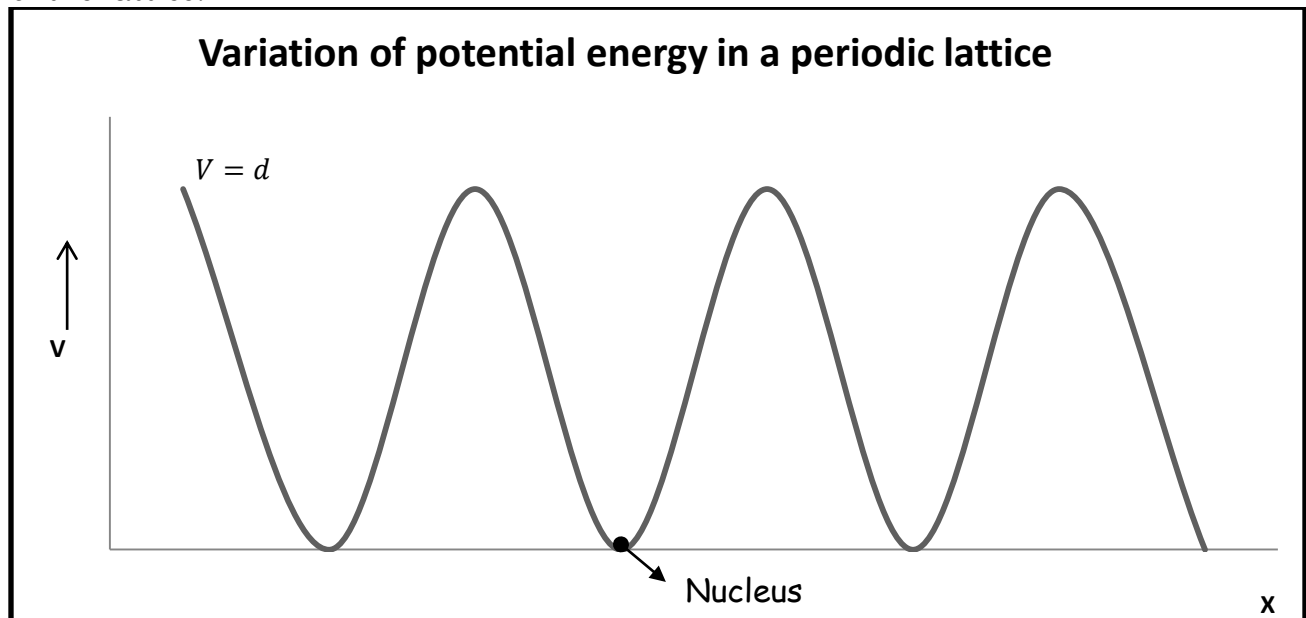


Band Theory of Solids & Semiconductor Physics

Bloch theorem (qualitative)

According to free electron model, a conduction electron in metal experiences constant potential. But in real crystal, there exists a periodic arrangement of positively charged ions through which the electrons move. As a consequence, the potential experienced by electrons is not constant but it varies with the periodicity of the lattice.



The potential is minimum at positive ions and maximum in between ions.

Consider Schrodinger's time independent wave equation in one dimension,

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

The periodic potential $V(x)$ changes with the help of lattice constant ' a ',

$$V(x) = V(x + a) \quad ('a' \text{ is the periodicity of the lattice})$$

Bloch's 1-D solution for Schrodinger wave equation

$$\Psi_k(x) = u_k(x)e^{ikx}$$

Where, $u_k(x) = u_k(x + a)$

' K ' is propagation vector corresponding to K^{th} State

$$P = \hbar K = \frac{h}{2\pi}K$$

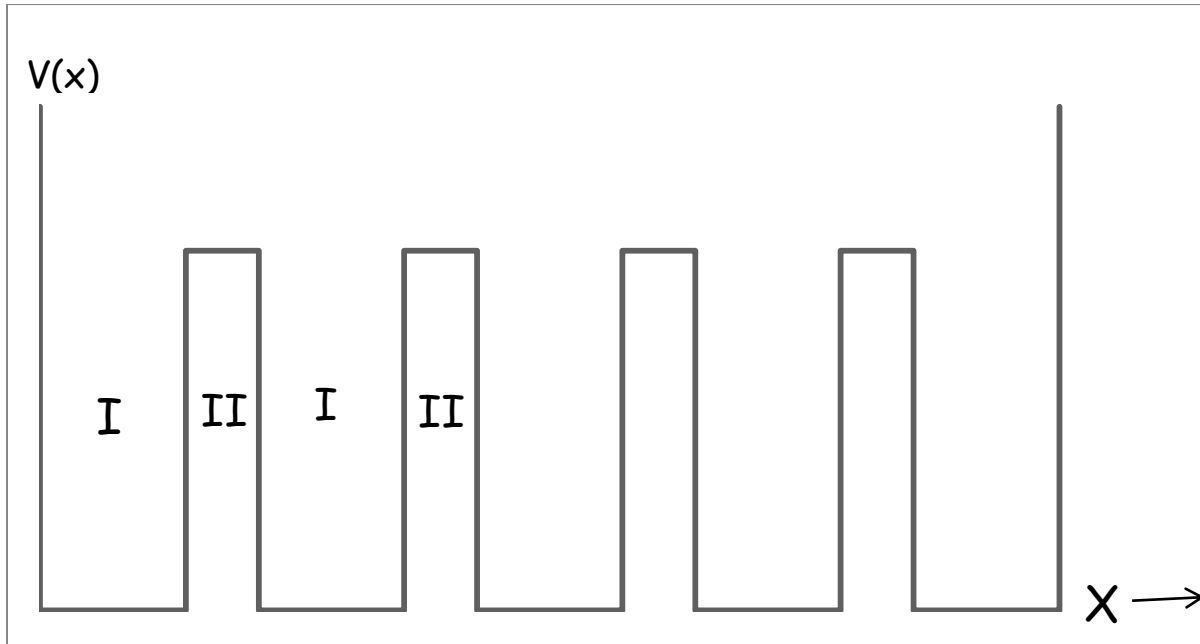
Three dimensional solutions for Schrodinger's Equation is

