv^2$

$\therefore \quad E = \frac{1}{2} mv^2 + V$

$\frac{1}{2} mv^2 = E - V$

$m^2 v^2 = 2m (E - V) \qquad \rightarrow (5)$

Substituting eq (5) in eq (4), we get

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m(E - V)}{h^2} \psi = 0 \qquad \rightarrow (6)$$

In quantum mechanics, the value $\frac{h}{2\pi}$ occurs most frequently. Hence we denote $\hbar = \frac{h}{2\pi}$ using this notation, we have

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m(E - V)}{\hbar^2} \psi = 0 \qquad \rightarrow (7)$$

For simplicity, we have considered only one dimensional wave extending eq(7) for a 3 – dimensional wave

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m(E - V)}{\hbar^2} \psi = 0 \qquad \rightarrow (8)$$

Where ψ (x, y, z); here, we have considered only stationary states of ψ after separating the time dependence of ψ

The Laplacian operator is defined as

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \qquad \rightarrow (9)$$

Hence eq (10) can be written as

$$\nabla^2 \psi + \frac{2m(E - V)}{\hbar^2} \psi = 0 \qquad \rightarrow (10)$$

This is Schrodinger wave equation. Since time factor doesn't appear, eq(8) or eq(10) is called 'time independent Schrodinger wave equation' in three dimensions.

4.4.2 Physical significance of wave function ψ

(1) The wave function ψ has no direct physical meaning. It is a complex quantity representing the variation of matter wave.
(2) It connects the practical nature and its associated wave nature statically.
(3) $|\psi|^2$ (or $\psi\psi *$ if function is complex) at a point is proportional to the probability of finding the particle at that point at any given time. The probability density at any point is represented by $|\psi|^2$.
(4) If the particle is present in a volume dxdydz, then $|\psi|^2$ dxdydz =1

If a particle is present somewhere in space

$$\int_{-\infty}^{\infty} \psi^2 \, dx \, dy \, dz = 1$$

$$\text{Or} \quad \int_{-\infty}^{\infty} \psi\psi * \, dx \, dy \, dz = 1$$

The wave function satisfying the above condition is said to be normalized.

4.5.1 Particle in Infinite square potential well

A free electron trapped in a metal or charge carriers trapped by barriers trapped by the potential barriers of a double hetero junction can be approximated by an electron in an infinitely deep one- dimensional potential well.

Consider one – dimensional potential well of width L as shown in fig. Let the potential

66

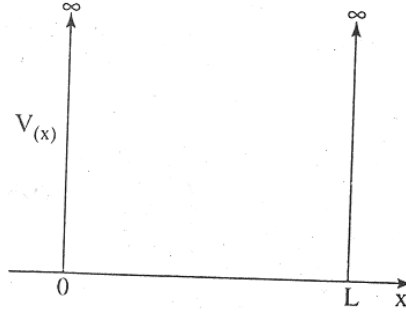V = 0 inside well and V = ∞ outside the well.

Fig.4.4 Square potential well infinite height

The time independent Schrödinger wave equation in one dimensional case

$$\frac{d^2\psi}{dx^2} + \frac{2m(E - V)}{\hbar}\psi = 0 \qquad \rightarrow (1)$$

For a particle present inside the well where V=0 and $\psi = \psi(x)$

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \qquad \rightarrow (2)$$

Let the general solution of eq (2) be

$$\psi(x) = A \sin kx + B \sin kx \qquad \rightarrow (3)$$

Where A and B are constants which can be determined from boundary conditions

$$\left. \begin{array}{l} \psi(x) = 0 \text{ at } \quad x = 0 \\ \psi(x) = 0 \quad \text{ at } x = L \end{array} \right\} \qquad \rightarrow (4)$$

And

Since $\psi(x) = 0$ at $x = 0$

$$0 = A \sin k(0) + B \cos k(0)$$

$\Rightarrow \qquad$ B = 0 $\qquad \rightarrow (5)$

Since $\psi(x) = 0$ at $x = L$

$$0 = A \sin kL$$

Which means A =0 or $\sin kL = 0$ since both A and B cannot be zero, A≠ 0. If A = 0, then $\psi = 0$ everywhere. This means that the particle is not in the well. The only meaningful way to satisfy the condition is

$$\sin kL = 0,$$

or kL = nπ ; n = 1,2,3,…

$$\therefore \quad k = \frac{n\pi}{L} \qquad \rightarrow (6)$$

Thus, eq (3) simplifies to

$$\psi(x) = A \sin\frac{n\pi}{L}x \qquad \rightarrow (7)$$

Differentiating ψ in eq (7)

$$\frac{d\psi}{dx} = A \frac{n\pi}{L} \cos\frac{n\pi}{L} x$$

Again Differentiating, we get

$$\frac{d^2\psi}{dx^2} = - A \frac{n^2\pi^2}{L^2} \sin\frac{n\pi}{L} x$$

67

$$\frac{d^2\psi}{dx^2} = -\frac{n^2\pi^2}{L^2}\ \psi\ = 0$$

$$\frac{d^2\psi}{dx^2} + \frac{n^2\pi^2}{L^2}\ \psi\ = 0 \qquad\qquad \rightarrow (8)$$

Comparing eq (2) and eq (8), we get

$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2}\ = k^2$$

$$E = \frac{n^2\ \pi^2\ \hbar^2}{2mL^2}$$

 n is called the quantum number. Thus we obtain an important result. The particle cannot possess any value of energy as assumed in classical case, but it possesses only discrete set of energy values.

The energy of the nth quantum level,

$$E_n = \frac{n^2\ \pi^2\ \hbar^2}{2mL^2}\ = \frac{n^2\ h^2}{8mL^2} \qquad (\text{since } \hbar\ = \frac{h}{2\pi}\ ) \qquad \rightarrow (9)$$

The wave functions and the corresponding energy levels of the particles are as suggested in Figure 3.5
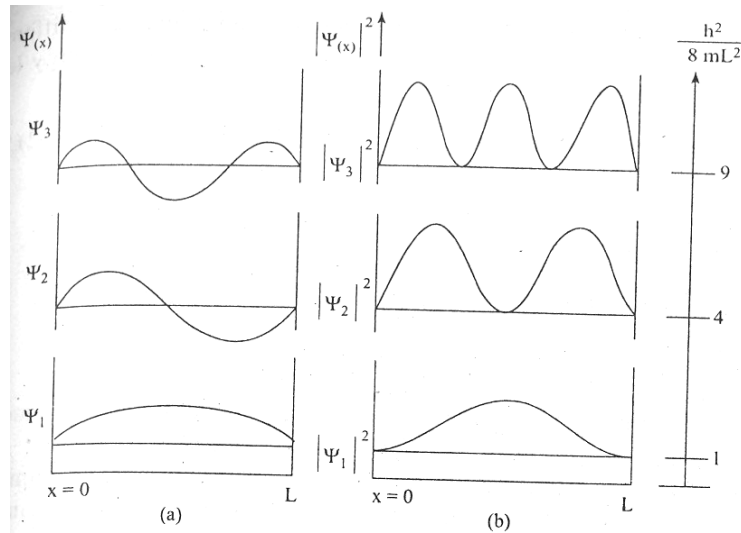

Fig.4.5 Ground state and first two excited states of an electron in a potential well: a) the electron wave functions and b) the corresponding probability density functions. The energies of these three states are shown on the right.

We are still left with an arbitrary constant 'A' in eq (7). It can be obtained by applying normalization condition i.e.; the probability of finding the particle inside the box is unity.

$$\int\limits_0^L |\psi\ x|^2\ dx\ =\ 1$$

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

$$A^2\ \int_0^L \frac{1}{2}\left[1 - cos\frac{2n\pi}{l}x\right] dx\ =\ 1$$

$$\frac{A^2}{2}\left[\text{x} - \frac{L}{2\pi n}\ sin\frac{2\pi nx}{L}\ \right]^L_{\ 0}\quad = 1$$

$$\Rightarrow \qquad \frac{A^2}{2}\left[(L-0) - (0-0)\right]\ =\ 1$$

$$\frac{A^2L}{2}\ =\ 1\ or\ \ A = \sqrt{\frac{2}{L}} \qquad\qquad \rightarrow 10)$$

∴   The normalized wave function is

$$\psi_n\ =\ \sqrt{\frac{2}{L}}\ sin\frac{n\pi x}{L} \qquad\qquad\qquad \rightarrow (11)$$

4.5.2 Particle in Three dimensional potential box

Let us consider the case of a single particle, i.e., a gas molecule of mass m, confined within a rectangular box with edges parallel to X, Y and Z axes as shown in figure.
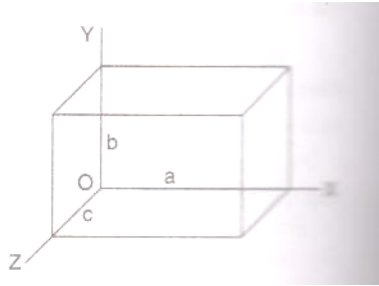

Fig 4.6 Three dimensional potential box

Let the sides of the rectangular box be a, b and c respectively. The particle can move freely within the region $0 < \text{x} < a$, $0 < y < b$ and $0 < z < c$, i.e., inside the box where potential V is zero, i.e.,

$$V\ (\text{x, y, z}) = 0, \qquad for \qquad 0 < \text{x} < a$$
$$V\ (\text{x, y, z}) = 0, \qquad for \qquad 0 < y < b$$
and $\qquad V\ (\text{x, y, z}) = 0, \qquad for \qquad 0 < z < c$

The potential rises suddenly to have a large value at the boundaries, i.e., the potential outside the box is infinite.

The Schrodinger wave equation inside the box is given by

$$\frac{\partial^2\psi}{\partial x^2}\ +\ \frac{\partial^2\psi}{\partial y^2}\ +\frac{\partial^2\psi}{\partial z^2}\ +\frac{2m}{\hbar^2}E\psi\ = 0 \qquad\qquad \rightarrow (1)$$

This is partial differential equation in three independent variables and may be solved by the method of separation of variables. The solution of equation (1) is of the form

$$\psi\ (\text{x, y, z}) = X\ (\text{x})\ Y(y)\ Z\ (z) \qquad\qquad \rightarrow (2)$$

Where X (x) is a function of x alone, Y(y) is a function of y alone and Z (z) is a function of z alone.

69

Differentiating ψ in eq (2) partially with respect to 'x', we get

$$\frac{\partial \psi}{\partial x} = \frac{\partial X(x)}{\partial x} Y(y) Z(z) \qquad \rightarrow (3)$$

Again differentiating eq (3) partially with respect to 'x', we get

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial^2 X(x)}{\partial x^2} Y(y) Z(z)$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial^2 X(x)}{\partial x^2} \frac{X(x) Y(y) Z(z)}{X(x)}$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{X} \frac{\partial^2 X}{\partial x^2} \psi \qquad \rightarrow (4)$$

Where $X = X(x)$ and $\psi = \psi(x, y, z)$

Similarly,
$$\frac{\partial^2 \psi}{\partial y^2} = \frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} \psi \qquad \rightarrow (5)$$

And
$$\frac{\partial^2 \psi}{\partial z^2} = \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} \psi \qquad \rightarrow (6)$$

Substituting eqs.(4),(5) and (6) in eq (1), we get

$$\left[\frac{1}{X} \frac{\partial^2 X}{\partial x^2} \psi + \frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} \psi + \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} \psi \right] + \frac{2m}{\hbar^2} E \psi = 0$$

$$\left[\frac{1}{X} \frac{\partial^2 X}{\partial x^2} + \frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} + \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} \right] + \frac{2m}{\hbar^2} E = 0 \qquad \rightarrow (7)$$

This equation can be written as

$$\frac{1}{X} \frac{\partial^2 X}{\partial x^2} = -\frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} - \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} - \frac{2mE}{\hbar^2} \qquad \rightarrow (8)$$

The left hand side of eq (8) is a function of x alone, while the right hand side is a function of y and z and is independent of x. both sides are equal to each other. Both sides are equal to each other. This is possible only when they are separately equal to a constant quantity, i.e.

$$\frac{1}{X} \frac{\partial^2 X}{\partial x^2} = k_x \qquad \rightarrow (9)$$

And
$$-\frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} - \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} - \frac{2mE}{\hbar^2} = k_x$$

Or
$$\frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} = -\frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} - \frac{2mE}{\hbar^2} - k_x \qquad \rightarrow (10)$$

In eq (10), the left hand side is a function of y alone while right hand side is a function of z and is independent of y. If the above equation is to be satisfied, both sides must be equal to a constant say k_y, i.e.

$$\frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} = k_y \qquad \rightarrow (11)$$

and
$$-\frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} - \frac{2mE}{\hbar^2} - k_x = k_y$$

Or
$$\frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} = -\frac{2mE}{\hbar^2} - k_x - k_y \qquad \rightarrow (12)$$

Again, we have
$$\frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} = k_z \qquad \rightarrow (13)$$

And
$$-\frac{2mE}{\hbar^2} - k_x - k_y = k_z$$

Or
$$\frac{2mE}{\hbar^2} = -k_x - k_y - k_z \qquad \rightarrow (14)$$

For convenience, introduce

70

$$k_x = -\frac{2mE_x}{\hbar^2}, \quad k_y = -\frac{2mE_y}{\hbar^2} \quad \text{and} \quad k_z = -\frac{2mz}{\hbar^2}$$

Now, the differential equations in x, y and z coordinates may be written as

$$\frac{\partial^2 X}{\partial x^2} + \frac{2mE_x}{\hbar^2} X = 0 \qquad \rightarrow (15a)$$

$$\frac{\partial^2 Y}{\partial y^2} + \frac{2mE_y}{\hbar^2} Y = 0 \qquad \rightarrow (15b)$$

And $\frac{\partial^2 Z}{\partial z^2} + \frac{2mE_z}{\hbar^2} Z = 0 \qquad \rightarrow (15c)$

The general solution of eq [(15a)] will be a sine function of the arbitrary amplitude, frequency and phase, i.e.,

$$X(x) = A \sin (Bx + C) \qquad \rightarrow (16)$$

Where A, B and C are constants whose values are determined by boundary conditions.

