MODULE 4
Material Science

Classical free electron theory (Drude Lorentz theory)

Metals are good conductors of heat and electricity. Such a high conductivity is due to the presence of free electrons in the metals. The Classical free electro theory developed by Drude and Lorentz was able to explain certain experimental observations. Theory was based on certain assumptions which are listed below.

Assumptions of classical free electron theory:

1) A metal is imagined as the structure of 3-dimensional array of ion cores (consists of a nucleus surrounded by the inner electrons) in between which there are freely moving valence electrons confined to the body of the materials. Such freely moving electrons cause electrical conduction under an applied field and hence referred to as conduction electrons.

2) The free electrons are treated as equivalent to gas molecules and thus they are assumed to obey the laws of kinetic theory of gases.
   The energy associated with each electron at a temperature T is $\frac{1}{2} mv_{th}^2 = 3/2kT$
   Where k is the Boltzmann constant and v_{th} is the thermal velocity or rms velocity.

3) The electric potential due to the ionic cores is taken to be constant throughout the body of the metal

4) The electrostatic repulsion between the electrons and the attractive force between the free electrons and the ion cores are considered to be negligible.

Expression for electrical conductivity

Based on classical free electron theory the expression for electrical conductivity of a conductor is

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

Where σ is the electrical conductivity, n is the number of free electrons per unit volume, 'τ' is the mean collision time, 'm' is the mass of the electron and 'e' is the charge on the electron.

Failures of classical free electron theory

1. **specific heat:**
   Molar specific heat of gas at constant volume is $C_v = 3/2R$
   According to classical free electron theory electron gas is expected to behave as gas molecules. Therefore, it must have specific heat 3/2R, which is independent of the temperature.
   But experimentally it is found that $C_v \approx 10^{-4} RT$
   It is far smaller than the expected value and also proportional to the temperature T.

2. **Temperature dependence of electrical conductivity**
   According to the classical free electron theory, electrical conductivity is inversely proportional to $\sqrt{T}$ i.e. $\sigma \alpha \frac{1}{\sqrt{T}}$

But experimentally it is observed that for metals electrical conductivity is inversely proportional to the temperature T i.e. $\sigma \alpha \dfrac{1}{T}$

3. Dependence of electrical conductivity on the electron concentration

According to classical free electron theory, electrical conductivity $\sigma = \dfrac{ne^2\tau}{m}$ where n is the electron concentration. Therefore $\sigma \alpha$ n

Since electron concentration n is more for the trivalent metals than the monovalent metals electrical conductivity σ should be more for trivalent metals than that for monovalent metals. But experimentally it is observed that monovalent metals are good conductors compared to trivalent metals.

For example, copper (monovalent metal) is having electrical conductivity $5.88 \times 10^7/\Omega$-m whereas aluminium (trivalent metal) is having conductivity $3.65 \times 10^7/\Omega$-m.

Quantum free electron theory

Applying the quantum mechanical principles Arnold Somerfield succeeded in overcoming many of the drawbacks of the classical free electron theory. Main assumptions of quantum free electron theory are

1. The energy values of the conduction electrons are quantized. The allowed energy values are realized in terms of a set of energy levels.
2. The distribution of the electron in the various allowed energy levels occurs as per Pauli's exclusion principle.

The following assumptions of the classical free electron theory continue to be applicable in quantum free electron theory.
3. The electrons travel in a constant potential inside the metal but stay confined within its boundaries.
4. The attractive force between electron and lattice and repulsive force between electrons are ignored.

Density of states

There are large numbers of allowed energy levels in solid materials. A group of energy levels close to each other is called as energy band. The number of energy levels in each band will be extremely large. The distribution of energy levels in the band follows certain pattern and it is realized by what is called density of states.

The density of states is the number of available energy states per unit volume per unit energy interval at a particular energy E. It is denoted by a function g(E).

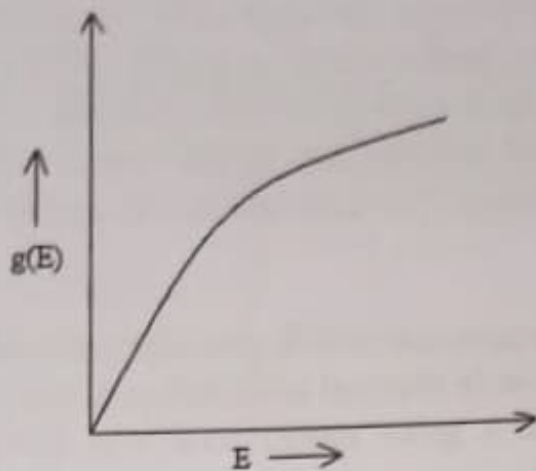The number of energy states between energies E and E+dE per unit volume is given by

$$g(E)dE = \left[\dfrac{8\sqrt{2}\pi m^{\frac{3}{2}}}{h^3} \right] E^{\frac{1}{2}} dE$$

$$= CE^{\frac{1}{2}} dE \qquad \text{Where } C = \left[\dfrac{8\sqrt{2}\pi m^{\frac{3}{2}}}{h^3} \right] \text{ is a constant}$$

Plot of g(E) Vs. E is as shown in the figure.

Fermi Energy

We know that for a metal containing N atoms there will be N allowed energy levels in each band. As per the Pauli's exclusion principle each energy level can accommodate a maximum of two electrons, one with spin up and other with spin down. Any system always tries to be in the state of lowest energy state. At absolute zero the conduction electron starts occupying each of the allowed levels starting from the lowest one. Thus pair of electrons one with spin up and another with spin down occupy the lowest level. The next pair of electrons will occupy the next higher level, and so on. When all the electrons are accommodated, still there are number of energy levels are left vacant. Therefore below a particular energy level all the energy levels are completely filled and all the energy levels above it will remain completely vacant.

