# <u>UNIT-2</u>

# **Band Theory of Solids**

#### Introduction:

- The electrons in the outermost orbitals of the atoms determine its electrical properties. The electron theory of solids aims to explain the electrical, thermal and magnetic properties of solids.
- This theory has been developed in three main stages.
  - 1. Classical free electron theory
  - 2. Quantum free electron theory
  - 3. Band theory of solids.

### **Classical free electron theory:**

• Drude and Lorentz developed this theory in 1900. According to this theory the metals containing free electrons obey the laws of Classical Mechanics.

### Quantum free electron theory:

• Somerfield developed this theory during 1928. According to this theory free electrons obey the Quantum laws.

# Band theory of solids or Zone theory:

• Bloch stated this theory in 1928. According to this theory, the free electrons move in a Periodic field provided by the lattice and the theory is also called Band theory of solids.

# **Classical free electron theory:**

# Postulates:

- Metal is an aggregate of positive lattice ions (immobile) and negative free electrons.
- The valance electrons are free to move about the whole volume of metals like the molecules of a perfect gas in a container.
- These free electrons moves in random directions and collide with either positive ions fixed to the lattice or other free electrons.
- These all collisions are elastic that means there is no loss of energy.
- The free electrons move in a completely uniform potential field which is provided by lattice ions in the metal.
- When an electric field is applied to the metal, the free electrons are accelerated in the direction opposite the direction of applied electric field.
- When an electric field E is applied on an electron of charge e then it moves in opposite the direction of applied electric field with a velocity  $V_d$ .



Fixed Positive metallic ions

- Lorenz force acting on electron is F = -eE....(1)
- From Newton's law  $F = -ma = -\frac{mv_d}{t_r}$ .....(2) Therefore from 1 &2 we get  $-eE = -\frac{mv_d}{t_r} \Rightarrow v_d = \left(-\frac{et_r}{m}\right)E$ .

# **Drift velocity (**v<sub>d</sub>):

• The amount of velocity gained by the electron by the application of unit electric field is known drift velocity.

#### Relaxation time (t<sub>r</sub>):

- The duration of a time required for an electron to decay its drift velocity to 1/e times of its initial velocity.
- When electric field is applied on an electron then it drifts in opposite direction to the field applied. After removal of electric field the drift velocity decays exponentially.
- Let us assume that the applied field is cut off after the drift velocity of the electron has reached its steady value.

# Mean free Path ( $\lambda$ ):

- The average distance travelled by an electron between two successive collisions in the presence of applied field is known as mean free path.
- If **n** is the number of conduction electrons per unit volume, then the charge per unit volume is **-ne**.
- The amount of charge crossing a unit area per unit time is given by the current density J.

$$J = \frac{i}{A} = (-ne)\boldsymbol{v}_d = (-ne)\left(-\frac{et_r}{m}\right)E = \left(\frac{ne^2t_r}{m}\right)E = \boldsymbol{\sigma}E, \text{ where } \boldsymbol{\sigma} = \left(\frac{ne^2t_r}{m}\right) \text{ conductivity.}$$

Mobility  $\mu$ :

• Mobility of the electron is defined as the steady state drift velocity per unit electric field.  $u = \frac{v_d}{m} = \frac{\left|-\frac{et_r}{m}E\right|}{m} = \frac{et_r}{et_r}$ 

$$\mu = \frac{1}{E} = \frac{1}{E} = \frac{1}{E} = \frac{1}{m}.$$

• Electrical conductivity  $\boldsymbol{\sigma} = \left(\frac{ne^2 t_r}{m}\right) = ne\mu.$ 

Drawbacks of Classical free electron theory:

1. The phenomena such as photoelectric effect, Compton Effect and black body radiation couldn't be explained by classical free electron theory.

2. Electrical conductivity of semiconductor or insulators couldn't be explained using this model.

3. Ferromagnetism couldn't be explained by this theory.

4. Wiedemann-franz law  $\frac{K}{\sigma T} = L$ , according to the classical free electron theory, it is not constant at low temperature.

# Kroning – Penney Model :

- According to Kroning Penney model the electrons move in a periodic potential field which is provided by the lattice ions.
- To study the behavior of electron moving in a periodic potential field Kronig & Penny modified the above periodic curve into rectangular potential wells with width 'a'.
- By considering Schrodinger's wave equation  $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E V(x)]\psi = 0$  we can find the existence of energy gap and allowed energy bands.
- For one dimensional periodic potential field.....