$|\psi|^2$ represents the probability of finding the particle at any point within the box. Therefore, $|X(x)|^2$ which is a function of x coordinates only represents the probability of Finding the particle at any point along the X-axis. As the potential is very high at the walls of the box, the probability of finding the particle at the walls will be zero, i.e.,

$$|X(x)|^2 = 0 \text{ when } x = 0 \text{ and } x = a$$
$$X(x) = 0 \text{ when } x = 0 \text{ and } x = a$$

Using the above boundary conditions in eq (16), we have

$$0 = A \sin (0 + C); \quad A \neq 0$$

$\therefore$ Sin C = 0 and $\qquad 0 = A \sin (Ba + C)$

\\ $\qquad\qquad$ Or $\qquad 0 = \sin Ba . \cos C + \cos Ba . \sin C$

$$0 = \sin Ba \cos C$$

$\therefore$ Sin Ba = 0 [since $\sin C = 0$, $\cos C$ is not zero]

$$\leftrightarrow \qquad Ba = n_x \pi$$

$$\text{Or} \quad B = \frac{n_x \pi}{a} \qquad\qquad \rightarrow (17)$$

$$\therefore \quad X(x) = A \sin \frac{n_x \pi}{a} x \qquad\qquad \rightarrow (18)$$

Applying the normalization condition between x=0 to x=a, we have

$$\int_0^a |X(x)|^2 \, dx = 1$$

$$\int_0^a \left| A \sin \frac{n_x \pi}{a} x \right|^2 dx = 1$$

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

$$\frac{A^2}{2} \int_0^a \left[1 - \cos \frac{2 n_x \pi}{a} x \right] dx = 1$$

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

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

$$A^2 = \frac{2}{a} \quad \text{or} \quad A = \sqrt{\frac{2}{a}}$$

Therefore, $X(x) = \sqrt{\frac{2}{a}} \sin \frac{n_x \pi x}{a} \qquad\qquad \rightarrow (19)$

Similarly, we can solve equations [15(b)] and [15(c)] to obtain

$$Y(y) = \sqrt{\frac{2}{b}} \text{ Sin } \frac{n_y \pi y}{b} \qquad \rightarrow (20)$$

$$Z(z) = \sqrt{\frac{2}{c}} \text{ Sin } \frac{n_z \pi z}{c} \qquad \rightarrow (21)$$

The complete wave function ψ_{n_x}, n_y, n_z has the form

$$\psi_{n_x}, n_y, n_z = \sqrt{\frac{2}{a}} \text{ Sin } \frac{n_x \pi}{a} x \sqrt{\frac{2}{b}} \text{ Sin } \frac{n_y \pi}{b} Y \sqrt{\frac{2}{c}} \text{ Sin } \frac{n_z \pi}{c} Z$$

$$= \frac{2\sqrt{2}}{\sqrt{abc}} \text{ Sin } \frac{n_x \pi}{a} x \sqrt{\frac{2}{b}} \text{ Sin } \frac{n_y \pi}{b} Y \sqrt{\frac{2}{c}} \text{ Sin } \frac{n_z \pi}{c} Z \qquad \rightarrow (22)$$

The wave function of a particle in a finite box and its probability density are shown in Figure 3.7.
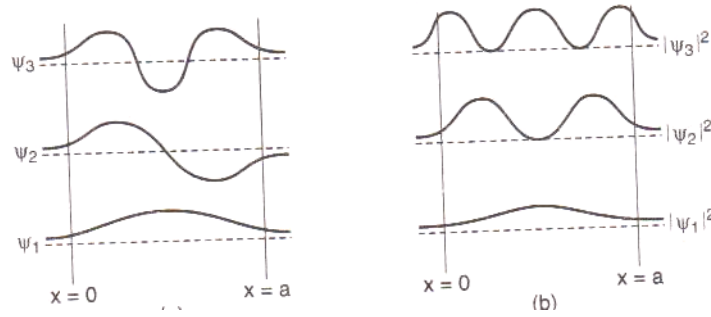

Fig 4.7 a) wave functions and b) probability densities of a particle in three dimensional box

Differentiating eq (19) twice with respect to 'x', we get

$$\frac{\partial^2 X}{\partial x^2} = -[\frac{\pi n_x}{a}]^2 \sqrt{\frac{2}{a}} \text{ Sin } \frac{n_x \pi x}{a} = -[\frac{\pi n_x}{a}]^2 X(x) \qquad \rightarrow (23)$$

Substituting eq (23) in eq [15(a)], we get

$$-[\frac{\pi n_x}{a}]^2 X(x) + \frac{2mE_x}{\hbar^2} X(x) = 0$$

$$\text{Or} \qquad \frac{2mE_x}{\hbar^2} = [\frac{\pi n_x}{a}]^2$$

$$\text{Or} \qquad E_x = \frac{\pi^2 n_x^2}{a^2} \frac{h^2}{4\pi^2} \frac{1}{2m}$$

$$E_x = \frac{h^2 n_x^2}{8ma^2} \qquad \rightarrow (24)$$

$$\text{Similarly,} \qquad E_y = \frac{h^2 n_y^2}{8mb^2} \qquad \rightarrow (25)$$

$$\text{And} \qquad E_z = \frac{h^2 n_z^2}{8mc^2} \qquad \rightarrow (26)$$

The allowed values of total energy are given by

$$E = E_x + E_y + E_z$$

$$= \frac{h^2}{8m^2} [\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}] \qquad \rightarrow (27)$$

72

Where n_x, n_y and n_z denote any set of three positive numbers.

When the box is a cube, i.e., a = b= c, the energy expression is given by

$$E = \frac{h^2}{8ma^2} \left[\frac{n_x{}^2 + n_y{}^2 + n_z{}^2}{a^2} \right] \qquad \rightarrow (28)$$

With n_x, n_y, $n_z =$

Objective Questions

I choose the correct answer

1. Davisson and germens experiment relates to: [   ]
   (a) Interference   (b) Polarization
   (c) Phosphorescence   (d) electron diffraction

2. Uncertainty principle was discovered by   _____   [   ]
   (a) Bohr   (b) de-Broglie   (c) Heisenberg   (d) Schrodinger

3. The wavelength if de-Broglie wave associated with an electron accelerated through 50 volts is   [   ]
   (a)1 A^0 (b) 1.5 A^0 (c) 1.27 A^0 (d) 1.28 A^0

4. Among the following practices moving with velocity, the particle having shortest wave associated with it is: [   ]
   a) Proton   (b) Neutron   (c) α-particle   (d) $\beta -$ Particle

5. The wavelength associated with a particle moving with velocity v is: [   ]
   (a) $\lambda = $h/$mv$ (b)$\lambda = $h^2/$mv$
   (c) $\lambda = mv$/h (d) $\lambda = \frac{(mv)^2}{h}$

6. the quantized energy do a particular of mass 'm' confined in one dimensional box of length L is   _____   [   ]
   (a) $\frac{n^2 h^2}{8mL^2}$ (b) $\frac{n^2 h^2}{8m^2 L^2}$
   (c) $\frac{n^2 h}{8mL}$ (d) $\frac{n^2 h^2}{8Lm^2}$

7 Fermi energy is the of the state at which the probability of electron is_____ at any temperature above ok   [   ]
   (a) 1   (b) 0
   (c) 0.5   (d) Any value between 0 and 1

9. If E is the kinetic energy of the material particle of mass ' m' then the de-Broglie wavelength is given by   _____   [   ]
   (a)$\frac{h}{\sqrt{2ME}}$ (b)$\frac{\sqrt{2ME}}{h}$
   (c) $h\sqrt{2ME}$ (d)$\frac{h}{2ME}$

10. If E is the kinetic energy of the material particle of mass 'm' then de-broglie wavelength is given by

                                                                [   ]

(a) Lesser than velocity of light   (b) Equal to velocity of light

(c) Greater than velocity of light   (d) none of these

11. Existence of matter waves was experimentally first demonstrated by   [   ]

     (a) Newton   (b) Planck

     (c) de-Broglie   (d) Davisson and Germer

12. Wave nature and particle nature called dual nature is exhibited by   [   ]

     (a)Waves only   (b) Particles only

     (c)Photons   (d) By both particles and waves

16. The lowest energy state of a particle of mass M confined in a linear box of size L

is: [   ]

(a) $\dfrac{h^2}{8mL^2}$ (b) $\dfrac{2h^2}{8mL^2}$ (c) $\dfrac{4h^2}{8mL^2}$ (d) $\dfrac{9h^2}{8mL^2}$

19. The wavelength associated with an electron which has been accelerated from rest application of potential of 900V is   [   ]

     (a) 0. 613A^0 (b) 0. 365A^0

     (c) 0. 4086A^0 (d) None of these

20. The normalized wave function of a particle n a one dimensional potential well

is: [   ]

(a) $\sqrt{\dfrac{L}{2}}\sin\dfrac{n\pi x}{L}$ (b) $\dfrac{\sqrt{2}}{L}\sin\dfrac{n\pi x}{L}$

(c) $\dfrac{2}{\sqrt{L}}\sin\dfrac{n\pi x}{L}$ (d) $\sqrt{\dfrac{2}{L}}\sin\dfrac{n\pi x}{L}$

21. When the potential barrier strength is zero, then E-k curve is: [   ]

                (a) Continuous parabola

                (b) Discrete energy levels

                (c) Parabola with discontinuities

                (d) Exponentially decaying function of k

II. Fill in the blanks:

        1.   Uncertainty principle was proposed by _____

        2.   Lighter the particle, _____the de-Broglie wavelength associated with it.

        3.   According to uncertainty principle, it is not possible to measure both energy and _____ of a process very accurately and simultaneously.

        4.   _____ can travel faster than velocity of light.

        5.   According to Planck's quantum theory, energy is emitted in the form of packets or quanta called _____

        6.   One dimensional time independent Schrodinger wave equation is _____

7. The wavelength associated with an electron moving under a potential of 1600V is _____

8. Fermi energy is the energy of the state at which the probability of electron occupation is _____ at any temperature above 0K.

9. At 0K, all the energy levels above Fermi level are _____

10. Lighter is the particle, _____ is the wavelength associated with it.

11. Three dimensional time independent Schrodinger's wave equation is _____

12. Matter wave is associated with _____ particle.

13. Wave functions representing _____ are ant symmetric.

14. He^4 atoms obey _____ statistics.

15. _____ is the velocity of the particle greater is the wavelength associated with it

16. The subject which deals with the relationship between the overall behavior of the system and the properties of the particles is called _____

17. Single crystal target of nickel is used in _____ experiment to prove wave nature of electrons.

18. If E_{F_0} is the Fermi-energy of an electron at 0K, then its Fermi – energy at any temperature above 0K is _____

19. .