The energy of the level corresponding to the highest occupied state at absolute zero is called Fermi energy. Fermi energy is denoted by E_F, and the corresponding level is Fermi level. Thus at T=0K all the energy levels lying above the Fermi level is completely empty and those lying below the Fermi level is completely filled.

vacant energy levels

E_F

Filled Energy levels
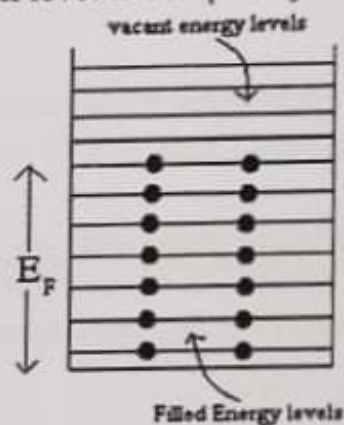
Fermi-Dirac statistics

In a metal there will be very large number of free electrons and each one of them can possess energy corresponding to any of the energy states in the conduction band. But number of energy states available will be much more than the number of free electrons. Therefore, no orderliness is expected. However, there exists orderliness in the energy possessed by the electron when the temperature is same throughout the body. Under thermal equilibrium the free electrons acquire energy obeying the statistical rule known as Fermi-Dirac statistics.

Fermi-Dirac statistics is applicable to the assembly of particles which obey the Pauli's exclusion principle. They must also be identical particles of spin ½ and are indistinguishable. Since electrons satisfy these conditions they obey Fermi-Dirac statistics

Fermi-Dirac statistics permits the evaluation of probability of finding electrons occupying energy levels in a certain energy range. The evaluation is done through a function called Fermi factor. With the knowledge of Fermi factor f(E) and density of states g(E) one can find the distribution of electrons among the various energy levels of material under thermal equilibrium conditions. This distribution is known as Fermi-Dirac distribution.

Fermi factor

The Fermi factor is an expression which gives the probability of occupation of a given energy state for a material in thermal equilibrium at any temperature.

The probability f(E) that a given energy level with energy E is occupied at steady temperature T is given by

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

This is called **Fermi factor**

Let us consider the different cases of distribution as follows

1. Probability of occupation when $E < E_F$ at T=0K

   when T=0K and $E < E_F$

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

   $\therefore$ f(E) = 1 When $E < E_F$

   $\therefore$ At T=0K all the energy levels below the Fermi level are occupied.

2. Probability of occupation when $E > E_F$ at T=0K

   when T=0K and $E > E_F$

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

   $\therefore$ f(E) = 0 When $E > E_F$

At T=0 all the energy levels above Fermi level are unoccupied.
The variation of f(E) for different energy values at T=0 is as shown in the figure.

3. Probability of occupation at ordinary temperature:

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

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

Further for $E > E_F$ the probability value falls off to zero very rapidly.
Variation of f(E) for T > 0K is as shown in the figure.

VARIATION OF f(E) WITH E
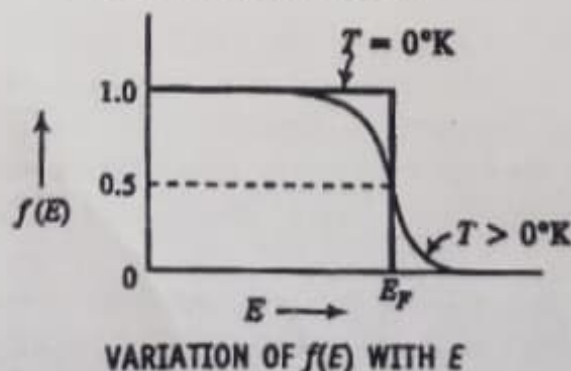
Carrier Concentration in metals

The number of charge carriers per unit volume is called *carrier concentration*

The number of electrons per unit volume having the energy between E and E+dE is given by

$$N(E)dE = g(E)dE \times f(E)$$

The elecron concentration is given by

$$n = \int_0^\infty N(E)dE = \int_0^\infty g(E).f(E)dE$$

Fermi temperature

Fermi temperature T_F is that temperature at which the average thermal energy of the free electron in the solid becomes equal to Fermi energy at 0K.

But thermal energy is kT

$\therefore kT_F = E_{F0}$

But for all practical purposes $E_{F0} = E_F$

$\therefore kT_F = E_F$

or $T_F = E_F/k$

Fermi temperature is the theoretical concept If $E_F = 5eV$ then $T_F = 66000K$. At such a temperature system is no longer in the solid form.
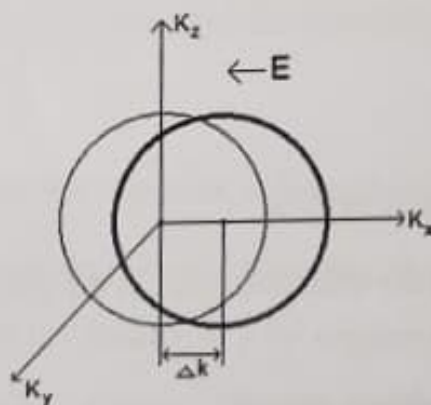
Fermi velocity

The energy of the electrons which are at the Fermi level is E_F. **The velocity of the electrons which occupy the Fermi level is called Fermi velocity v_F.**

$\therefore E_F = \frac{1}{2}mv_F^2$

or $v_F = \left(\frac{2E_F}{m}\right)^{\frac{1}{2}}$

Electrical conductivity based on quantum free electron theory:

The momentum of the conduction electron is given by

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

If the momenta of electron are plotted in k-space, we obtain points, each point corresponds to the tip of the k vectors. The maximum value of k is k_F. The sphere having radius k_F represents the Fermi surface. All points inside the Fermi sphere are occupied. Thus Fermi

surface separates occupied states from the unoccupied states. For every occupied state k there will be occupied state $-k$ as a consequence the net momentum of the electrons is zero. Therefore, there is no current flow across the material.