V(x) = 0, 0 < x < a for region -1 and  $V(x) = V_0$ , -b < x < 0. for region -2



 $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E]\psi = \mathbf{0} \text{ in region (1)} \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E - V_0(x)]\psi = \mathbf{0} \text{ in region (2)}.$  $\frac{d^2\psi}{dx^2} + \alpha^2\psi = \mathbf{0}.....(1) \text{ where } \alpha^2 = \frac{2m}{\hbar^2} E \text{ and } \frac{d^2\psi}{dx^2} - \beta^2\psi = \mathbf{0}....(2) \text{ where } \beta^2 = \frac{2m}{\hbar^2} [V_0(x) - E]$ 

- According to Bloch, the solution of a Schrodinger equation  $\psi(x) = U_k(x) \cdot e^{ikx}$ .
- By substituting this solution in equations (1) & (2)then we get  $coska = P.\left(\frac{sin\alpha a}{\alpha a}\right) + cos\alpha a \dots \dots (3)$ , where  $P = \frac{mV_0ab}{\hbar^2}$  scattering power of potential barrier.
- A graph is drawn between  $\alpha a \& P.\left(\frac{\sin \alpha a}{\alpha a}\right) + \cos \alpha a$  (on X-axis  $\alpha a \&$  on Y-axis



#### • Conclusions

- 1. The motion of electrons in a periodic lattice is characterized by the bands of allowed energy separated by forbidden regions.
- 2. As the value of  $\dot{\alpha}a$  increases, the width of allowed energy bands also increases and the width of the forbidden bands decreases. i.e., the first term of equation deceases on the average with increasing  $\dot{\alpha}a$ .
- Let us now consider the effect of varying barrier strength P. if V<sub>0</sub>b is large ,i.e. if p is large ,the function described by the left hand side of the equation crosses +1 and -1 region as shown in figure. Thus the allowed bands are narrower and the forbidden bands are wider.
- 4. If  $\mathbf{P} \to \infty$  The allowed band reduces to one single energy level. The eq.(3) has only one solution i.e.

 $\sin\alpha a = 0 \ \Rightarrow \ \alpha = \pm \frac{n\pi}{a} \Rightarrow \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2} \Rightarrow \ E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \Rightarrow E_n = \frac{n^2h^2}{8mL^2}$ 

5. If  $\mathbf{P} \rightarrow \mathbf{0}$  No energy levels exist all energies are allowed to the electrons.

$$coska = cos\alpha a \Rightarrow k = \alpha \Rightarrow k^2 = \alpha^2 \Rightarrow \frac{2mE}{\hbar^2} = k^2 \Rightarrow E_n = \left(\frac{\hbar^2}{2m}\right)k^2.$$





- When we consider isolated atom, the electrons are tightly bound and have discrete, sharp energy levels.
- When two identical atoms are brought closer the outer most orbits of these atoms overlap and interact.
- If more atoms are brought together more levels are formed and for a solid of N atoms, each of the energy levels of an atom splits into N levels of energy.
- The levels are so close together that they form an almost continuous band.
- The width of this band depends on the degree of overlap of electrons of adjacent atoms and is largest for outer most atomic electrons.

•	E <sub>1</sub>	СВ
	E <sub>1</sub> E <sub>2</sub>	
		VB
•	E <sub>1</sub> E <sub>2</sub> E <sub>3</sub>	
8888	N atoms ΔE	

Valance band: The highest filled energy band is called valance band.

**Conduction band:** Lowest unfilled energy band is called conduction band.

Forbidden energy gap: The gap between valance band and conduction band is called energy gap.

# Classifications of materials into Conductors, Semiconductors & Insulators:

• On the basis of magnitude of forbidden band the solids are classified into insulators, semiconductors and conductors.