20. All the energy levels below Fermi-level are completely filled at a temperature _____

21. Thin metallic film of gold or silver or aluminium is used as target in _____ experiment to prove wave nature of electrons.

22. When an electron moves in a periodic potential of lattice, its mass varies and this mass is called _____of the electron.

23. _____ Model proposed a simpler potential in the form of an array of square wells.

24. The representation of permissible values of K of the electrons in one, two or three dimensions is known as _____

25. The periodicity of the potential of zone theory of solids is given by _____ theorem.

26. _____ have relatively wide forbidden gaps.

27. _____ have relatively narrow band gaps.

28. According to zone theory of solids, free electrons move inside _____ potential field

29. When the band gap is in the order of 1ev in a solid, it behaves as a _____

30. _____ have either partially filled valence band or overlap of completely filled valence band with partially filled conduction band.

31. When the band gap is in the order of 7ev in a solid, it behaves as a
_____

Problems

1. **A body at 1500K emits maximum energy at a wavelength 20,000 A^0.If the sun emits maximum temperature of wavelength 5500 A^0, what would be the temperature of the Sun.**

    Solution: According to Wien's displacement law,
    $$\lambda_m T = \text{constant}$$
    $$\text{Or } \lambda_m T = \lambda_m^1 T^1$$
    $$T^1 = \frac{\lambda_m T}{\lambda_m^1} = \frac{20000 \text{ X } 1500}{5500} = 5454K$$

2. **At what temperature we can expect a 10% probability that electrons in silver have an energy which is 1% above the Fermi energy? (The Fermi energy of silver is 5.5eV.)**

    Solution: probability function
    $$F(E) = \frac{1}{1 + exp\left(\frac{E - E_F}{K_T}\right)}$$

    Given data: F (E) =10%=0.1
    $$E_F = 5.5eV$$
    $$E = E_F + \frac{1}{100} E_F$$
    $$(5.5 + 0.055) = 5.555eV$$
    $$E - E_F = 0.055eV = 0.055 \times 1.6 \times 10^{-19}J$$

    Substituting in the formula
    $$0.1 = \frac{1}{1 + exp\left(\frac{0.055 \times 1.6 \times 10^{-19}}{T \times 1.38 \times 10^{-23}}\right)}$$

    i.e.
    $$0.1 = \frac{1}{exp\left(\frac{637.7}{T}\right) + 1}$$
    $$exp\left(\frac{637.7}{T}\right) + 1 = 10$$
    $$\left(\frac{637.7}{T}\right) = \ln 9$$
    $$T = \frac{637.7}{T} = \ln 9$$
    $$T = \frac{637.7}{\ln 9}$$
    $$T = \frac{637.7}{2.197} = 290.2K$$

3. **Evaluate the Fermi function for an energy KT above the Fermi energy.**

Solution: Fermi function $F(E) = \dfrac{1}{1+exp\left(\frac{E-E_F}{K_T}\right)}$

Given that $E-E_F=KT$

$F(E) = \dfrac{1}{1+exp(1)} = \dfrac{1}{1+2.718}$

$= \dfrac{1}{3.718}$

$= 0.269$

4. **Calculate the wavelength of an electron raised to a potential 1600V.**

Solution: de-Broglie wavelength

$$\lambda = \dfrac{12.26}{\sqrt{v}} A^0$$

$$= \dfrac{12.26}{\sqrt{1600}}$$

$$= \dfrac{12.26}{40}$$

$$= 0.3065 A^0$$

5. **If the kinetic energy of the neutron is 0.025eV calculate its de-Broglie wavelength (mass of neutron =1.674X10^{-27} Kg)**

Solution: Kinetic energy of neutron

$$E = \dfrac{1}{2} mv^2 = 0.025eV$$

$$= 0.025 \times 1.6 x10^{-19} J$$

$$v = \left(\dfrac{2X0.025 \times 1.6 \times 10^{-19}}{1.674 \times 10^{-27}}\right)^{\frac{1}{2}} = (0.04779 \times 10^8)^{\frac{1}{2}}$$

$$= 0.2186 x10^4 m/s$$

$\therefore$ de- Broglie wavelength $\lambda = \dfrac{h}{mv}$

$$\lambda = \dfrac{6.626 \times 10^{-34}}{1.67 \times 410^{-27} \times 0.2186 \times 10^4}$$

$=0.181$nm

6. **Calculate the energies that can be possessed by a particle of mass 8.50 x10^{-31}kg which is placed in an infinite potential box of width 10^{-9}cm.[June 2012]**

Solution: The possible energies of a particle in an infinite potential box of width L is given by $E_n = \dfrac{n^2h^2}{8mL^2}$

M=8.50 x 10^{-31}Kg

L=1 x 10^{-11}m

h=6.626$\times$ 10^{-34}J-s

For ground state n=1

$$E_1 = \dfrac{6.626 \, X \, 10^{-34}}{8(8.50 \times 10^{-31})(1 \times 10^{-11})^2}$$

$=6.456 \times 10^{-16}$joule

For first excited state $E_2 = 4 \times 6.4456 \times 10^{-16}$

$= 258.268 \times 10^{-16}$ Joule

7. **Calculate the wavelength of matter wave associated with a neutron whose kinetic energy is 1.5times the rest mass of electron.[Given that mass of neutron=1.676×10^{-27}kg,mass of electron 9.1×10^{-31}Kg,Mass of electron 9.1×10^{-31}J-Sec,velocity of light is 3×10^{8}m/s](June 2010,set1).**

Solution: For neutron $\frac{1}{2}mv^2 = 1.5 \times 9.1 \times 10^{-31}$ Joules

Or $v^2 = \frac{2(1.5 \times 9.1 \times 10^{-31})}{1.676 \times 10^{-27}}$

$= 16.288 \times 10^{-4}$

$v = \sqrt{16.288 \times 10^{-4}}$

$= 4.046 \times 10^{-2}$ m/s

The de-Broglie wavelength expression is

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

$$= \frac{6.62 \times 10^{-34}}{1.676 \: X \: 10^{-2} \times 4.046 X 10^{-2}}$$

$= 9.76 X 10^{-6}$ m

Questions

1) Drive Schrodinger's wave equation for the motion of an electron
2) describe the experimental verification of matter waves using Davisson-Germen experiment
3) Derive an expression for the de-Broglie wavelength of an electron
4) What are the important conclusions of G.P Thomson's experiment

(Or)

Describe the experimental verification of matter waves using G.P Thomson experiment
7) Write the physical significance of wave function
8) Write short notes on:
    i)De Broglie wavelength and
    ii)Heisenberg's uncertainty principle
9) What are matter waves? Derive an expression for the wavelength of matter waves
10) Describe an experiment to establish the wave nature of electron
11) Show that the energies of a particle in a potential box are quantized .

UNIT – V

SEMICONDUCTOR PHYSICS

Introduction to Semiconductor Physics

Based on electrical conductivity, materials are divided into conductors, insulators, & semiconductors. Metals are good conductors of electricity. All dielectrics are insulators (non-conducting). Semiconductors electrical conductivity lies between metals & insulators. Good examples are Silicon and Germanium. They belong to IV-A group. At 0K, Semiconductors behave like Insulators. At temperature greater than 0K they behave like conductors. Pure germanium and silicon are called intrinsic semiconductors. By adding a small quantity of either group-III, group-V element atoms as impurity into pure Ge or Si, the electrical conductivity of the materials increases. This impure semiconductor is called extrinsic semiconductors.
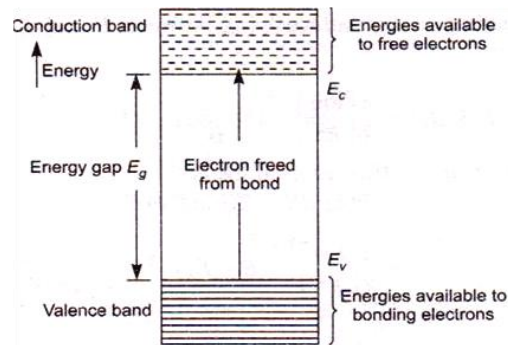
2 The energy diagram for a semiconductor, showing the energy gap
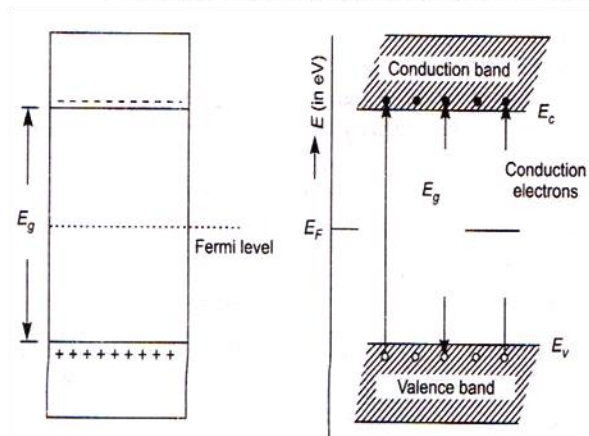
Figure 5.1 (a) Energy band diagram of a semiconductor
(b) Fermi level at T=0K & Thermal excitation of electrons at T>0K

5.1 Intrinsic Semiconductor

Pure germanium or silicon called an intrinsic semiconductor. Each atom possesses four valence electrons in outer most orbits. At T = 0K a 2-D representation of the crystal of silicon & band diagram is shown in the figure 2.
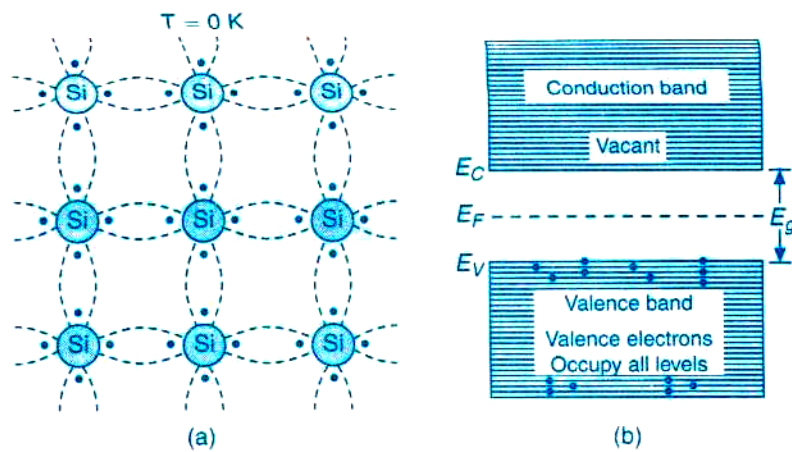

Figure5.2: Intrinsic silicon crystal at T =0K (a) 2-D representation of silicon crystal
(c) Energy band diagram of intrinsic semiconductor

Explanation: At 0K, all the valence electrons of silicon atoms are in covalent bonds and their energies constitute a band of energies called valance band (VB). So at 0K, VB is completely filled & conduction band (CB) is empty.