When an electric field is applied, electrons experience a force F which is given by

$$F = \frac{dp}{dt} = -eE$$

$$h\frac{dk}{dt} = -eE$$

$$dk = -\frac{eE}{h}dt$$

Above equation represents the equation of motion of electron in the presence of applied field. Due to the change in the momentum of electrons the Fermi sphere is displaced opposite to the field direction. Integrating the above equation, we get

$$k(t) - k(o) = -\frac{eE}{h}t$$

Thus if the electric field is applied at time t=0 to a filled Fermi sphere centered at the origin of the k space then in a characteristic time $\tau_F = \frac{\lambda_F}{v_F}$ the Fermi sphere moved to a new center at

$$\Delta k = -\frac{eE}{h}\tau_F = -\frac{eE}{h}\left(\frac{\lambda_F}{v_F}\right)\text{----------(1)}$$

Collision of electrons with impurities, imperfections and phonons oppose the displacement and tend to restore the Fermi surface back to its equilibrium position. Ultimately a steady state is reached.

If n is the free electrons per unit volume of the conductor, the steady current density would be given by

$$J = n(-e)\Delta v$$

$$= -ne\left(\frac{h\Delta k}{m}\right) \quad \text{because } \Delta v = \frac{\Delta p}{m} = \frac{h\Delta k}{m}$$

Substituting for Δk from equation (1)

$$J = -\frac{neh}{m}\left(-\frac{eE}{h}\right)\left(\frac{\lambda_F}{v_F}\right)$$

$$= \frac{ne^2}{m}\left(\frac{\lambda_F}{v_F}\right)E$$

But we know that

$$J = \sigma E$$

$$\therefore \quad \sigma = \frac{ne^2}{m}\left(\frac{\lambda_F}{v_F}\right)$$

Rigorous expression for conductivity is

$$\boxed{\sigma = \frac{ne^2}{m^*}\left(\frac{\lambda_F}{v_F}\right)}$$ where m* is the effective mass of the electron.

Merits of quantum free electron theory:

1. **specific heat:**

   The small value of specific heat is explained as follows

   According to classical free electron theory all the conduction electrons are capable of absorbing the heat energy irrespective of the what energy they already possess. Thus the theory predicts very large value of specific heat. According to quantum free electron

theory only those electrons those are occupying energy level very close to E_F which absorbs the heat energy. It means only the small percentage of the conduction electrons is capable of receiving the thermal energy and hence specific heat takes a very small value. Further it is possible to calculate the specific heat on the basis of quantum free electron theory that

$$C_v = \left(\frac{2k}{E_F}\right)RT$$

If the E_F is 5eV then $\left(\frac{2k}{E_F}\right) = 10^{-4}$

$\therefore$ Cv= 10^{-4} RT which is in conformity with the experimental value.

2. Temperature dependence of electrical conductivity

The experimentally observed fact that the electrical conductivity(σ) dependence on($1/T$) but according to classical free electron theory it depends on($1/\sqrt{T}$) can be explained as follows

According to quantum free electron theory electrical conductivity is

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

Here v_F is independent of the temperature but λ depends on the temperature.
Therefore $\sigma \alpha \lambda$

Mean free path $\lambda \propto \dfrac{1}{\pi r^2}$ 　　where r is the amplitude of vibration

Since energy of the vibrating body is proportional to square of the amplitude and energy of the ions is proportional to the temperature, $r^2 \alpha$ T. Where T is the temperature
$\therefore \lambda \alpha 1/T$

Since $\sigma \alpha \lambda$ 　　　　　　$\sigma \alpha 1/T$
Thus dependence of electrical conductivity on temperature can be correctly explained on the basis of quantum free electron theory.

3. Electrical conductivity and electron concentration

As per the quantum free electron theory we have the equation for the electrical conductivity

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

From the above equation it is clear that electrical conductivity depends on n, ratio $\left(\frac{\lambda}{v_F}\right)$ and

m^*. If we compare the copper and aluminium, the value of n for aluminum is 2.13 times higher than that of the copper but the value ($\frac{\lambda}{v_F}$) for copper is 3.73 times higher than that of aluminium. Thus the conductivity of the copper exceeds that of the aluminium.
Further the value of m^* for aluminium is 1.08 times that of copper. This also reduces the conductivity of the aluminium.

Physics of Semiconductors

Introduction to semiconductor

The material which has electrical conductivity between that of a conductor and that of an insulator is called as semiconductor. Silicon, germanium and graphite are some examples of semiconductors. In semiconductors, the forbidden gap between valence band and conduction band is very small. It has a forbidden gap of about 1 electron volt (eV).

Intrinsic semiconductor

Pure semiconductors are called intrinsic semiconductors. Silicon and germanium are the most common examples of intrinsic semiconductors. The conductivity in intrinsic semiconductor is due to only the thermal excitation.