Insulator	Semiconductor	Conductor
Energy of electro Conduction Band Large energy gap between valence and conduction bands. Values Band a. Insulator	Conduction Band Isvel Valence Band b. Semiconductor	Conduction Band Valence Band c. Conductor
2. FEG more than 3eV	FEG nearly 1eV	FEG=0eV
3. No free electrons exist	Free electrons & holes exist	Only free electrons exist.
4. Resistivity high	Resistivity moderate	Resistivity low

5.Ex: wood, stone, rubber, etc.	Si, Ge, graphite etc.	Cu, Al, etc.
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# **Semiconductors**

Introduction:

- Semiconductors are materials whose electronic properties are intermediate between those of Metals and Insulators.
- The interesting feature about semiconductors is that they are bipolar and current is transported by two charge carriers of opposite sign.
- Semiconductors are mainly two types 1. Intrinsic (Pure) Semiconductors
  - 2. Extrinsic (Impure) Semiconductors

# Intrinsic semiconductors:

- A Semiconductor which does not have any kind of impurities behaves as an Insulator at 0k and behaves as a Conductor at higher temperature is known as Intrinsic Semiconductor or Pure Semiconductor.
- Ex: Germanium & Silicon (4th group elements) and they possess diamond cubic crystalline structure.

# **Extrinsic semiconductors:**

- A semiconductor which is in an impure form (with doping) is called an extrinsic semiconductor.
- Adding a suitable impurity to pure semiconductor is known as doping.
- Extrinsic semiconductors are further divided into two types
  - 1. P- type semiconductors
  - 2. N-type semiconductor

#### P- type semiconductors:

- Adding the trivalent impurity to pure semiconductor (like Al, Ga, In etc) then it becomes P-type semiconductor.
- In P-type semiconductors majority charge carriers are holes.

# N- type semiconductors:

- Adding the penta-valent impurity to pure semiconductor (like P, As, Sb etc) then it becomes N-type semiconductor.
- In N-type semiconductors majority charge carriers are electrons

# Carrier concentration:

• The number of charge carriers per unit volume is defined as carrier concentration. Units: number of electrons/m<sup>3</sup>





Note:

• In Intrinsic Semiconductor the Number of Conduction electrons will be equal to the Number of Vacant sites or holes in the valence band

# **Carrier Concentration in Intrinsic Semiconductors:**

#### **Calculation of Density of Electrons:**

• Let 'dn' be the Number of Electrons available between energy interval 'E and E+ dE' in the Conduction band

$$dn = Z(E) dE F(E)$$

• Where **Z**(**E**)**dE** is the Density of states in the energy interval **E** and **E** + **dE** and **F**(**E**) is the Probability of Electron occupancy.



• We know that the density of states i.e., the number of energy states per unit volume within the energy interval **E** and **E** + **dE** is given by

$$n = \int_{E_c}^{\text{topof the band}} z(E)F(E)dE.....(1)$$

$$Z(E)dE = \frac{4\pi}{h^3} (2m)^{\frac{3}{2}} E^{\frac{1}{2}} dE$$
$$Z(E)dE = \frac{4\pi}{h^3} (2m_e^*)^{\frac{3}{2}} (E - E_c)^{\frac{1}{2}} dE$$

• Probability of an electron occupying an energy state **E** is given by

$$F(E) = \frac{1}{1 + \exp(\frac{E - E_f}{kT})}$$

For all possible temperatures  $E - E_F >> kT$ 

$$F(E) = \frac{1}{\exp(\frac{E - E_f}{kT})}$$
$$F(E) = \exp(\frac{E - E_F}{kT}) = \exp(\frac{E_F - E}{kT})$$

• Substitute **Z**(**E**) and **F**(**E**) values in Equation (1)

$$n = \int_{E_c}^{\text{topof the band}} z(E)F(E)dE$$

$$n = \int_{E_c}^{\infty} \frac{4\pi}{h^3} (2m_e^*)^{\frac{3}{2}} (E - E_c)^{\frac{1}{2}} \exp(\frac{E_F - E}{kT})dE$$

$$n = \frac{4\pi}{h^3} (2m_e^*)^{\frac{3}{2}} \exp(\frac{E_F}{kT}) \int_{E_c}^{\infty} (E - E_c)^{\frac{1}{2}} \exp(\frac{-E}{kT})dE.....(2)$$

• To solve equation **2**, let us put

$$E - E_{c} = x \Longrightarrow E = E_{c} + x \Longrightarrow dE = dx$$

$$n = \frac{4\pi}{h^{3}} (2m_{e}^{*})^{\frac{3}{2}} \exp(\frac{E_{F}}{kT}) \int_{0}^{\infty} (E - E_{c})^{\frac{1}{2}} \exp(\frac{-E}{kT}) dE$$

$$n = \frac{4\pi}{h^{3}} (2m_{e}^{*})^{\frac{3}{2}} \exp(\frac{E_{F}}{kT}) \int_{0}^{\infty} (x)^{\frac{1}{2}} \exp(-(\frac{E_{c} + x}{kT})) dx$$

$$n = \frac{4\pi}{h^{3}} (2m_{e}^{*})^{\frac{3}{2}} \exp(\frac{E_{F} - E_{c}}{kT}) \int_{0}^{\infty} (x)^{\frac{1}{2}} \exp(-(\frac{x}{kT})) dx$$
(3)