If we rise temperature (T>0K), some of the electrons which are in covalent bonds break the bonds become free and move from VB to CB. The energy required should be greater than the energy gap of a semiconductor (E>E_g). The electron vacancy or deficiency created in VB is called holes. This is shown in the figure 3 below.
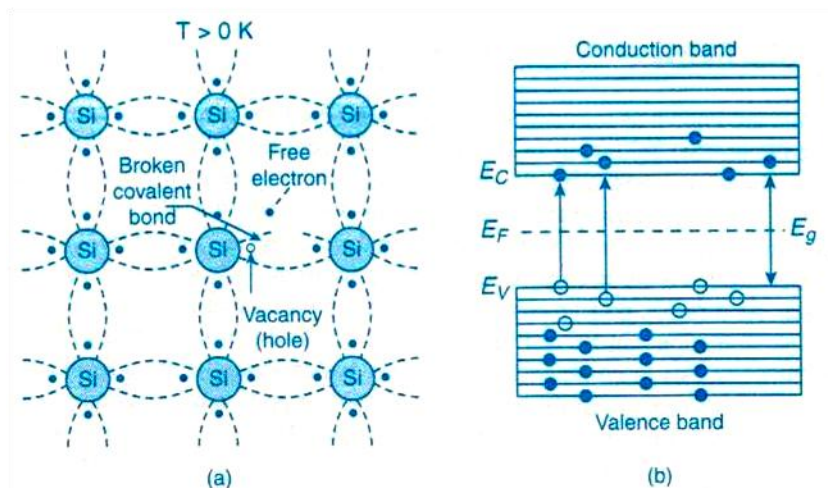

Figure5.3 Silicon crystal at temperature above 0K (a) Due to thermal energy breaking of Covalent bonds take place (b) Energy band representation

5.2 Electron concentration in intrinsic semiconductor in conduction band (n)

Definition: The no. of free electrons per unit volume of the conduction band of a given intrinsic semiconductor is called electron concentration, represented by 'n'.
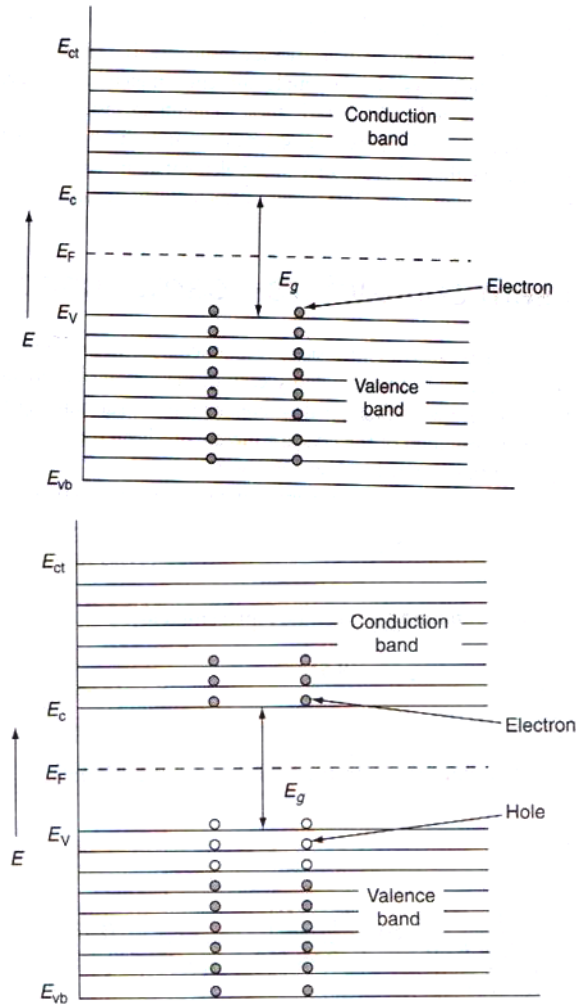

Figure5.4 (a) Energy band diagram of silicon at T = 0K
(b) Energy band diagram of silicon at T > 0K

Derivation: Let the no. of free electrons per unit volume of the semiconductor having energies E and E + dE in CB is represented by n (E) dE. It is obtained by multiplying the density of energy states Z_C (E) d (E). [No. of energy states per unit volume] and Fermi – Dirac distribution function for the Probability of occupation of electrons F_C (E)

Therefore $\quad\quad$ n (E) dE = [Z_C (E) d (E)] [F_C (E)] → (1)

Where Z_v (E) d (E) = Density of energy states

$\quad\quad$ F_h (E) = Probability of occupation of electrons given by Fermi – Dirac function

The total no. of electrons in CB per unit volume between the energies E_C to E_{ct} is given by integrating equation (1) with limits E_C to E_{ct}

$$n = \int_{E_C}^{E_{ct}} n(E)dE \rightarrow (2)$$

But equation (2) can be written as

81

$$n = \int_{E_C}^{\infty} n(E)dE + \int_{\infty}^{E_{ct}} n(E)dE \rightarrow (3)$$

$$n = \int_{E_C}^{\infty} n(E)dE - \int_{E_{ct}}^{\infty} n(E)dE \rightarrow (4)$$

In equation (4) the second term vanishes (disappears).

Since, above E_{ct} electrons do not present. Hence equation (4) becomes

$$n = \int_{E_C}^{\infty} n(E)dE$$

$$n = \int_{E_C}^{\infty} [Z_C (E) \, dE] \times [F_C (E)] \rightarrow (5)$$

{Since from equation (1)}

But $[F_C (E)]$ is Fermi – Dirac distribution function;

$$F_C (E) = \frac{1}{1+e^{\frac{E-E_F}{K_B T}}} \rightarrow (6)$$

Here $\quad E > E_F, \quad i.e. \quad e^{\frac{E-E_F}{K_B T}} \gg 1$

Hence '1' can be neglected in equation (6)

$$F_C (E) = \frac{1}{e^{\frac{E-E_F}{K_B T}}}$$

$$F_C (E) = e^{\frac{E_F - E}{K_B T}} \rightarrow (7)$$

Also the density of electrons

$$Z_C (E) \, d (E) = \frac{\pi}{2} \left[\frac{8 m_e^*}{h^2}\right]^{\frac{3}{2}} (E)^{\frac{1}{2}} \, dE \rightarrow (8)$$

Here $E > E_C$ .Since E_C is the minimum energy state in CB. Hence equation (8) becomes

$$Z_C (E) \, d (E) = \frac{\pi}{2} \left[\frac{8 m_e^*}{h^2}\right]^{\frac{3}{2}} (E - E_C)^{\frac{1}{2}} \, dE \rightarrow (9)$$

Substituting equations (7) & (9) in equation (5) we get

$$n = \int_{E_C}^{\infty} \frac{\pi}{2} \left[\frac{8 m_e^*}{h^2}\right]^{\frac{3}{2}} (E - E_C)^{\frac{1}{2}} \, e^{\frac{E_F - E}{K_B T}} \, dE$$

$$n = \frac{\pi}{2} \left[\frac{8 m_e^*}{h^2}\right]^{\frac{3}{2}} \int_{E_C}^{\infty} (E - E_C)^{\frac{1}{2}} \, e^{\frac{E_F - E}{K_B T}} \, dE \rightarrow (10)$$

Let $\quad \varepsilon = E - E_C$

$\quad d\varepsilon = dE$ { E_C is constant} . The limits are $\varepsilon = 0$ to $\varepsilon = \infty$

Hence equation (10) can be written as

$$n = \frac{\pi}{2} \left[\frac{8 m_e^*}{h^2}\right]^{\frac{3}{2}} \int_{\varepsilon=0}^{\infty} (\varepsilon)^{\frac{1}{2}} \, e^{\frac{E_F - (\varepsilon + E_C)}{K_B T}} \, d\varepsilon$$

$$n = \frac{\pi}{2} \left[\frac{8 m_e^*}{h^2}\right]^{\frac{3}{2}} \, e^{\frac{(E_F - E_C)}{K_B T}} \int_{\varepsilon=0}^{\infty} (\varepsilon)^{\frac{1}{2}} \, e^{\frac{-\varepsilon}{K_B T}} \, d\varepsilon \rightarrow (11)$$

In equation (11) But $\int_{\varepsilon=0}^{\infty} (\varepsilon)^{\frac{1}{2}} \, e^{\frac{-\varepsilon}{K_B T}} \, d\varepsilon = \frac{\sqrt{\pi}}{2} \, (k_B T)^{\frac{3}{2}} \rightarrow (12)$

Substituting (12) in (11) we get

$$n = \frac{\pi}{2} \left[\frac{8 m_e^*}{h^2}\right]^{\frac{3}{2}} \, e^{\frac{(E_F - E_C)}{K_B T}} \, \frac{\sqrt{\pi}}{2} \, (k_B T)^{\frac{3}{2}}$$

$$n = \frac{1}{4}\left[\frac{8\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}} e^{\frac{(E_F - E_C)}{K_B T}}$$

$$n = \frac{8}{4}\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}} e^{\frac{(E_F - E_C)}{K_B T}}$$

$$n = 2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}} e^{\frac{-(E_C - E_F)}{K_B T}} \rightarrow (13)$$

{Here $N_C = 2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}}$} Therefore $n = N_C \ e^{\frac{-(E_C - E_F)}{K_B T}}$

5.3 Hole concentration in the valance band of intrinsic semiconductor(p)

Definition: The number of holes per unit volume of the valance band of a given intrinsic semiconductor is called hole concentration, represented by 'p'.

Derivation: Let the number of holes per unit volume of the semiconductor having energies E, E + dE in VB is represented by p (E) dE. It is obtained by multiplying the density of energy states Z_V (E) d (E) [No. of energy states per unit volume] and Fermi – Dirac distribution function for the Probability of occupation of holes F_h (E).
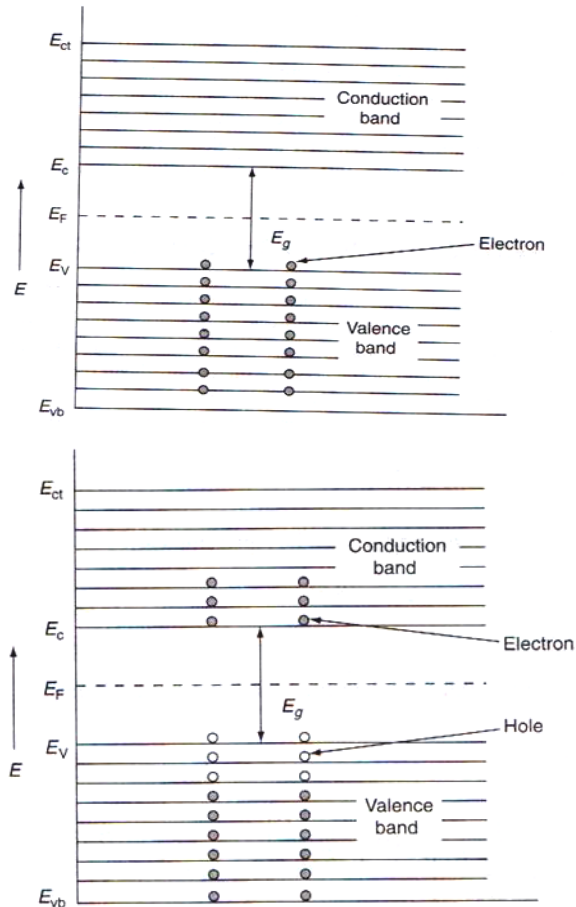

Figure5.5 (a) Energy band diagram of silicon at T = 0K
(b) Energy band diagram of silicon at T > 0K

Therefore   p (E) dE = [Z_v (E) d (E)] [F_h (E)] → (1)
Where Z_v (E) d (E) = Density of energy states.

$$F_h(E) = \text{Hole probability given by Fermi} - \text{Dirac function}$$

The total no. of holes in VB per unit volume between the energies E_{vb} to E_v is given by integrating equation (1) with limits E_{vb} to E_v

$$p = \int_{E_{vb}}^{E_v} p(E)dE \rightarrow (2)$$

But equation (2) can be written as

$$p = \int_{E_{vb}}^{-\infty} p(E)dE + \int_{-\infty}^{E_v} p(E)dE \rightarrow (3)$$

$$p = -\int_{-\infty}^{E_{vb}} p(E)dE + \int_{-\infty}^{E_v} p(E)dE \rightarrow (4)$$

In equation (4) the first term vanishes (disappears).