In intrinsic semiconductor the number of electrons in the conduction band is equal to the number of holes in the valence band.

Extrinsic semiconductor

The semiconductor in which very small amount of impurities are added to a pure semiconductor in a controlled manner is called extrinsic semiconductor. The process of adding impurities to the semiconductor is called doping. Doping increases, the electrical conductivity of semiconductor. Extrinsic semiconductor has high electrical conductivity than intrinsic semiconductor.

Based on the type of impurities added, extrinsic semiconductors are classified in to two types.

n- type semiconductor

When pentavalent impurity (phosphorus, arsenic, antimony etc.) is added to an intrinsic or pure semiconductor (silicon or germanium), then it is said to be an n-type semiconductor. In n-type semiconductors electrons are the majority carriers and holes are minority carriers.
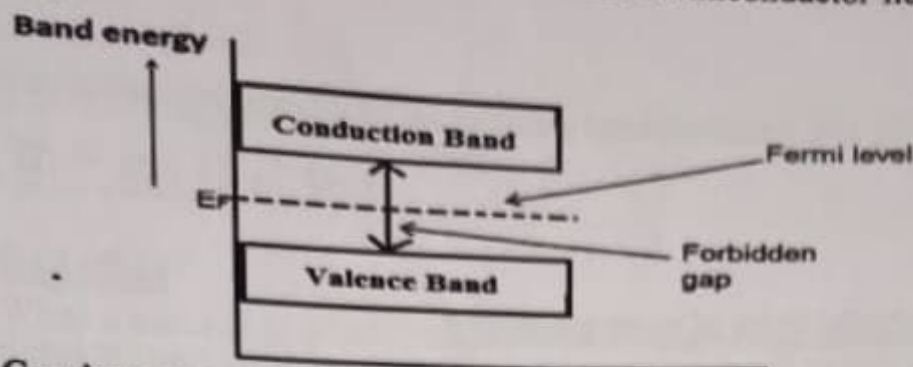
p- type semiconductor

When the trivalent impurity (Boron, Gallium, Aluminium etc) is added to an intrinsic or pure semiconductor (silicon or germanium), then it is said to be an p-type semiconductor. In p-type semiconductors holes are the majority carriers and electrons are minority carriers.

Fermi level in intrinsic semiconductor

In intrinsic semiconductor at absolute zero all the energy levels in the valence band are completely filled and all the energy levels in the conduction band are completely empty. But at ordinary temperatures such as room temperature, due to thermal excitation some of electrons at the top of the valence band are able to jump the energy gap and occupy some energy levels at bottom part of the conduction band. These electrons return soon to the energy levels which they had left vacant in the valence band. The electrons in this set of energy levels continue to undergo excitation and de-excitation and thus become conduction electrons. Thus conduction electrons are distributed between the energy levels in the bottom of the conduction band and top portion of the valence band. Because of such distribution the average energy of the electrons taking part in conduction will be almost equal to $(1/2)E_g$.

Therefore, the Fermi level for the intrinsic semiconductor lies in the middle of forbidden band.

Carrier concentrations in intrinsic semiconductors

In intrinsic semiconductor all the energy states of the electrons in a valence band (VB) are occupied while in the conduction band (CB) they are empty at 0 K.

At room temperature covalent bonds are broken and electron –hole pairs are generated. Large numbers of electrons are available in the conduction band and large number of holes is created in the valence band. As electrons and holes are charged particles they are together called charge carriers. Carrier concentration is the number of electrons in the conduction band per unit volume (N_e) and the number of holes in the valence band per unit volume (N_h) of the material.

Expression for electron concentration (N_e)

The number of electrons in the conduction band/unit volume of the material is called electron concentration. Expression for the electron concentration is given by.

$$N_e = 2\left[\frac{2\pi m_e^* kT}{h^2}\right]^{\frac{3}{2}} e^{-\frac{(E_C - E_F)}{kT}}$$

Where N_e is the electron concentration, m_e^* is the effective mass of the electrons, k is the Boltzmann constant, T is the absolute temperature, h is the Planck's constant, E_c is the lowest energy value in the conduction band and E_F is the Fermi energy.
Designating

$$N_C = 2\left[\frac{2\pi m_e^* kT}{h^2}\right]^{\frac{3}{2}}$$ we obtain

$$N_e = N_C e^{-\frac{(E_C - E_F)}{kT}}$$

Hole concentration (N_h)

The number of holes in the valence band/unit volume of the material is called hole concentration. Expression for the hole concentration is given by

$$N_h = 2\left[\frac{2\pi m_h^* kT}{h^2}\right]^{\frac{3}{2}} e^{-\frac{(E_F - E_V)}{kT}}$$

Where N_h is the electron concentration, m_h^* is the effective mass of the electrons, k is the Boltzmann constant, T is the absolute temperature, h is the Planck's constant, E_V is the highest energy value in the valence band and E_F is the Fermi energy.
Designating

$$N_V = 2\left[\frac{2\pi m_h^* kT}{h^2}\right]^{\frac{3}{2}}$$

we obtain

$$N_e = N_V e^{-\frac{(E_F - E_V)}{kT}}$$

Expression for Electrical conductivity of semiconductor:

On the basis of free electron theory the charge carrier can be assumed to be moving inside the semiconductor. Both the holes and electrons contribute to the conductivity of the semiconductor. Let us consider to start with the conductivity in a semiconductor due to the flow of electrons only.