• By using Gamma function

$$\int_{0}^{\infty} (x)^{\frac{1}{2}} \exp(\frac{-x}{a}) dx = (a)^{\frac{3}{2}} \frac{\pi^{\frac{1}{2}}}{2}$$
$$n = \frac{4\pi}{h^{3}} (2m_{e}^{*})^{\frac{3}{2}} \exp(\frac{E_{F} - E_{c}}{kT}) \{ (kT)^{\frac{3}{2}} \frac{\pi^{\frac{1}{2}}}{2} \}$$

1

$$n = 2(\frac{2\pi m_e^* kT}{h^2})^{\frac{3}{2}} \exp(\frac{E_F - E_c}{kT})$$

• The above equation represents Number of electrons per unit volume of the Material Calculation of Density of Holes:

• Let 'dp' be the Number of Electrons available between energy interval 'E and E+ dE' in the Valancy band

$$dp = Z(E)dE\{1 - F(E)\}$$

$$p = \int_{\text{bottomof the band}}^{E_{\gamma}} z(E)\{1 - F(E)\}dE....(1)$$

- Where Z(E)dE is the Density of states in the energy interval E and E + dE and 1-F(E) is the Probability of Hole occupancy.
- We know that the density of states i.e., the number of energy states per unit volume within the energy interval  $\mathbf{E}$  and  $\mathbf{E} + \mathbf{dE}$  is given by

$$Z(E)dE = \frac{4\pi}{h^3} (2m_h^*)^{\frac{3}{2}} E^{\frac{1}{2}} dE$$
$$Z(E)dE = \frac{4\pi}{h^3} (2m_h^*)^{\frac{3}{2}} (E_v - E)^{\frac{1}{2}} dE$$

• Probability of an electron occupying an energy state **E** is given by

$$1 - F(E) = 1 - \left\{\frac{1}{1 + \exp(\frac{E - E_f}{kT})}\right\}$$
$$1 - F(E) = 1 - \left\{1 + \exp(\frac{E - E_f}{kT})\right\}^{-1}$$

neglect higher order terms in above expansion for higher T values

$$1 - F(E) = \exp(\frac{E - E_f}{kT})$$

• Substitute **Z**(**E**) and **1**-**F**(**E**) values in Equation (1)  $E_{2}$ 

$$p = \int_{\text{bottomof the band}}^{E_{v}} z(E) \{1 - F(E)\} dE$$

$$p = \int_{-\infty}^{E_{v}} \frac{4\pi}{h^{3}} (2m_{h}^{*})^{\frac{3}{2}} (E_{v} - E)^{\frac{1}{2}} \exp(\frac{E - E_{F}}{kT}) dE$$

$$p = \frac{4\pi}{h^{3}} (2m_{h}^{*})^{\frac{3}{2}} \exp(\frac{-E_{F}}{kT}) \int_{-\infty}^{E_{v}} (E_{v} - E)^{\frac{1}{2}} \exp(\frac{E}{kT}) dE....(2)$$

• To solve equation **2**, let us put

$$E_{v} - E = x \Longrightarrow E = E_{v} - x \Longrightarrow dE = -dx$$

$$p = \frac{4\pi}{h^{3}} (2m_{h}^{*})^{\frac{3}{2}} \exp(\frac{-E_{F}}{kT}) \int_{-\infty}^{E_{v}} (E_{v} - E)^{\frac{1}{2}} \exp(\frac{E}{kT}) dE$$

$$p = \frac{4\pi}{h^{3}} (2m_{h}^{*})^{\frac{3}{2}} \exp(\frac{-E_{F}}{kT}) \int_{\infty}^{0} (x)^{\frac{1}{2}} \exp(\frac{E_{v} - x}{kT}) (-dx)$$

$$p = \frac{4\pi}{h^{3}} (2m_{h}^{*})^{\frac{3}{2}} \exp(\frac{E_{v} - E_{F}}{kT}) \int_{0}^{\infty} (x)^{\frac{1}{2}} \exp(\frac{-x}{kT}) dx$$

$$p = \frac{4\pi}{h^3} (2m_h^*)^{\frac{3}{2}} \exp(\frac{E_v - E_F}{kT}) (kT)^{\frac{3}{2}} \frac{\pi^{\frac{1}{2}}}{2}$$
$$p = 2(\frac{2\pi m_h^* kT}{h^2})^{\frac{3}{2}} \exp(\frac{E_v - E_F}{kT})$$