Since, below E_{vb} holes do not present. Hence equation (4) becomes

$$p = \int_{-\infty}^{E_v} p(E)dE$$

$$p = \int_{-\infty}^{E_v} [Z_v(E)dE] \times F_h(E) \rightarrow (5)$$

{Since from equation (1)}

But $[F_h(E)]$ is Fermi − Dirac distribution function;

$$F_h(E) = 1 - F_C(E) \rightarrow (6)$$

$$= 1 - \frac{1}{1+e^{\frac{E-E_F}{K_B T}}}$$

Simplifying; $\qquad F_h(E) = \dfrac{e^{\frac{E-E_F}{K_B T}}}{1+e^{\frac{E-E_F}{K_B T}}}$

Divide by $\quad e^{\frac{E-E_F}{K_B T}}\quad$ we get

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

$$F_h(E) = \frac{1}{1+e^{\frac{E_F-E}{K_B T}}} \rightarrow (6)$$

Here $\qquad E_F > E, \qquad i.e.\ e^{\frac{E_F-E}{K_B T}} \gg 1$

Hence '1' can be neglected in equation (6)

$$F_h(E) = \frac{1}{e^{\frac{E_F-E}{K_B T}}}$$

$$F_h(E) = e^{\frac{E-E_F}{K_B T}} \rightarrow (7)$$

Also the density of holes

$$Z_v(E)\ d(E) = \frac{\pi}{2}\left[\frac{8m_p^*}{h^2}\right]^{\frac{3}{2}} (E)^{\frac{1}{2}}\ dE \rightarrow (8)$$

Here $E < E_v$. Since E_v is the maximum energy state in VB. Hence equation (8) becomes

$$Z_v(E)\ d(E) = \frac{\pi}{2}\left[\frac{8m_p^*}{h^2}\right]^{\frac{3}{2}} (E_V - E)^{\frac{1}{2}}\ dE \rightarrow (9)$$

Substituting equations (7) & (9) in equation (5) we get

$$p = \int_{-\infty}^{E_v} \frac{\pi}{2}\left[\frac{8m_p^*}{h^2}\right]^{\frac{3}{2}} (E_V - E)^{\frac{1}{2}}\ e^{\frac{E-E_F}{K_B T}}\ dE$$

$$p = \frac{\pi}{2}\left[\frac{8m_p^*}{h^2}\right]^{\frac{3}{2}} \int_{-\infty}^{E_v} (E_V - E)^{\frac{1}{2}} e^{\frac{E-E_F}{K_BT}} \, dE \rightarrow (10)$$

Let $\quad \varepsilon = E_V - E$

$\quad\quad d\varepsilon = -dE$ { E_V is constant} . The limits are $\varepsilon = \infty \; to \; \varepsilon = 0$

Hence equation (10) can be written as

$$p = \frac{\pi}{2}\left[\frac{8m_p^*}{h^2}\right]^{\frac{3}{2}} \int_{\varepsilon=\infty}^{0} (\varepsilon)^{\frac{1}{2}} e^{\frac{(E_V-\varepsilon)-E_F}{K_BT}} \, d\varepsilon$$

$$p = \frac{\pi}{2}\left[\frac{8m_p^*}{h^2}\right]^{\frac{3}{2}} e^{\frac{(E_V-E_F)}{K_BT}} \int_{\varepsilon=0}^{\infty} (\varepsilon)^{\frac{1}{2}} e^{\frac{-\varepsilon}{K_BT}} \, d\varepsilon \rightarrow (11)$$

In equation (11) But $\quad \int_{\varepsilon=0}^{\infty} (\varepsilon)^{\frac{1}{2}} e^{\frac{-\varepsilon}{K_BT}} \, d\varepsilon = \frac{\sqrt{\pi}}{2} (k_BT)^{\frac{3}{2}} \rightarrow (12)$

Substituting (12) in (11) we get

$$p = \frac{\pi}{2}\left[\frac{8m_p^*}{h^2}\right]^{\frac{3}{2}} e^{\frac{(E_V-E_F)}{K_BT}} \frac{\sqrt{\pi}}{2} (k_BT)^{\frac{3}{2}}$$

$$p = \frac{1}{4}\left[\frac{8\pi m_p^* K_BT}{h^2}\right]^{\frac{3}{2}} e^{\frac{(E_V-E_F)}{K_BT}}$$

$$p = \frac{8}{4}\left[\frac{2\pi m_p^* K_BT}{h^2}\right]^{\frac{3}{2}} e^{\frac{(E_V-E_F)}{K_BT}}$$

$$p = 2\left[\frac{2\pi m_p^* K_BT}{h^2}\right]^{\frac{3}{2}} e^{\frac{-(E_F-E_V)}{K_BT}} \rightarrow (13)$$

{Here $N_V = 2\left[\frac{2\pi m_p^* K_BT}{h^2}\right]^{\frac{3}{2}}$}

$$p = N_V \, e^{\frac{-(E_F-E_V)}{K_BT}}$$

5.4 Fermi energy level in intrinsic semiconductor

At temperature T k , the electron concentration 'n' is equal to hole concentration 'p' in intrinsic semiconductor.

i.e. $\quad\quad\quad\quad\quad\quad\quad\quad\quad n = p$

$$2\left[\frac{2\pi m_e^* K_BT}{h^2}\right]^{\frac{3}{2}} e^{\frac{-(E_C-E_F)}{K_BT}} = 2\left[\frac{2\pi m_p^* K_BT}{h^2}\right]^{\frac{3}{2}} e^{\frac{-(E_F-E_V)}{K_BT}}$$

On simplifying we get

$$(m_e^*)^{\frac{3}{2}} e^{\frac{-(E_C-E_F)}{K_BT}} = (m_p^*)^{\frac{3}{2}} e^{\frac{-(E_F-E_V)}{K_BT}}$$

$$\frac{e^{\frac{-(E_C-E_F)}{K_BT}}}{e^{\frac{-(E_F-E_V)}{K_BT}}} = \frac{(m_p^*)^{\frac{3}{2}}}{(m_e^*)^{\frac{3}{2}}}$$

$$e^{\frac{E_C+E_F+E_F-E_V}{K_BT}} = \left[\frac{m_p^*}{m_e^*}\right]^{\frac{3}{2}}$$

$$e^{\frac{2E_F}{K_BT}-\frac{(E_C-E_V)}{K_BT}} = \left[\frac{m_p^*}{m_e^*}\right]^{\frac{3}{2}}$$

Taking logarithms on both sides we get

$$\frac{2E_F}{K_BT} - \frac{(E_C-E_V)}{K_BT} = \frac{3}{2} \, ln\left[\frac{m_p^*}{m_e^*}\right]$$

85

$$\frac{2E_F}{K_BT} = \frac{(E_C - E_V)}{K_BT} + \frac{3}{2} \, ln[\frac{m_p^*}{m_e^*}]$$

$$E_F = \frac{(E_C + E_V)}{2} + \frac{3}{4} K_B T \, ln[\frac{m_p^*}{m_e^*}] \qquad \{At\ T > 0K\}$$

Let T = 0K $\qquad E_F = \frac{(E_C + E_V)}{2}$

This means E_F lies in the middle between $(E_C\ \&\ E_V)$ of the energy gap 'E $_g$'

As the temperature increases the electrons move from VB to CB. Also the Fermi level slightly rises upwards towards CB. Hence $E_F = \frac{(E_C + E_V)}{2} + \frac{3}{4} K_B T \, ln[\frac{m_p^*}{m_e^*}]$. It is shown in the figure 6 below.
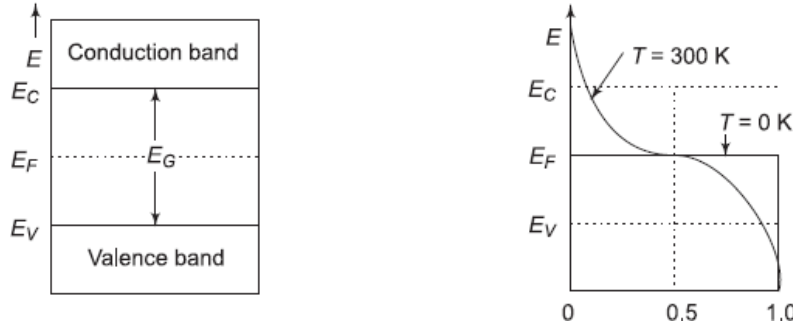
Figure5.6 (a) Fermi level E_F at T = 0K (b) Upward shift of E_F near E_C at T> 0k

5.5 Intrinsic carrier concentration (n$_i$)

Definition: The no. of free electrons and holes per unit volume of the intrinsic semiconductor is called intrinsic carrier concentration (n $_i$) remains constant.

i .e. $\qquad$ n = p = n$_i$

n p = (n$_i$) (n$_i$)

$n_i^2 = (n\ p) \rightarrow (1)$

$n_i = (np)^{\frac{1}{2}} \rightarrow (2)$

Consider equation (1) $\qquad n_i^2 = (n\ p)$

$$n_i^2 = 2[\frac{2\pi m_e^* K_B T}{h^2}]^{\frac{3}{2}} \, e^{\frac{-(E_C - E_F)}{K_B T}} \times 2[\frac{2\pi m_p^* K_B T}{h^2}]^{\frac{3}{2}} \, e^{\frac{-(E_F - E_V)}{K_B T}}$$

$$= 4\left[\frac{2\pi K_B T}{h^2}\right]^3 (m_e^* m_p^*)^{\frac{3}{2}} \, e^{\frac{-E_C + E_F - E_F + E_V}{K_B T}}$$

$$n_i^2 = 4\left[\frac{2\pi K_B T}{h^2}\right]^3 (m_e^* m_p^*)^{\frac{3}{2}} \, e^{\frac{-E_g}{K_B T}} \{Since\ E_C - E_V = E_g\}$$

$$n_i = 2\left[\frac{2\pi K_B T}{h^2}\right]^{\frac{3}{2}} (m_e^* m_p^*)^{\frac{3}{4}} \, e^{\frac{-E_g}{2K_B T}}$$

If $m_e^* = m_p^* = m^*$, the above equation becomes

$$n_i = 2\left[\frac{2\pi K_B T}{h^2}\right]^{\frac{3}{2}} (m^*)^{\frac{3}{2}} \, e^{\frac{-E_g}{2K_B T}}$$

$$n_i = 2\left[\frac{2\pi m^* K_B T}{h^2}\right]^{\frac{3}{2}} e^{\frac{-E_g}{2K_B T}}$$

Let $\qquad 2\left[\frac{2\pi m^* K_B T}{h^2}\right]^{\frac{3}{2}} = C.$

Then $\qquad\qquad\qquad\qquad n_i = C\,[T]^{\frac{3}{2}}\,e^{\frac{-E_g}{2K_B T}}$

5.6. Extrinsic (or) Impure semiconductor

Introduction: The conductivity of an intrinsic semiconductor can be increased by adding small amounts of impurity atoms, such as III rd or Vth $_{group}$ atoms. The conductivity of silica is increased by 1000 times on adding 10 parts of boron per million part of silicon. The process of adding impurities is called doping and the impurity added is called dopant.

5.6.1 N – Type semiconductor

In a pure (intrinsic) semiconductor, when pentavalent an impurity like Phosphorous atom consisting of five valance electrons is doped, and then concentration of electrons increases than holes. Hence the given semiconductor formed is called N – type semiconductor. This is shown in the figure 7a below. By adding donor impurities, the free electrons generated or donated, form an energy level called as "Donor energy level" i.e. E_D is shown in the figure 9.7b below.
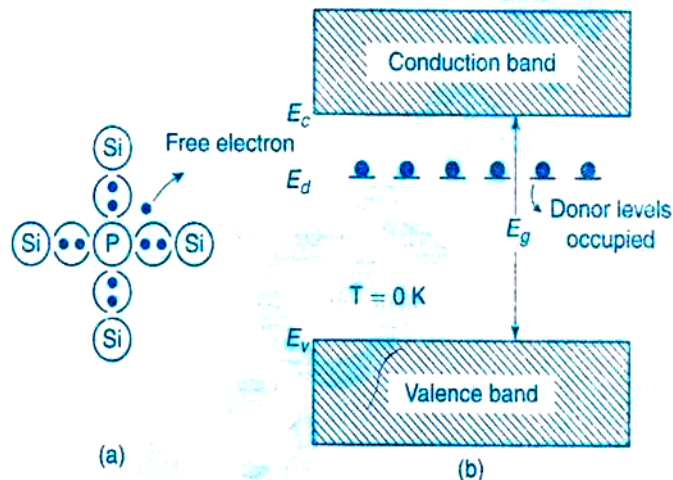

Figure5.7 (a) Representation of n- type silicon at T = 0K (b) Energy band diagram at T = 0K

In the figure (b) E_F is Fermi energy level is in between E_C & E_D at T = 0K.

Hence $E_F = \frac{E_C + E_D}{2}$. The donor level 'E_D' is near to E_F consisting of free electrons. But CB is empty.