Consider a semiconductor of area of cross section A in which a current 'I' is flowing. Let 'v' is the drift velocity of the electrons. The electrons move the distance v in one second.
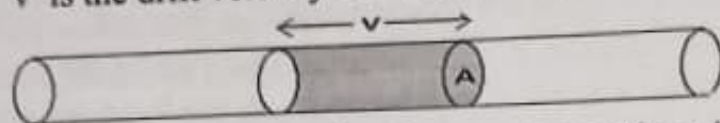
The volume swept by the electrons / second = vA

If N_e is the number of electrons per unit volume, No of electrons crossing the cross sectional area per second is = N_e vA

e is the charge on the electrons then the charge flow per second is= N_e evA

Since charge flow per second is the current I

I= N_e evA

Current density J= I/A= N_e ev----(1)

The electron mobility is μ_e= v/E where E is the electric field.

Substituting for v in equation (1)

J=(N_e e μ_e)E----(2)

But from the Ohms law

J=σE

Where σ is the conductivity of the charge carriers. If σ_e is the conductivity due to the electrons in the semiconductor, then Ohms law becomes

J=σ_eE----(3)

Comparing equations (2) and (3) conductivity of electrons is given by

σ_e = (N_e e μ_e)------(4)

Now let us consider the contribution of holes to the conduction of electricity. If σ_h is the conductivity due holes, N_h is the number of holes per unit volume and μ_h is the mobility of the holes then conductivity due to holes is given by

σ_h = (N_h e μ_h)------(5)

The total conductivity is given by the sum of σ_e and σ_h

i.e. σ = σ_e+ σ_h=(N_e e μ_e)+ (N_h e μ_h)

σ =e(N_e μ_e+ N_h μ_h)

For n Type semiconductor N_e >> N_h

Therefore conductivity σ = N_e eμ_e

For p-type semiconductor N_h >> N_e

Therefore conductivity σ = N_h eμ_h

In the case of intrinsic semiconductor the number of holes is always equal to number of electrons

i.e. $N_e = N_h = n_i$

If σ_i is the conductivity of the intrinsic semiconductor it is given by

$$\boxed{\sigma_i = n_i e \left(\mu_e + \mu_h\right)}$$

Hall effect

When a material in which a current flow is placed in a magnetic field at right angles to the direction of the current, an electric field is induced across the material in a direction perpendicular to both the direction of the magnetic field and the direction of the current flow. This phenomenon is called Hall Effect and the potential difference obtained is called Hall voltage.
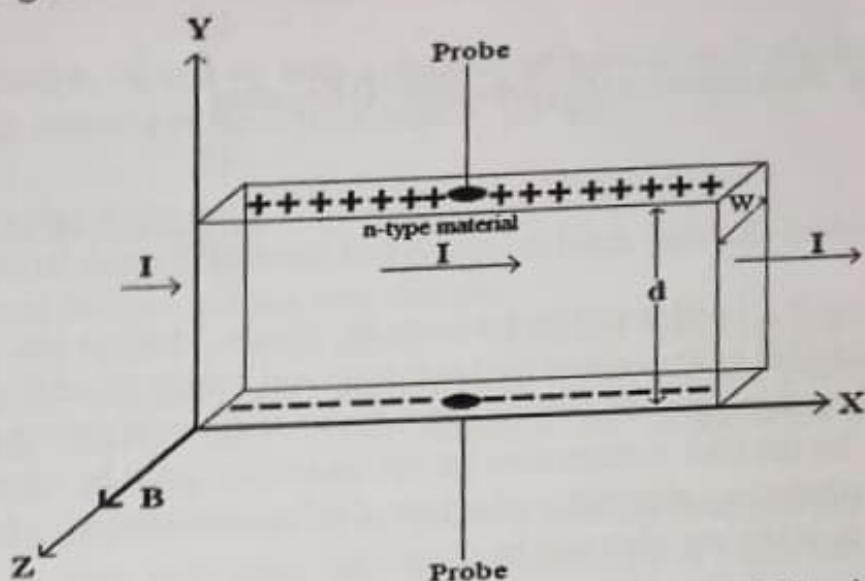
Let us consider a thin rectangular sheet of conductor with current I flowing in X-direction. Let the magnetic field B be applied on the conductor in Z-direction. Then the Lorentz force acting on an electron is given by

$$F_L = -Bev \qquad \text{------(1)}$$

Where 'e' is the electronic charge and v is the drift velocity.

According to Fleming's left hand rule, we see that the force is exerted on the electrons in the negative Y direction. Electrons are therefore tend to move towards the lower surface and accumulate at this surface. Therefore the lower surface of the conductor becomes negative. On the other hand, the loss of electrons on the upper end gives rise to the positive charge to the upper surface.

The potential difference developed between the two opposite surfaces is known as Hall voltage (V_H) The electric field so developed prevents the further motion of electrons towards the lower end.

Let E_H be the electric field due to Hall voltage. This field exerts upward force on the electron. Then force on electron in the upward direction is given by

$$F_H = -e E_H \qquad \text{-----(2)}$$

In equilibrium position two forces becomes equal

i.e. $F_L = F_H$

$-Bev = -e E_H$

$$E_H = Bv \qquad \text{-----(3)}$$

If 'd' is the distance between the lower and upper ends then

$E_H = \dfrac{V_H}{d}$

$\qquad\qquad\qquad\qquad\qquad\qquad$ -----(4) from equation(3)

Or $V_H = d \times E_H = Bvd$

If 'w' is the width of the conductor in Z direction then its area of cross section normal to the direction of the current I is $= wd$

Therefore the current density

$J = \dfrac{I}{wd}$

But we know that $J = nev = \rho v$ $\qquad\qquad\qquad\qquad$ -----(5)

where n is the charge carrier concentration and $\rho(=ne)$ is the charge density.