• The above equation represents Number of holes per unit volume of the Material Intrinsic Carrier Concentration:

 In intrinsic Semiconductors n = p, Hence n = p = n<sub>i</sub> is called intrinsic Carrier Concentration

$$n_{i}^{2} = np$$

$$n_{i} = \sqrt{np}$$

$$n_{i} = \sqrt{\left\{2 \left(\frac{2\pi m_{e}^{*}kT}{h^{2}}\right)^{\frac{3}{2}} \exp\left(\frac{E_{F} - E_{c}}{kT}\right)\right\} \left\{2\left(\frac{2\pi m_{h}^{*}kT}{h^{2}}\right)^{\frac{3}{2}} \exp\left(\frac{E_{v} - E_{F}}{kT}\right)\right\}}$$

$$n_{i} = 2\left(\frac{2\pi kT}{h^{2}}\right)^{\frac{3}{2}} \left(m_{e}^{*}m_{h}^{*}\right)^{\frac{3}{4}} \exp\left(\frac{E_{v} - E_{c}}{2kT}\right)$$

$$n_{i} = 2\left(\frac{2\pi kT}{h^{2}}\right)^{\frac{3}{2}} \left(m_{e}^{*}m_{h}^{*}\right)^{\frac{3}{4}} \exp\left(\frac{-E_{g}}{2kT}\right)$$

# PN junction diode and VI-characteristics:

#### **PN junction diode:**

- When a P-type Semiconductor is joined together with an N-type Semiconductor a PN junction is formed. And it is also known as a Semiconductor Diode.
- The two kinds of majority carriers diffusing across the junction meet each other near the junction and undergo recombination's, leaving negative ions on the P-side and positive ions on the N-side of the junction. This distribution of Positive and Negative Charges is called Space charge.





#### V - I Characteristics of PN Junction:

- The diode can be operated in two different ways, as Forward and Reverse bias.
- When positive terminal of the battery is connected to the P-type & negative terminal is to the N-type of the PN-junction diode, known the diode is kept in forward bias.
- When negative terminal of the battery is connected to the P-type & positive terminal is to the N-type of the PN-junction diode, known the diode is kept in reverse bias.





- From the graph the following points are noted.
- The region between knee voltage & breakdown voltage is known as non-ohmic region.
- Above the knee & breakdown voltage the current increases.



- Breakdown voltage is due to thermally broken covalent bonds.
- Diode is conducting in forward bias & non-conducting in reverse bias.

# Hall Effect:

- When a Magnetic field is applied perpendicular to a current Carrying Conductor or Semiconductor, Voltage is developed across the specimen in a direction perpendicular to both the current and the Magnetic field. This phenomenon is called the Hall effect and voltage so developed is called the Hall voltage.
- Let us consider, a thin rectangular slab carrying Current in the X-direction. If we place it in a Magnetic field B which is in the Z-direction. Potential difference V<sub>pq</sub> will develop between the faces p and q which are perpendicular to the Y-direction.
- Magnetic deflecting force  $F = q(v_d \times B)$
- Hall eclectic deflecting force  $F = qE_H$
- When an equilibrium is reached, the Magnetic deflecting force on the charge carriers are balanced by the electric forces due to electric Field.

 $q(v_d \times B) = qE_H$  $E_H = (v_d \times B)$ Where v<sub>d</sub> is drift velo city



- The relation between current density and drift velocity is  $v_d = \frac{J}{ne}$
- Where 'n' is the number of charge carriers per unit volume.

$$E_{H} = (v_{d} \times B) \Longrightarrow E_{H} = (\frac{J}{ne} \times B) \Longrightarrow E_{H} = (\frac{1}{ne} J \times B) \Longrightarrow E_{H} = R_{H}(J \times B)$$
$$R_{H}(Hall, coefficient) = \frac{1}{ne} \Longrightarrow \frac{E_{H}}{J \times B}$$

• If  $V_H$  be the Hall Voltage in equilibrium, the Hall Electric field.