5.6.2 Variation of Fermi level E_F with respect to temperature in N -type

As temperature increases the electrons in the Donor level $'E_D'$ moves into CB leaving holes. Also The Fermi level slightly shifts upwards towards CB. If further increase of temperature is done, the hole concentration also increases with respect to electron concentration. Hence it reaches again the concentration of n = p i.e. an intrinsic semiconductor. At lasts the Fermi level drops in the middle of the energy gap (or) Forbidden band gap, indicating a pure semiconductor that is towards 'E_i'. This happens only for very high temperatures as shown in the figure 8 below.
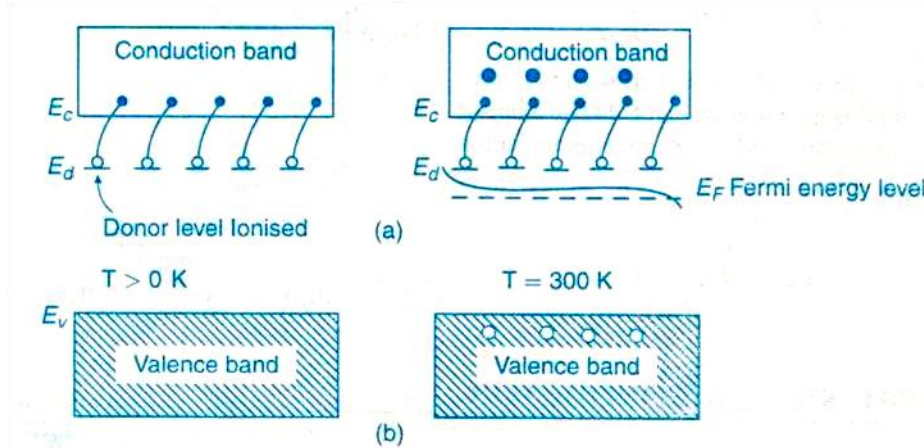
Fig5.8 Variation of Fermi level wrt temperature in n- type semiconductor

5.6.3 Variation of E_F with respect to donor concentration

As the donor concentration increases the Fermi level decreases (lowers) as in case of intrinsic semiconductor 'E_i. This is shown in the figure below
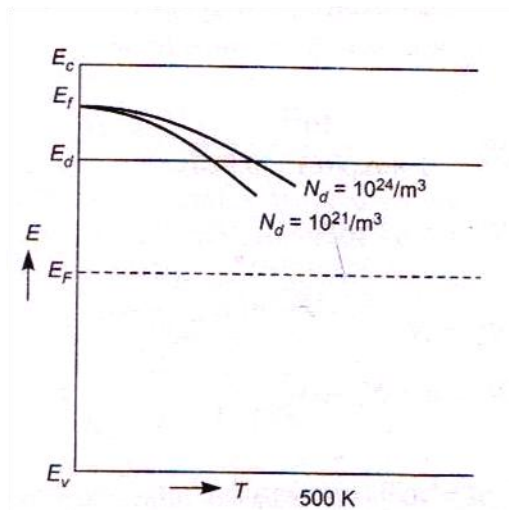

Figure5.9 Variation of Fermi level with temperature for different donor concentrations in an n-type semiconductor

5.6.4. Carrier concentration in N – type semiconductor & Density of electrons in CB

Let N_D is the donor concentration (no. of donor atoms per unit volume). Let it be written as

Or written as
$$= N_D \exp\left[\frac{-(E_F - E_D)}{K_B T}\right]$$

$$= N_D e^{\frac{-(E_F - E_D)}{K_B T}} \rightarrow (1)$$

The density of electrons in CB in pure semiconductor is given by

$$= 2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}} e^{\frac{-(E_C - E_F)}{K_B T}} \rightarrow (2)$$

At very low temperatures the no. of electrons in CB must be equal to the no. of donor atoms per unit volume. Hence equating equations (1) & (2) we get

$$2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}} e^{\frac{-(E_C - E_F)}{K_B T}} = N_D e^{\frac{-(E_F - E_D)}{K_B T}}$$

$$\frac{e^{\frac{-(E_C + E_F)}{K_B T}}}{e^{\frac{-(E_F + E_D)}{K_B T}}} = \frac{N_D}{2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}}}$$

$$e^{\frac{-E_C + E_F + E_F - E_D}{K_B T}} = \frac{N_D}{2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}}}$$

$$e^{\frac{2E_F - (E_C + E_D)}{K_B T}} = \frac{N_D}{2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}}}$$

Taking logarithms on both sides we get

$$\frac{2E_F - (E_C + E_D)}{K_B T} = \log\left[\frac{N_D}{2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}}}\right]$$

$$2E_F - (E_C + E_D) = K_B T \log\left[\frac{N_D}{2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}}}\right]$$

$$E_F = \frac{(E_C + E_D)}{2} + \frac{K_B T}{2} \log\left[\frac{N_D}{2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}}}\right] \quad \{At\ T>0K\} \rightarrow (3)$$

Case I: At T= 0K

$$E_F = \frac{(E_C + E_D)}{2}. \text{ That is } E_F \text{ lies between } E_C \ \& \ E_D$$

Case II: At T>0K. As temperature increases the Fermi level slightly shifts upwards towards CB, hence
$$E_F = \frac{(E_C + E_D)}{2} + \frac{K_B T}{2} \log\left[\frac{N_D}{2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}}}\right]$$

Density of electrons in CB in extrinsic semiconductor:

Here consider equation (2). That is

$$= 2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}} e^{\frac{-(E_C - E_F)}{K_B T}}$$

OR

$$= 2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}} e^{\frac{(E_F - E_C)}{K_B T}}$$

Substitute the value of E_F from equation (3) in equation (2), it becomes

$$n_{(Extrinsic\ N-type)}$$

$$n_{(Extrinsic\ N-type)} =$$

$$2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}} \exp\left\{\frac{\frac{(E_C+E_D)}{2}+\frac{K_B T}{2}\log\left[\frac{N_D}{2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}}}\right]-E_C}{K_B T}\right\}$$

On simplifying

We know that $\exp(a+b) = \exp(a) \times \exp(b)$

Also $\quad \exp(\log x) = x$

$$= 2\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{2}} \exp\left[\frac{(E_D-E_C)}{2K_B T}\right]\left\{\frac{(N_D)^{\frac{1}{2}}}{(2)^{\frac{1}{2}}\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{4}}}\right\}$$

$$n_{(Extrinsic\ N-type)} = (2N_D)^{\frac{1}{2}}\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{4}} \exp\left[\frac{-(E_C-E_D)}{2K_B T}\right]$$

OR

$$n_{(Extrinsic\ N-type)} = (2N_D)^{\frac{1}{2}}\left[\frac{2\pi m_e^* K_B T}{h^2}\right]^{\frac{3}{4}} e^{\left[\frac{-(E_C-E_D)}{2K_B T}\right]}$$

5.6.5 P- type semiconductor

P – Type semiconductor is formed by doping with trivalent impurity atoms (acceptor) like III rd group atoms i.e. Aluminum, Gallium, and Indium etc to a pure semiconductor like Ge or Si. As the acceptor trivalent atoms has only three valance electrons & Germanium , Silicon has four valence electrons; holes or vacancy is created for each acceptor dopant atom. Hence holes are majority and electrons are minority. It is shown in the figure 10a below. Also an acceptor energy level 'E_A' is formed near VB consisting of holes, as shown in the figure 10b below.
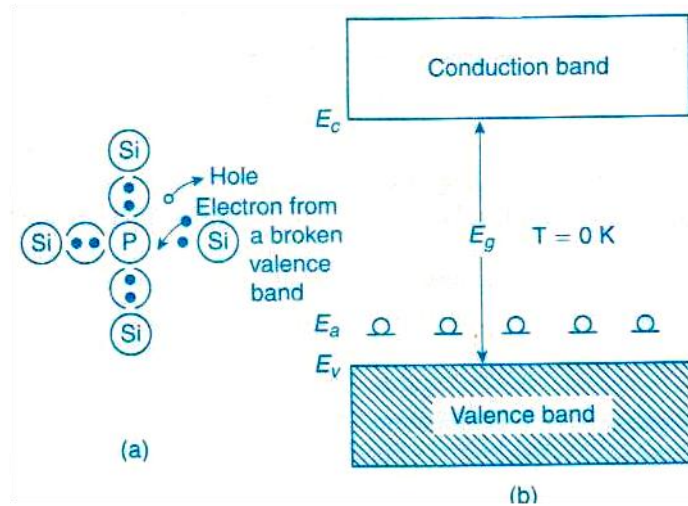

Fig.5.10 (a) Representation of p- type silicon at T = 0K (b) Energy band diagram at T =0K

As temperature increases (T>0K) the electrons in VB which are in covalent bonds break the bonds become free and move from VB to acceptor energy level E_A.

90

Variation of Fermi level E_F with respect to temperature in P- type semiconductor

As temperature increases the Fermi level E_F slightly drops towards VB. For further increase of high temperatures the electron concentration also increases with respect to hole concentration. Hence a condition is reached such that 'n = p' i.e. it becomes an intrinsic or pure semiconductor. Hence the Fermi level increases and reaches to intrinsic level E_i as in case of pure semiconductor. This is shown in the figure 11 below
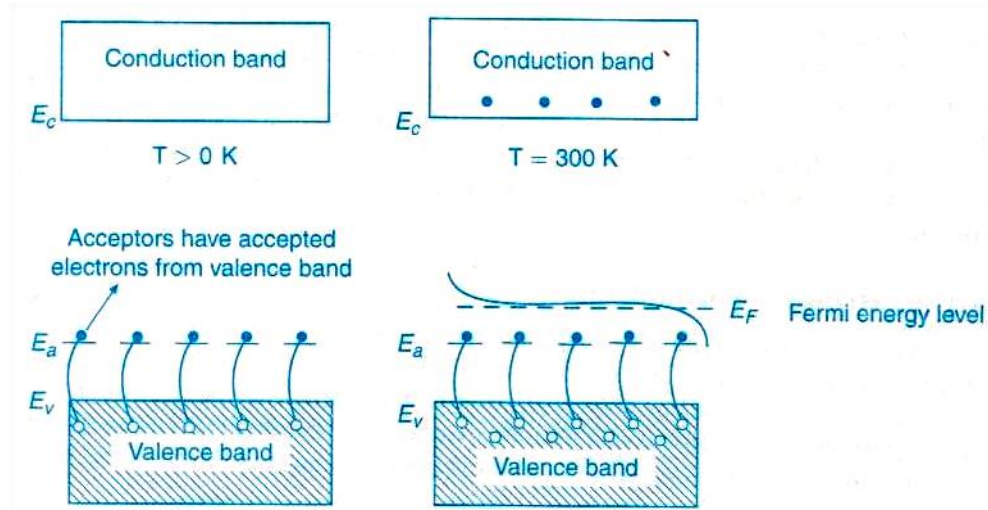

Figure5.11 Variation of Fermi level wrt temperature in p- type

Variation of Fermi level with respect to acceptor concentration:

Also as the acceptor concentration increases we find that Fermi level E_F reaches (increases) towards intrinsic level E_i as in case of pure or intrinsic semiconductor. This is shown in the figure 12 below.
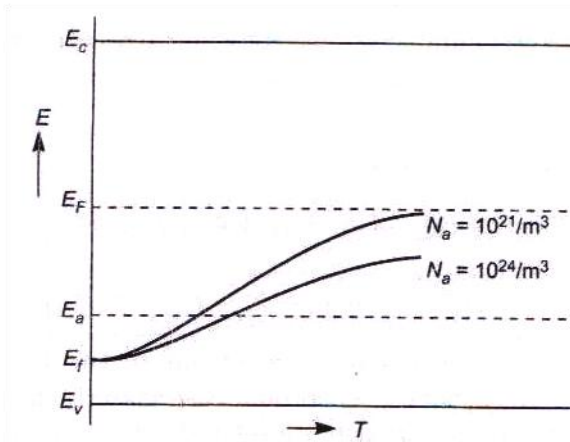

Fig 5.12 Variation of Fermi level with temperature for different acceptor concentrations in a p-type

Carrier concentration of P- type semiconductor & Density of holes in VB

Let N $_A$ is the acceptor concentration (no. of acceptor atoms per unit volume). Let it be written as

$$= N_A \exp \left[\frac{-(E_A - E_F)}{K_B T}\right]$$

Or written as

$$= N_A \, e^{\frac{(E_F - E_A)}{K_B T}} \rightarrow (1)$$

The density of holes in VB in pure semiconductor is given by

$$= 2\left[\frac{2\pi m_P^* K_B T}{h^2}\right]^{\frac{3}{2}} e^{\frac{-(E_F - E_V)}{K_B T}} \rightarrow (2)$$

At very low temperatures the no. of holes in VB must be equal to the no. of acceptor atoms per unit volume. Hence equating equations (1) & (2) we get

$$2\left[\frac{2\pi m_P^* K_B T}{h^2}\right]^{\frac{3}{2}} e^{\frac{(-E_F + E_V)}{K_B T}} = N_A e^{\frac{(E_F - E_A)}{K_B T}}$$

$$\frac{e^{\frac{(-E_F + E_V)}{K_B T}}}{e^{\frac{(E_F - E_A)}{K_B T}}} = \frac{N_A}{2\left[\frac{2\pi m_P^* K_B T}{h^2}\right]^{\frac{3}{2}}}$$

$$e^{\frac{-E_F + E_V - E_F + E_A}{K_B T}} = \frac{N_A}{2\left[\frac{2\pi m_P^* K_B T}{h^2}\right]^{\frac{3}{2}}}$$

$$e^{\frac{-2E_F + (E_V + E_A)}{K_B T}} = \frac{N_A}{2\left[\frac{2\pi m_P^* K_B T}{h^2}\right]^{\frac{3}{2}}}$$