$\therefore \rho v = \dfrac{I}{wd}$

Or $v = \dfrac{I}{\rho wd}$ $\qquad\qquad\qquad\qquad\qquad\qquad$ -----(6)

Substituting for v, from equation (6) , Equation (4) becomes

$V_H = \dfrac{BI}{\rho w}$ $\qquad\qquad\qquad\qquad\qquad\qquad$ -----(7)

Or $\rho = \dfrac{BI}{V_H w}$ $\qquad\qquad\qquad\qquad\qquad\qquad$ -----(8)

Thus by measuring V_H, I and w and by knowing B , charge density ρ can be determined. The polarity of the Hall voltage developed at the top and bottom edges of the specimen can be identified by using probes. For the setup shown in figure if the top edge acquires positive polarity for the Hall voltage then the charge carriers must be electrons which means that semiconducting material is of n-type. On the same reasoning for the material of p-type the polarity at the top edge will be negative.

Hall coefficient R_H:

For a given semiconductor, the Hall field E_H depends upon the current density J and the applied field B.

i.e. $E_H \alpha JB$

or $E_H = R_H JB$

Where R_H is called the Hall coefficient.

Now from the above equation

$R_H = \dfrac{E_H}{JB}$ $\qquad\qquad\qquad\qquad\qquad\qquad$ -----(9)

Substituting for E_H and J from equation (3) and (5) in equation (9) we hqve

$R_H = \dfrac{Bv}{\rho vB}$

Or $R_H = \dfrac{1}{\rho}$

Thus the Hall coefficient can be evaluated once ρ is known.

Expression for Hall voltage in term of Hall coefficient:

From equation (7)

$V_H = \dfrac{BI}{\rho w} = \dfrac{1}{\rho}\left(\dfrac{BI}{w}\right) = R_H \left(\dfrac{BI}{w}\right)$ because $R_H = 1/\rho$

DIELECTRICS:

Introduction

A **dielectric** is an electrically nonconducting material. Examples: glass, wood, rubber etc. If its main purpose is just to provide insulation it is called **insulating material**. If it is employed for charge storage then its name is **dielectric**.

Unlike in the case of metals there are no free electrons in dielectrics. In dielectrics all the electrons are bound very strongly to the respective nuclei of the parent molecule.

Electric dipole and dipole moment

A pair of equal and opposite charges which are separated by a very small distance is called **electric dipole**.

+q   d   -q
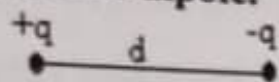
The product of magnitude of one of the charges and distance of their separation is called **dipole moment**.

Consider two charges −q and +q with a distance of separation d which is assumed to be small. The dipole moment of the arrangement is $\mu = qd$

Polar and non polar dielectrics

A dielectric material doesn't have any free electrons. Each molecule in the material consists of equal number of positive and negative charges.

In the molecules(or atoms) of some dielectric materials effective centre of the negative charge distribution coincides with the effective center of the positive charges thus neutralizing each other's effect. Such materials are called **non- polar dielectrics**. Examples: methane, Benzene etc.

In some materials effective centers of the positive and negative charges in the molecules will not coincides with each other they are separated by a small distance constituting permanent dipole. Such materials are called **polar dielectrics**. Examples: water, NH_3, HCl etc.

Dipoles are oriented randomly in polar dielectrics. It results in a net zero dipole moment for the materials as a whole.

Electric polarization

When the electric field is applied to the non polar dielectrics, positive and negative charges of the various molecules in it experience pulling forces in opposite directions. Thus the effective centers of positive and negative charges in molecules get separated by a small distance. Therefore each molecule develops dipole in the direction of the applied field.

When the electric field is applied to the polar dielectrics molecular dipoles tends to align their dipole moment in the direction of the applied electric field. Some alignment is achieved in relatively stronger field.

The **polarization** of the dielectric is the process of formation of dipoles (or alignment of already existing dipoles) by the application of the electric field on the dielectric material.

Or

The **polarization (P)** of the dielectric material is the induced dipole moment per unit volume of the dielectric material.

The ratio of induced dipole moment to the effective applied electric field is called **polarisability (α)** $\alpha = (\mu/E)$

Where μ is the electric dipole moment acquired by an atom, α is the polarisability and E the electric field.

Static dielectric constant

The electric flux density D in a material is related to electrical field strength E in any point in space. $D = \epsilon_0 \epsilon_r E$

Where $\epsilon_0 = 8.854 \times 10^{-12}$ farad /m represents the permittivity of vacuum & ϵ_r the relative permittivity of the material. Further $\epsilon = \epsilon_0 \epsilon_r$ which ϵ is known as absolute permittivity of the material. ϵ_r which is a constant & dimensionless, is known as **dielectric constant** of the material.

The relative dielectric constant ϵ_r is referred to as static dielectric constant or simply dielectric constant which is constant under static field conditions.

ϵ_r is a dimensionless quantity and has a value of unity for vacuum, which is the lowest value it can possess. For air it is 1.0006. ϵ_r varies widely from material to material for example its value for pyrex glass is 5.6 and for water is 80. ϵ_r varies with frequency of the voltage applied to the plates of the capacitor.

Relation between the polarization, dielectric constant and electric susceptibility.

The relation between the polarisation P and dielectric constant ϵ_r is given by

$$P = \epsilon_0 (\epsilon_r - 1) E$$ Where E is the applied electric field.

or $P = \epsilon_0 \chi E$ Where $\chi = (\epsilon_r - 1)$ is the dielectric susceptibility of the material.