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

Where 'd' is the width of the slab.

$$R_{\mu} = \frac{E_{H}}{E_{H}} \Longrightarrow R_{\mu} = \frac{1}{E_{H}} \times \frac{V_{H}}{E_{H}}$$

$$R_{H} = \frac{V_{H}t}{IB} (\because A = d \times t)$$

- Since all the three quantities  $E_H$ , J and B are Measurable, the Hall coefficient  $R_H$  and hence the carrier density can be find out.

#### Applications of Hall effect:

- Determination of type of semiconductor('n' type or 'p' type)
- Calculation of carrier concentration:  $n=1/eR_H$
- Determination of mobility:  $\mu = (\sigma/ne)$
- Measurement of magnetic flux density:  $B = (V_H t / IR_H)$

# **Thermistors:**

- Thermistors are made of semiconductor materials (metallic compounds including oxides such as manganese, copper, cobalt, and nickel, as well as single-crystal semiconductors silicon and germanium).
- A Thermistor is another special type of resistor. Its resistance changes as its temperature changes.
- When the temperature of the thermistor is low, its resistance is high. This is because a Thermistor is made of a material which does not conduct electricity well at low temperatures. The outer electrons are loosely bound to the atoms and are not free to flow through the Thermistor.

Assume a simple linear relationship between resistance and temperature for the following discussion

 $\Delta R = k \Delta T$ 

where

 $\Delta R$  = change in resistance

 $\Delta T$  = change in temperature

k = first-order temperature coefficient

of resistance



- This graph shows the thermistor's resistance against temperature.
- Remember, the resistance of a thermistor decreases as the temperature increases.
- Thermistors can be classified into two types depending on the sign of k.
- If k is positive, the resistance increases with increasing temperature, and the device is called a positive temperature coefficient (PTC) thermistor, Posistor.
- If k is negative, the resistance decreases with increasing temperature, and the device is called a negative temperature coefficient (NTC) thermistor.
- Thermisters are used temperature related sensors.

# **Dielectrics**

#### Introduction:

- Dielectrics are insulating materials which do not contain free electrons or the number of such electrons is too low to constitute the electric current. The electrons are tightly bound to the nucleus of the atom in dielectrics.
- Dielectrics are the materials having electric dipole moment permanently.

Ex: Mica, glass, plastic, water & polar molecules...

#### **Electric Dipole:**

• A system of two equal and opposite charges separated by a distance is called electric dipole.

# Dipole Moment(µ):

• The product of charge and distance between two charges is called dipole moment.  $\mu = qd$  Units: Coulomb-meter or Debye

#### Dielectric Constant(ε<sub>r</sub>):

Y	d	-4
~		

• The dielectric constant or relative permittivity of a medium is defined as the ratio between the permittivity of that medium and the permittivity of free space.  $C_{c}$ 

I	nee space	$\mathcal{F} \cdot \mathcal{C}$
	E = :	= —
	$\mathcal{E}_0$	$C_0$

• The characteristics of a dielectric material are determined by the dielectric constant and it has no units.

#### Electric Polarization:

• The process of producing electric dipoles by influence of an electric field is called electric polarization.

# Polarizability(α):

• The induced dipole moment per unit electric field is called Polarizability. The induced dipole moment of a system is proportional to the electric field(**E**) applied.

Therefore,  $\mu \alpha E_{\mu=\alpha E}$ 

where ' $\alpha$ ' is Polarizability

 $\alpha = \mu/E$ 

#### Various polarization processes:

- When the specimen is placed inside a electric field, polarization is due to four types of processes....
  - 1). Electronic polarization
  - 2). Ionic polarization
  - 3). Orientation polarization
  - 4). Space charge polarization.

# 1). Electronic Polarization:

- When an Electric field is applied to an atom, +vely charged nucleus displaces in the direction of field and electron cloud in opposite direction. This kind of displacement will produce an electric dipole with in the atom.
- i.e., dipole moment is proportional to the magnitude of field strength and is given by  $\mu_e \alpha E$

or  $\mu_e = \alpha_e E$ 

where ' $\alpha_{e}$ ' is called electronic Polarizability.