Taking logarithms on both sides we get

$$\frac{-2E_F + (E_V + E_A)}{K_B T} = \log\left[\frac{N_A}{2\left[\frac{2\pi m_P^* K_B T}{h^2}\right]^{\frac{3}{2}}}\right]$$

$$-2E_F + (E_V + E_A) = K_B T \log\left[\frac{N_A}{2\left[\frac{2\pi m_P^* K_B T}{h^2}\right]^{\frac{3}{2}}}\right]$$

$$E_F = \frac{(E_V + E_A)}{2} - \frac{K_B T}{2} \log\left[\frac{N_A}{2\left[\frac{2\pi m_P^* K_B T}{h^2}\right]^{\frac{3}{2}}}\right] \quad \{At\ T>0K\} \rightarrow (3)$$

Case I: At T= 0K

$$E_F = \frac{(E_V + E_A)}{2} . \text{That is } E_F \text{ lies between } E_V \ \& \ E_A$$

Case II: At T>0K. As temperature increases the Fermi level slightly drops towards VB, hence

$$E_F = \frac{(E_V + E_A)}{2} - \frac{K_B T}{2} \log\left[\frac{N_A}{2\left[\frac{2\pi m_P^* K_B T}{h^2}\right]^{\frac{3}{2}}}\right]$$

Density of electrons in CB in extrinsic semiconductor

Here consider equation (2). That is

$$= 2\left[\frac{2\pi m_p^* K_B T}{h^2}\right]^{\frac{3}{2}} e^{\frac{-(E_F - E_V)}{K_B T}}$$

OR

$$= 2\left[\frac{2\pi m_p^* K_B T}{h^2}\right]^{\frac{3}{2}} e^{\frac{(-E_F + E_V)}{K_B T}}$$

Substitute the value of E_F from equation (3) in equation (2), it becomes

$n_{(Extrinsic\ P-type)}$

$$n_{(Extrinsic\ P-type)} = 2\left[\frac{2\pi m_p^* K_B T}{h^2}\right]^{\frac{3}{2}} \exp\left\{\frac{\left[\frac{-(E_V+E_A)}{2}+\frac{K_B T}{2}\log\left[\frac{N_A}{2\left[\frac{2\pi m_p^* K_B T}{h^2}\right]^{\frac{3}{2}}}\right]\right]+E_V}{K_B T}\right\}$$

On simplifying

We know that exp (a + b) = exp (a) × exp (b)

    Also   exp (log x) = x

$$= 2\left[\frac{2\pi m_p^* K_B T}{h^2}\right]^{\frac{3}{2}} \exp\left[\frac{(E_V-E_A)}{2K_B T}\right]\left\{\frac{(N_A)^{\frac{1}{2}}}{(2)^{\frac{1}{2}}\left[\frac{2\pi m_p^* K_B T}{h^2}\right]^{\frac{3}{4}}}\right\}$$

$$n_{(Extrinsic\ P-type)} = (2N_A)^{\frac{1}{2}}\left[\frac{2\pi m_p^* K_B T}{h^2}\right]^{\frac{3}{4}} \exp\left[\frac{-(E_A-E_V)}{2K_B T}\right]$$

$$OR$$

$$n_{(Extrinsic\ P-type)} = (2N_A)^{\frac{1}{2}}\left[\frac{2\pi m_p^* K_B T}{h^2}\right]^{\frac{3}{4}} e^{\left[\frac{-(E_A-E_V)}{2K_B T}\right]}$$
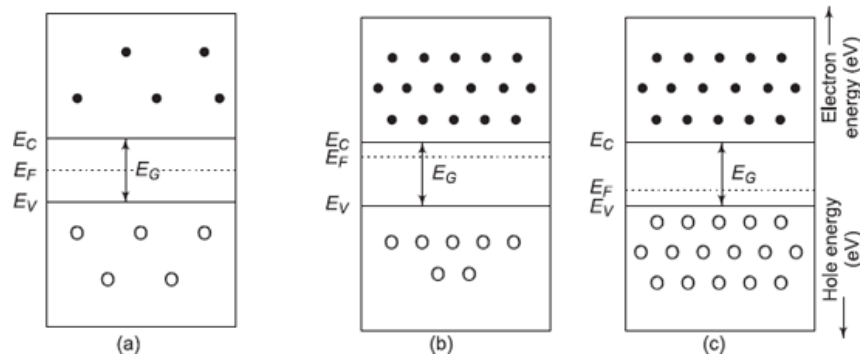

Fig. 5.13Energy band diagrams of (a) Intrinsic semiconductor (b) N- type & (c) P- type   semiconductors

Direct and Indirect band gap semiconductors

Direct band gap semiconductor	Indirect band gap semiconductor

1.These are impure   or Extrinsic or compound
  semiconductors
	1.These are pure or intrinsic or elemental
	  Semiconductors
	
	2. Examples : Ge, Si

2. Examples : InP, GaAs, GaAsP etc 3.	3.

Figure: E-K curve

Figure: E-K curve

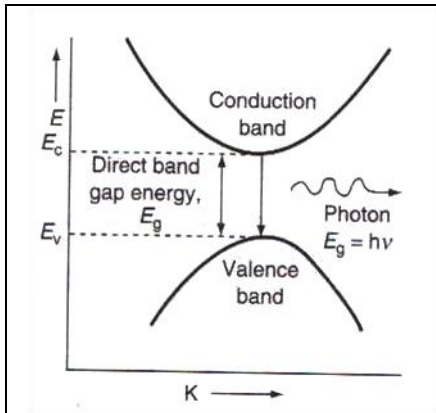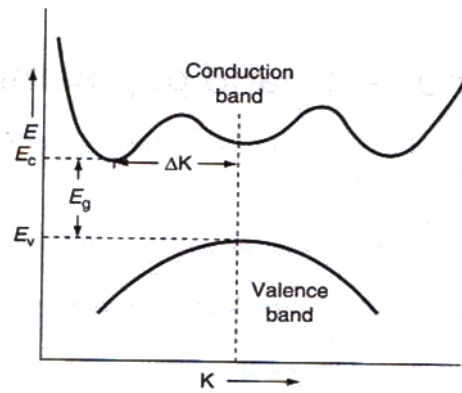|	
4. The minimum energy of Conduction band (CB) and maximum energy of valence band (VB) have the same value of wave vector , i.e. $k_1 = k_2$	4. The minimum energy of Conduction band (CB) and maximum energy of valence band (VB) have the different values of wave vector, i.e. $k_1 \neq k_2$
5. Here an electron from CB to can recombine with a hole in VB directly by emitting light of photon of energy 'hϑ'.	5. Here an electron from CB cannot recombine directly with holes in VB. But can recombine through traps by emitting light without emission of photon or light.
6. They are used to fabricate LEDs, Laser Diodes etc.	6. They are used to amplify the signals in electronic devices like rectifiers, transistors, amplifiers etc.
7. Life time (recombination rate) of charge carriers is less.	7. Life time of charge carriers is more.
8. Emission of light has energy gap is $$E_g = \frac{hC}{\lambda} \text{ eV}$$	8. No emission of light. It conducts only Electricity.

Hall Effect

Determination of Hall coefficient R_H, Hall voltage V_H & Applications of Hall Effect
Definition:
If a piece of semiconductor carrying a current 'I' is placed in a transverse or perpendicular magnetic field, then an Electric field 'E_H' is generated in perpendicular to

both 'I' and 'B'. Hence production of Hall electric field 'E$_H$' and generation of Hall voltage V$_H$ by applying current 'I' & 'B' in perpendicular directions is called Hall Effect.

Derivation of R$_H$, V$_H$, & E$_H$:

Assume an N – type semiconductor. Let 'I' be the current passed along X- axis. Let 'B' the magnetic field applied along 'Z' axis. Due to current 'I', due to the flow of electrons, the force acting on electrons is in opposite direction to the direction of conventional current.

Due to the magnetic field 'B' there is a down ward force act on each electron given by Bev. This makes the electrons deviated in a down ward direction along Z – axis. This causes a negative charge to accumulate on the bottom face.

Hence $\qquad\qquad\qquad$ F$_{B =}$ Bev

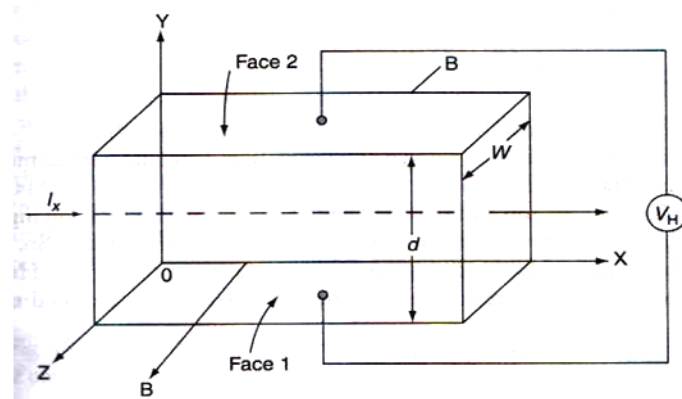Where 'e' = charge of electron, v = velocity of electron

Fig. 9.14 A semiconductor applied to current and magnetic field perpendicularly in Hall Effect

A potential difference is formed from top to bottom of the specimen. The potential difference causes a field E$_H$ to flow along negative Y- axis. Due to E$_H$ along negative Y- direction a force of eE$_H$ acts in upward direction along positive Y- axis.

Hence $\qquad\qquad\qquad$ F$_E$ = e E$_H$

Under equilibrium condition

Upward force due to E$_H$ = Downward force due to B.

$$F_B = F_E$$
$$e\ E_H = Bev$$
$$v = \frac{E_H}{B} \to (1)$$

If J is the current density then J = nev

$$v = \frac{J}{ne} \to (2)$$

Equating (1) & (2) we get $\qquad \dfrac{E_H}{B} = \dfrac{J}{ne}$

$$E_H = \frac{JB}{ne}$$
$$E_H = [\frac{-1}{ne}]\ B\ J$$

Let Hall coefficient $\qquad\qquad$ R$_H$ = $\dfrac{-1}{ne}$ $\qquad$ for electrons

$$R_H = \frac{-1}{pe} \quad \text{for holes}$$

Hence $\quad E_H = R_H \, B \, J \rightarrow (4)$

$$R_H = \frac{E_H}{B \, J} \rightarrow (5)$$

Where n= electron density, P = hole density, E_H = Hall electric field, R_H = Hall coefficient

B = magnetic field, J = current density

Experimental determination of R_H

Consider equation (5)

$$R_H = \frac{E_H}{B \, J}$$

Let V_H is the Hall voltage across the sample of thickness 't'

Generally $\qquad\qquad V = Ed$

In Hall effect $\qquad\qquad V_H = E_H \times t$

$$E_H = \frac{V_H}{t} \rightarrow (6)$$

If 'b' is the width of the sample semiconductor, Area 'A', thickness 't'

Area = breadth × thickness

$$A = b \times t$$

We know that current density $\quad J = \frac{I}{A}$

$$J = \frac{I}{b \, t} \rightarrow (7)$$

Substituting equations (6) & (7) in (5) we get

$$R_H = \frac{[\frac{V_H}{t}]}{B[\frac{I}{b \, t}]}$$

Hall coefficient $\qquad R_H = \frac{V_H \times b}{B \times I} \rightarrow (8)$

Where V_H = Hall voltage, b = breadth of a semiconductor, B = magnetic field

I = current due to flow of electron

$$V_H = \frac{R_H \, B \, I}{b} \rightarrow (9)$$

Applications of Hall Effect

1. For determination of type of given semiconductor.
   For N-type, Hall coefficient R_H = negative; For P-type, Hall coefficient R_H = Positive

2. To determine carrier concentration 'n' and 'p' ; that is n = p= $\frac{1}{R_H \, e}$

3. Determination of mobility of charge carriers (μ)

$$\sigma = ne\mu$$

$$\mu = \left[\frac{1}{ne}\right]\sigma = R_H \, \sigma$$

$$\mu = [\frac{V_H \; b}{B \; I}]\sigma \; , \qquad \text{Where } \sigma = \text{electrical conductivity}$$

4. For measurement of magnetic flux density 'B' & Hall voltage.
5. To determine the sign of charge carriers, whether the conductivity is due to electrons or holes.