Types of polarizations

There are four different mechanisms through which electrical polarization can occur in the dielectric materials when they are subjected to electric field. They are
i)   The Electronic polarization
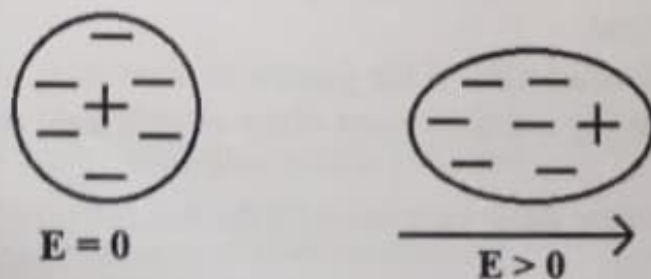ii)   The ionic polarization
iii)   Orientational polarization

1) The electronic polarization:

The atom can be considered to be made up of a point positive charge (nucleus) surrounded by a negative electron cloud. In the absence of the applied electric field, center of the electron cloud coincides with the center of the positive charge. When electric field is applied nucleus and the electron cloud tries to move in opposite directions. The nucleus moves in the direction of the applied field and electron cloud in the direction opposite to the applied field. The separation created between the charges leads to the development of an induced dipole moment. The polarization produced here is called electronic polarization.
Electronic polarizability is denoted by α_e. For rare gas atom α_e is given by

$$\alpha_e = \frac{\epsilon_r (\epsilon_0 - 1)}{N}$$ Where N is the number of atoms per unit volume.

$$E = 0 \qquad \qquad \xrightarrow{\quad\quad} E > 0$$

Electronic Polarisation

2) Ionic Polarization

This polarization mechanism occurs only in those dielectric materials which possess ionic bonds such as in NaCl. In an ionic material there will be an arrangement of positive and negative ions. If their arrangement is symmetrical there will be no permanent dipole present. When ionic solids are subjected to the external electric field, the positive ions move in the direction of the applied electric field and negative ions in the opposite direction. The displacement causes an increase or decrease in the distance of separation between the atoms depending upon the location of the ion pair in the lattice. This results in a net induced dipole moment. The ionic polarizability measures the shift of the ions relative to each other. The ionic polarization is denoted as α_i.


$$E = 0 \qquad E > 0$$
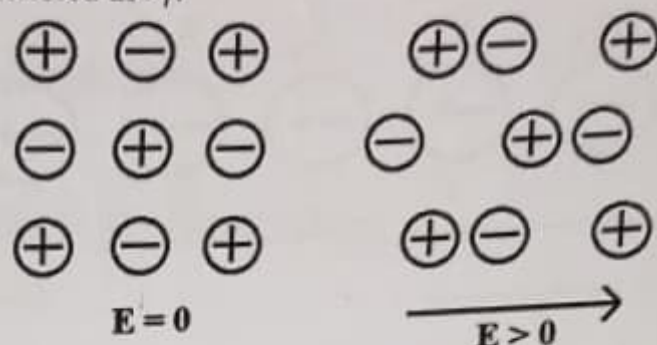
Ionic polarisation

3) Orientational polarization

Orientational polarization occurs in those dielectric materials which posses molecules with permanent dipole moment (polar dielctrics). They are normally randomly oriented due to thermal agitation. Because of randomness in the orientation the material has net zero dipole moment. When an external field is applied each of the dipoles under go rotation so as to reorient along the direction of the applied field. The orientation of these dipoles leads to polarization. This polarization is known as orientational polarization. The polarizability of this type is found to be proportional to square of the dipole moment 'μ' and inversely proportional to T (temperature). The orientational polarizability is given by α_0.

$$\alpha_0 = \frac{\mu^2}{3kT}$$

$$E = 0 \qquad E > 0$$
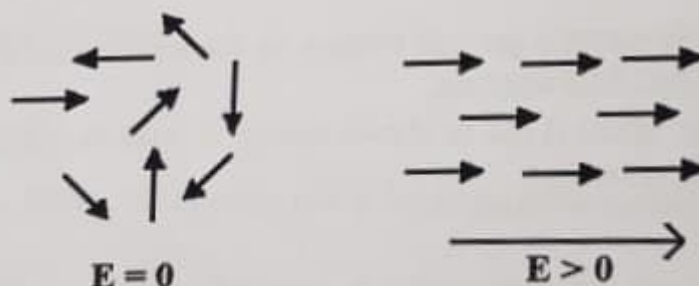
Orientational Polarisation

Total polarization α of the material is given by the sum of the electronic, ionic and orientational polarizations.

i.e. $\alpha = \alpha_e + \alpha_i + \alpha_0$

## Internal field in liquids & solids

When a dielectric material either solid or liquid is subjected to an external electric field each of the atoms develops a dipole moment and acts as electric dipole. Hence the resultant

field at any given atom is the sum of the applied electric field and the electric field due to the surrounding dipoles. This resultant local field is called internal field.

The internal field or local field is the electric field that acts at the sight of the given atom of a solid or liquid dielectric subjected to an external electric field and is the resultant of the applied electric field and the field due to all the surrounding dipoles.