# **Calculation of Electronic Polarizability:**

• In a simplified classical model of an atom, nucleus of charge 'Ze' is surrounded by an electron cloud of charge '-Ze' distributed in a sphere of radius 'R'.

$$\rho = \frac{-Ze}{\frac{4}{3}\pi R^3} = -\frac{3}{4} \left(\frac{Ze}{\pi R^3}\right)$$

The charge density ' $\rho$ ' is given by •



- When an electric field 'E' is applied, nucleus and electron cloud are pulled apart due to ٠ Lorentz force of magnitude 'ZeE' acting on them in opposite directions. Lorentz force = -ZeE
- When they are separated, a coulomb force develops between them which tends to ٠ oppose the displacement. When equilibrium is reached, Lorentz force and coulomb forces are equal and opposite. Let 'x' be the distance between nucleus and electron cloud under that condition.

$$=\frac{1}{4\pi\varepsilon_0}\frac{Ze\times(\text{Charge enclosed in the sphere of raduis 'x')}}{x^2}$$

Coulomb force

Charge enclosed

$$= \frac{4}{3}\pi x^{3}\rho$$
$$= \frac{4}{3}\pi x^{3} \left[ -\frac{3}{4} \left( \frac{Ze}{\pi R^{3}} \right) \right] = -\frac{Zex^{3}}{R^{3}}$$

 $=\frac{Ze}{4\pi\varepsilon_0 x^2} \left[-\frac{Zex^3}{R^3}\right] = -\frac{Z^2 e^2 x}{4\pi\varepsilon_0 R^3}$ Therefore, Coulomb force

 $4\pi\varepsilon_0$ 

$$-ZeE = -\frac{Z^2 e^2 x}{4\pi\varepsilon_0 R^3}$$
$$E = \frac{Zex}{4\pi\varepsilon_0 R^3}$$

• But, in the equilibrium position

• Induced electric dipole moment,  $\mu_e$ =Charge x Distance

=Zex  

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

$$= 4\pi\varepsilon_0 R^3 E$$

$$\mu_e = \alpha_e E$$

• Where  $\alpha_e = 4\pi\epsilon_0 \mathbf{R}^3$  is called electronic Polarizability. Thus ' $\alpha_e$ ' is depending on the volume of the atom and is independent of temperature.

# 2). Ionic Polarization:

- The ionic polarization occurs, when atoms form molecules and it is mainly due to a relative displacement of the atomic components of the molecule in the presence of an electric field.
- When a Electric Field is applied to the molecule, the positive ions displaced by  $x_1$  to the negative side electric field and negative ions displaced by  $x_2$  to the positive side of field.
- The resultant dipole moment  $\mu = e(x_1 + x_2)$ ..



# 3). Orientation Polarization

- In Polar dielectric substances all the molecular dipoles are oriented randomly when there is no Electric field. In the presence of the electric field these all dipoles orient themselves in the direction of field as a result the net dipole moment becomes enormous
- Expression for orientation polarization is

$$\alpha_{ori} = \frac{\mu_{ori}^2}{3kT}$$





• Thus the orientation polarization is inversely proportional to absolute

temperature.

# **Frequency Dependence and Temperature effect on Dielectric:**

• This behavior of Polarizability can be understood from various polarization processes and from the concept of the relaxation time for each process. On application of a.c field, the polarization P(t) as a function of time 't' is given by

 $P(t) = P[-exp(-t/t_r)]$ 

- Where P is maximum polarization attained and t<sub>r</sub> is the relaxation time for the particular polarization process.
- Electronic Polarization is extremely rapid and it's relaxation time is small.
   It occurs only at optical frequencies range(~10<sup>15</sup>Hz).

It is independent of temperature.

- Ionic Polarization is a slower process compared to electronic polarization. This polarization occurs at frequency ~10<sup>13</sup> Hz (IR). It is independent of temperature.
- Orientation Polarization is a slower process compare to electronic and ionic polarization. It occurs at a frequency 10<sup>6</sup> Hz to 10<sup>10</sup>Hz. It greatly depends on temperature.

# Determination of dielectric constant- Schering bridge method

• Schering bridge is particularly used for measuring the dielectric constant of given medium.

Dielectric constant of given material is  $\varepsilon_r = \frac{C^1}{C}$ , where C is the capacitance with medium and C<sup>1</sup> is capacitance with medium.