QUESTIONS

1) a) what is Hall Effect? Derive an expression for Hall efficient for p-type semiconductor

b) For semiconductor, the Hall efficient is $-68 \times 10^{-5} m^3$/coulomb & electrical conductivity is

$250 m^{-1} \Omega^{-1}$ calculate the density &mobility of charge carriers.

2) a) Derive an expression for density of holes in insect semiconductor.

b) For intense semiconductor of band gap of 0.78ev, find campier concentrations at $37^0 c$

[given that the effective mass of electron=effective mass of hole=rest mass of electron]

3) a) Derive an expression for campier concentrations of n-type.

b) Explain the variation of E_F wrt temperature in N - type

c) If effective mass of holes is 5 times that of elements at what temperature would the E_F be

shifted by 15% from middle of forbidden gap(E_g). Given $E_{g=}1.2ev$

4) a) Density of electron in N-type –Derivation

b) Explain Hall Effect &its significance

c) Calculate interstices carrier concentration for Ge at $27^0 c$ [for Ge atomic weight =72.6, Density=5400kg/m^3 Band gap Eg=0.7ev]

5)a) Draw & Explain the Energy Band diagram of a p-n junction diode in an unbiased Conduction.

6) a) Derive an expression for density of holes in intrinsic semiconductor

b) Write notes on direct &indirect Band gap.

7) a) Density of electrons-Derivation

b) Explain the variation of E_F wrt Donor &accepter concentration

c) Explain the variation of E_f wrt temperature in 'N & P' type.

8) a) Draw the energy band diagram of An Intrinsic N-Type, P- Type, E_F, E_D, E_A levels.

b) Define Hall effect derive R_H, V_H &applications of Hall effect

c) The current in P-N junction at $27^0 c$ is 0.18µA when a reverse bias voltage is applied. Calculate the current when FB of 0.98 V is applied.

) Distinguish between intrinsic &extrinsic semiconductor

SOLVED PROBLEMS

1) The intrinsic carrier density at room temperature in Ge is $2.37 \times 10^{19}/m^3$. If electron & hole nobilities are 0.38 &0.18 $m^2 v^{-1} s^{-1}$.calculate the resistivity

Given data:
$$n_i = 2.37 \times 10^{19}/m^3$$
$$\mu_n = 0.38 \ m^2 v^{-1} s^{-1}.$$
$$\mu_{p} = 0.18 \ m^2 v^{-1} s^{-1}.$$
$$P = ?$$

$$\sigma_i = (n \ e \ \mu_n + p \ e \ \mu_p)$$
$$n = p = n_i$$
$$\sigma_i = n_i e \ (\mu_n + \mu_p)$$
$$\frac{1}{\rho_i} = n_i e \ (\mu_n + \mu_p) \qquad \{since \qquad \sigma_i = \frac{1}{\rho_i}\}$$
$$\rho_i = \frac{1}{2.37 \times 10^{19} \times 1.6 \times 10^{-19} \times (0.38 + 0.18)}$$
$$\rho_i = 0.471 \Omega$$

2) For silicon E_g=1.12ev. Find E_F at 300k if $m_e^* = 0.12 m_o$ & $m_p^* = 0.28 \ m_o$

Given data:
$$E_g = 1.12ev$$
$$T = 300k$$
$$m_e^* = 0.12 m_o \quad \& \ m_p^* = 0.28 \ m_o$$
$$k_B = \frac{1.38 \times 10^{-23}}{1.61 \times 0^{-19}} \quad ev k^{-1} \quad [\text{Joules to eV}]$$
$$E_F = \frac{E_C + E_v}{2} + \frac{3}{4} K_B T \ln \left(\frac{mp^*}{me^*}\right)$$
$$\frac{E_C + E_V}{2} = E_F \quad (OR) \qquad E_C - E_V = E_g$$

$$E_F = \frac{E_C + E_V}{2} \quad (OR) \ \frac{E_C + E_V}{2} = \frac{E_g}{2}$$
$$E_F = \frac{1.12}{2} + \frac{3}{4} \times \frac{1.38 \times 10^{-23} \times 300}{1.6 \times 10^{-19}} \ln \left(\frac{0.28 m_o}{0.12 m_o}\right)$$

$$E_V = 0.576ev.$$

3) For intrinsic semiconductor with Band gap of E_g =0.78ev calculate intrinsic carrier at 37^0c (300k) if $m_e^* = m_p^* = m_0$=rest mass of electron.

Given data :
$$E_g = 0.78 \ ev = 0.78 \times 1.6 \times 10^{-19} \text{ Joules.}$$
$$T = 37^0 c = 300k$$
$$m_o = 9.1 \times 10^{-31} \text{ kg}$$
$$K_B = 1.38 \times 10^{-23} \text{ J/K}$$

$$\text{Formula } n_i = 2 \left[\frac{2\pi K_B T}{h^2} \right]^{\frac{3}{2}} \exp \left(\frac{-E_g}{2 k_B T}\right)$$
$$n_i = 2 \left[\frac{2 \times 3.14 \times 9.10 \times 10^{-31} \times 1.38 \times 10^{-23}}{(6.625 \times 10^{-34})^2} \right] \times \exp \left(\frac{-0.78 \times 1.6 \times 10^{-19}}{2 \times 1.38 \times 10^{-23} \times 300}\right)$$
$$n_i = 33.49 \times 10^{18}/m^3$$

4) If the effective mass of holes is 5 times that of electrons, at what temperature would the Fermi level be shifted by 15% from the middle of Eg. [Given$E_g = 1.2ev$]

5) For a semiconductor, the Hall coefficient is $-6.85 \times 10^{-5}/m^3$ & electrical conductivity is 250 $m^{-1}\Omega^{-1}$.calculate the coulomb density & mobility of charge carriers.

Given data **:** $\qquad\qquad R_H = -6.85 \times 10^{-5}/m^3 coulomb$

$$\sigma = 250 m^{-1}\Omega^{-1}$$

Density of elements 'n' =no of atoms/unit volume=?

Mobility μ =?

We know Hall coefficient $\quad R_H = \dfrac{-1}{ne}$

$$n = \dfrac{-1}{R_H e}$$

$$n = \dfrac{1}{6.85 \times 10^{-5} \times 1.6 \times 10^{-19}}$$

n = 9.124×10²²atoms/m³

Conductivity $\sigma = ne\mu$

Mobility μ $= \dfrac{\sigma}{ne}$

$$\mu = \dfrac{250 \times 1}{9.124 \times 10^{22} \times 1.6 \times 10^{-19}}$$

μ = 17.125×10⁻³m²v⁻¹s⁻¹

6) The R$_H$ is 33.66×10$^{-4}m^3c^{-1}$. its resistivity is 8.93×10^{-3}Ωm. find μ & n

Given data: $\qquad\qquad$ R$_H$=3.66×10$^{-4}m^3c^{-1}$

$$\sigma = \dfrac{1}{\rho} = \dfrac{1}{8.93 \times 10^{-3}} \Omega^{-1}m^{-1}$$

Formula:- $\quad R_H = \dfrac{-1}{ne}$

Density' n' $\quad = \dfrac{-1}{R_H e}$

$$= \dfrac{1}{3.66 \times 10^{-4} m^3 c^{-1}}$$

n=1.708 atoms/m³

Mobility μ=?

But σ=neμ

$$\mu = \dfrac{\sigma}{ne} = \dfrac{1}{\rho ne}$$

$$\mu = \dfrac{1}{8.93 \times 10^{-3}} \times \left(\dfrac{1}{ne}\right)$$

$$= \dfrac{R_H}{8.93 \times 10^{-3}}$$

$$= \dfrac{3.66 \times 10^{-3}}{8.93 \times 10^{-3}} = 0.041m²v⁻¹s⁻¹$$

OBJECTIVE QUESTIONS

Semiconductor physics and devices:

1. In intrinsic semiconductor the carrier concentration varies as $\underline{T^{3/2}}$.

2. At 0K pure silicon is insulator.

3. The majority charge carriers in p-type Ge are holes .

4. The electric current in a pure semiconductor when voltage is applied is due to holes and electrons.

5. In an intrinsic semiconductor .The resistivity of pure si at 0^0c is 300 m. The intrinsic carrier concentration per cubic metre is =0.14 and =0.05m^2 v^{-1} s^{-1} is 1.095×10^{17}

7. If the drift velocity of electrons under a field gradient of 1000vm^{-1} is 4ms^{-1}, their mobility is $\underline{4 \times 10^{-3}}$

8. In an intrinsic semiconductor at 0k, the fermi level lies at centre of top of the valence band and bottom of conduction band.

9. The density of charge carriers in a pure semiconductor is proportional to $\underline{\exp(-E_g/2KT)}$.

10. The ratio of the diffusion constant for hole(D_P) to the mobility of hole ( ) is proportional to $\underline{T}$.

11. The einstein relationship between the diffusion constant D and mobility for electron is $D_n/$ is $\underline{KT/e}$.

12. Since $m_h^* > m_e^*$ in the energy gap with increse of temoerature the fermi level is just above the middle and rises slightly.

13. Mobilities of electrons and holes are proportional to $\underline{T^{-3/2}}$.

14. To prepare a p-type semiconductor the element to be added with Ge is aluminium.

15. To prepare a n-type semiconductor,the element to be added with si is Arsenic .

16. In n-type semiconductors,density of electrons in the conduction band is given by $\underline{n=(2N_d)^{1/2}(2\pi\ m_e^* kT/h^2)^{3/4} \exp(E_d - E_c/2kT)}$.

17. In an intrinsic semiconductor the density of electrons is given by $\underline{n=2\ (2\pi\ me^* kT/h^2)^{3/2} \exp(E_f - E_c/2kT)}$.

18. In an intrinsic semiconductor the density of holes is given by $\underline{n=2\ (2\pi\ m_h^* kT/h^2)^{3/2} \exp(E_v - E_f/2kT)}$

19. Intrinsic carrier concentration is given by $\underline{n_i = 2(2\pi\ KT/h^2)^{3/2}\ (m_e^* m_h^*)^{3/4} \exp-(\ E_g/2kT)}$

20. In p-type semiconductor,density of holes in the valence band is given by $\underline{p=\ (\ 2N_a)^{1/2}\ (2\pi\ m_h^* kT/h^2)^{3/4} \exp(E_v - E_a/2kT)}$.

21. At moderately low temperatures the density of electrons in the conduction band of a n-type semiconductor is proportional to square root of the donor concentration.

22. At moderately low temperatures the density of holes in the valence band of a p-type semiconductor is proportional to square root of acceptor concentration.

23. Hall co.efficient is used to calculate mobility of charge carrier.

24. Concentration of charge carrier can be calculated by Hall co.efficient.

25. For an n-type semiconductor the hall co.efficient R_H is related to carrier concentration by $\underline{R_H = -1/ne}$.

26. If b is the width of the sample,V_h the hall voltage developed when placed in magnetic field of induction B,and current I flows through it,then hall co.efficient is given by $\underline{R_H = V_H t/IB}$.

27. The ratio of diffusion co.efficient to mobility of carriers is proportional to T.

28. Type of semiconductor can be identified using Hall co.efficient.

29. In an intrinsic semiconductor, the electrical conductivity is proportional to $T^{1/2}$.

30. Minority carrier life time is the time taken for the excess charge carriers to reduce to

1/e of its initial value.

31. Electrical conductivity of a semiconductor at absolute zero of temperature is zero.

32. In intrinsic semiconductor the electron concentration is equal to hole concentration.

33. For p-type semi conductor trivalent typr of atoms are added to si.

34. For n-type semiconductor pentavalent type of atoms are added to Ge.

35. Diffusion coefficients and mobility relation is given by Einstein relation.

36. If the effective mass of a hole is greater than the effective mass of an electron,then the position of fermi level in intrinsic semiconductor is just above the centre of energy gap.

37. The excess concentration of holes injected into a semiconductor decreases exponentially with time.

38. If the Hall coefficient is negative then the semiconductor is n-type.

39. Solids are classified into metals,semiconductors,insulators.

40. In metals the valence band and the conduction band overlap with each other.

41. Semiconductors have finite forbidden energy gap between the valence band and the CB.

42. Insulators have much larger band gaps.

43. Ge and Si are the important semiconductors which are widely used in manufacturng of diodes and transistors.

44. At room temperature the thermal energy is sufficient to break covalent bonds.When a covalent bond is broken a free electron-hole pair is generated.

45. Pentavalent impurities contribute through donor electrons.

46. Trivalent impurities contribute through acceptor holes.

47. The conductivity of semiconductor is dependent on the number of charge carriers, their mobilities and electron charge