Expression for Internal field in the case of liquid or solid (One dimensional case)

Consider a dielectric material either liquid or solid kept in an external uniform electric field of strength E. In the material let us consider an array of equidistant atomic dipoles arranged parallel to the direction of the field.
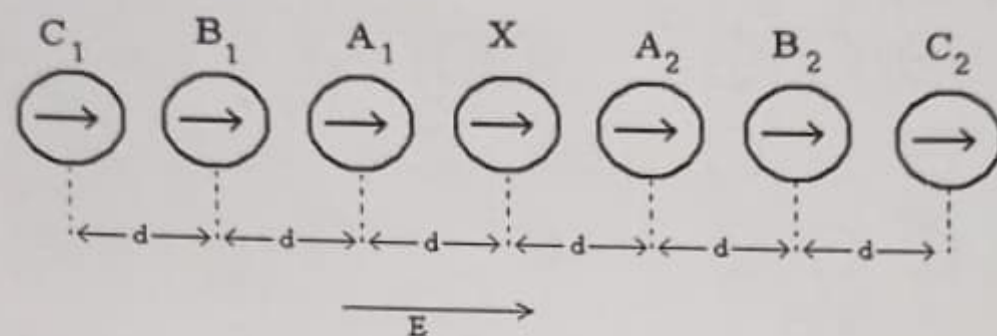
The expression for the internal field E_i is then given by

$$E_i = E + \frac{1.2\mu_{ind}}{\pi\varepsilon_0 d^3} \quad \text{-----------------------(1)}$$

Where d is the interatomic distance and $\mu_{ind}=\alpha_e E_i$ is the induced dipole moment of each atom.

Equation(1) represents expression for the internal field in case of one dimensional array of atoms in dielectric solids or liquids.

In the above equation since αe, E and ε_0 and d are all positive quantities $E_i > E$

Therefore internal field is more than the actual field. The internal field increases with decrease in d and increase in α.

For 3-dimentional cases expression for internal field is $E_i = E + \left(\frac{\gamma}{\varepsilon_0}\right)P$

Where P is the dipole moment per unit volume for the material and γ is the proportionality constant called internal field constant.

In the case of cubic lattice it can be shown that $\gamma = 1/3$ and the internal field is named as **Lorentz Field**. It is given by

$$E_{Lorentz} = E + \frac{P}{3\varepsilon_0}$$

Above equation is known as Lorentz relation.

Clasius- Mossotti relation

Elemental solids are those containing only one kind of atoms and the polarization is essentially due to the electronic polarizability of the atoms.

Consider an elemental solid dielectric material of dielectric constant ε_r.

If N is the number of atoms per unit volume of the material and μ is the atomic dipole moment then we have

Dipole moment / unit volume $= N\mu$ ....(1)

Here the field experienced by the atom is the internal field E_i. Hence if α_e is the electronic polarisability of the atoms, we can write the equation for the μ as $\mu = \alpha_e E_i$
Eq (1) becomes

Dipole moment / unit volume $= N\alpha_e E_i$ ....(2)
In Eq (2) its left side is same as polarization P

$\therefore P = N\alpha_e Ei$

or $E_i = \dfrac{P}{N\alpha_e}$ ----------(3)

But we have the relation for P as
$P = \varepsilon_0(\varepsilon r - 1)E$
Where E is the applied electric field.

$\therefore E = \dfrac{P}{\varepsilon_0(\varepsilon_r - 1)}$ -----------(4)

Also we have the equation for the internal field as

$E_i = E + \left(\dfrac{\gamma}{\varepsilon_0}\right)P$ ----------(5)

Where γ is the internal field constant.
Substituting for E_i and E from Eq(3) and Eq(4) in Eq(5)

$\dfrac{P}{N\alpha_e} = \dfrac{P}{\varepsilon_0(\varepsilon_r - 1)} + \gamma\dfrac{P}{\varepsilon_0}$

or $\dfrac{1}{N\alpha_e} = \dfrac{1}{\varepsilon_0}\left[\dfrac{1}{(\varepsilon_r - 1)} + \gamma\right]$

Considering the internal field in the material to be Lorentz field, we have $\gamma = 1/3$. Substituting the same in the above equation

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

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

By rearranging the above we have

$\dfrac{(\varepsilon_r - 1)}{(\varepsilon_r + 2)} = \dfrac{N\alpha_e}{3\varepsilon_0}$ --------(6)

Eq(6) is called Clasius –Mossotti equation and it holds good for crystal of high degree of symmetry.
The equation provides a relation between ε_r, the dielectric constant which is a macroscopically measurable quantity and α_e electronic polarisability, which is an atomic property.

Engineering Physics
Question Bank
(CBCS Scheme-2021-22)
Module-4

1. Give the assumptions of classical free electron theory

2. Explain the failure of the classical free electron theory.

3. Give the assumptions of quantum free electron theory.

4. Define of density of states and mention the expression for density of states.

5. What are Fermi energy and Fermi factor? Discuss the variation of Fermi factor with energy and temperature.

6. Explain Fermi Dirac statistics.

7. Define Fermi temperature and Fermi velocity give expression for them.

8. Obtain expression for electrical conductivity in metals on quantum model

9. Discuss the major success/merits of the quantum free electron theory.

10. Explain the Fermi level in an intrinsic semiconductor

11. Mention the expression for electron and hole concentration in intrinsic semiconductors.

12. Derive the expression for electrical conductivity of semiconductors

13. What is Hall Effect? Obtain the expression for Hall voltage in terms of Hall coefficient (Expression for Hall coefficient, determination of charge carriers)

14. What are dielectrics? Give the relation between dielectric constant and polarization.

15. Explain polar and non polar dielectric materials with examples.

16. What is polarization? Explain different polarization mechanisms.

17. Define internal field in case of solid dielectrics. Give the expression for it

18. Derive Clausius-Mossotti equation