- $r_1$  = a series resistance representing the loss in the capacitor  $C_1$ .
- $C_1$  = capacitor whose capacitance is to be measured.
- R<sub>3</sub>= variable resistance





- $C_4$  = variable capacitor.
- $R_4$ = fixed resistance.
- C<sub>2</sub>= standard capacitor
- D = A.C null detector and S = high frequency oscillator.
- First inserting  $C_1$ , the bridge should be balanced by adjusting  $C_4$  and  $R_3$ .

$$\frac{P}{Q} = \frac{R}{S} \text{ where } P = r_1 + \frac{1}{j\omega c_1}, Q = R_3, R = \frac{1}{j\omega c_2} \text{ and } \frac{1}{S} = \frac{1}{R_4} + \frac{1}{(\frac{1}{j\omega c_4})}$$

Therefore  $\mathbf{S} = \frac{\mathbf{R}_4}{1+j\omega\mathbf{R}_4\mathbf{C}_4}$ 

$$\begin{pmatrix} \frac{\mathbf{r}_1 + \frac{1}{j\omega c_1}}{\mathbf{R}_3} \end{pmatrix} = \left(\frac{\frac{1}{j\omega c_2}}{\frac{\mathbf{R}_4}{1 + j\omega \mathbf{R}_4 \mathbf{C}_4}}\right) \text{ then } (\mathbf{r}_1 + \frac{1}{j\omega c_1})\mathbf{R}_4 = \mathbf{R}_3 \left(\frac{1 + j\omega \mathbf{C}_4 \mathbf{R}_4}{j\omega \mathbf{C}_2}\right)$$
$$\mathbf{r}_1 \mathbf{R}_4 - \left(\frac{j\mathbf{R}_4}{\omega \mathbf{C}_1}\right) = -\left(\frac{j\mathbf{R}_3}{\omega \mathbf{C}_2}\right) + \frac{\mathbf{R}_3 \mathbf{R}_4 \mathbf{C}_4}{\mathbf{C}_2}$$

Equating real and imaginary parts we get

•  $r_1 = \frac{R_3 C_4}{C_2}$  and  $C_1 = \frac{R_4 C_2}{R_3}$ 

The dielectric specimen should be in the size of  $C_1$  and is inserted between the plates of  $C_1$ , again the bridge is balanced by adjusting  $R_3$ . And calculate  $C_1^{1}$ .

• Dielectric constant 
$$\varepsilon_r = \frac{c_1^2}{c_1}$$

# **Ferro electricity:**

- The phenomenon of possessing spontaneous polarization in absence of electric field is called ferro electricity. And these materials are called ferro electric materials.
- Examples for ferro electric materials:
  - 1. BaTio<sub>3</sub>(Barium titanate)
  - 2. KH<sub>2</sub> PO<sub>4</sub>(Potassium di hydrogen phosphate)
  - 3. NaKC<sub>4</sub>H<sub>4</sub>O<sub>6</sub>.4H<sub>2</sub>O(Rochelle salt)

# **Properties:**

- 1. All fero electric materials posses spontaneous polarization below certain temperature.
- 2. As temperature increases the spontaneous polarization decreases and at a particular temperature it vanishes. This temperature is called Curie temperature  $T_{C}$ .(graph)
- 3. Relation between dielectric constant and Curie temperature is given by

$$\epsilon_r = \frac{c}{T-T_c}$$
, where (T>T<sub>C</sub>).

# BaTio<sub>3</sub>(Barium titanate) structure:

• Above 120<sup>o</sup>C, BaTio<sub>3</sub> has cubic crystal structure with titanium ion exactly at the body centre, barium ions at the body corners and the oxygen ions at the six face centers as shown in the fig.

- Above 120<sup>o</sup>C the centre of positive and the centre of negative ions coincide, there is no dipole moment.
- If the crystal is cooled, below120<sup>0</sup>C the titanium ion shifts to one side of the body centre.
- This displaces the neibouring oxygen ions along one side of the crystal directions where the crystal gets elongated.
- Thus the cubic structure becomes tetragonal where dipoles are created throughout the crystal.
- All the dipoles of the adjacent unit cells get aligned in the same direction. Thus net dipole moment exists. Hence polarization arises in the material.

# Applications of ferro electrics: Ferro electrics are used in

- 1. Magnetic amplifiers and dielectric amplifiers.
- 2. Magnetic information storage devices.
- 3. Electro mechanical filters.
- 4. Capacitors etc.