$$\Psi_k(r) = u_k(r)e^{ikr}$$

Kronig-Penny Model (qualitative)

Kronig –penny approximated that the potentials of an electrons inside the crystal in terms of the shapes of rectangular steps, i.e. square wells is known as Kronig Penny model.

The periodic potential is taken in the form of rectangular one dimensional array of square well potentials.



It is assumed that the potential energy is zero when x lies between 0 and a , and is considered as **I** region. Potential energy is V_0 , when x lies between $-b$ and 0 and considered as **II** region.

Boundary Conditions:

$V(x) = 0$, where x lies between $0 < x < a$ –I region

$V(x) = V_0$, where x lies between $-b < x < 0$ –II region

This model explains many of the characteristic features and the behavior of electrons in a periodic lattice.

The wave function related to this model may be obtained by solving *Schrodinger equations* for the two regions,

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2} E\Psi = 0, \text{ for } 0 < x < a \text{ with } V(x) = 0$$

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2} (E - V_0)\Psi = 0, \text{ for } -b < x < 0 \text{ with } V(x) = V_0$$

Again,

$$\frac{d^2\Psi}{dx^2} + \alpha^2 \Psi = 0 \text{ Where } \alpha^2 = \frac{2mE}{\hbar^2} \quad \text{-----} \textcircled{1}$$

$$\frac{d^2\Psi}{dx^2} + \beta^2\Psi = 0 \text{ Where } \beta^2 = \frac{2m}{\hbar^2}(V_0 - E) \text{ -----} \textcircled{2}$$

$$\text{From Bloch function } \Psi_k(x) = u_k(x)e^{ikx} \text{ -----} \textcircled{3}$$

Differentiating equation③, we get

$$\frac{d\Psi}{dx} = ike^{ikx}u_k(x) + e^{ikx}\frac{du_k}{dx}$$

Again,

$$\frac{d^2\Psi}{dx^2} = -k^2e^{ikx}u_k(x) + 2ike^{ikx}\frac{du_k}{dx} + e^{ikx}\frac{d^2u_k}{dx^2} \text{ -----} \textcircled{4}$$

Substituting equation ③ & ④ in equation ① & ②, we get

$$\frac{d^2u_k}{dx^2} + 2ik\frac{du_k}{dx} + (\alpha^2 - k^2)u_k = 0 \quad \text{for } 0 < x < a$$

$$\frac{d^2u_k}{dx^2} + 2ik\frac{du_k}{dx} - (\beta^2 + k^2)u_k = 0 \quad \text{for } -b < x < 0$$

The general solutions of their equations are

$u_1 = Ae^{i(\alpha-k)x} + Be^{-i(\alpha+k)x} \quad 0 < x < a$ $u_2 = Ce^{i(\beta-ik)x} + De^{-i(\beta+ik)x} \quad -b < x < 0$
--

Boundary Conditions:

$$u_1(x)_{x=0} = u_2(x)_{x=0}$$

$$\left(\frac{du_1}{dx}\right)_{x=0} = \left(\frac{du_2}{dx}\right)_{x=0}$$

$$u_1(x)_{x=a} = u_2(x)_{x=-b}$$

$$\left(\frac{du_1}{dx}\right)_{x=a} = \left(\frac{du_2}{dx}\right)_{x=-b}$$

After applying boundary conditions:

$$A + B = C + D$$

$$Ai(\alpha - k) - Bi(\alpha + k) = C(\beta - ik) - D(\beta + ik)$$

$$Ae^{i(\alpha-k)a} - Be^{-i(\alpha+k)a} = Ce^{-(\beta-ik)b} + De^{(\beta+ik)b}$$

$$A(\alpha - k)e^{i(\alpha-k)a} - B(\alpha + k)e^{-i(\alpha+k)a} = C(\beta - ik)e^{-(\beta-ik)b} - D(\beta + ik)e^{(\beta+ik)b}$$

On solving the determinant of the above equations, we get

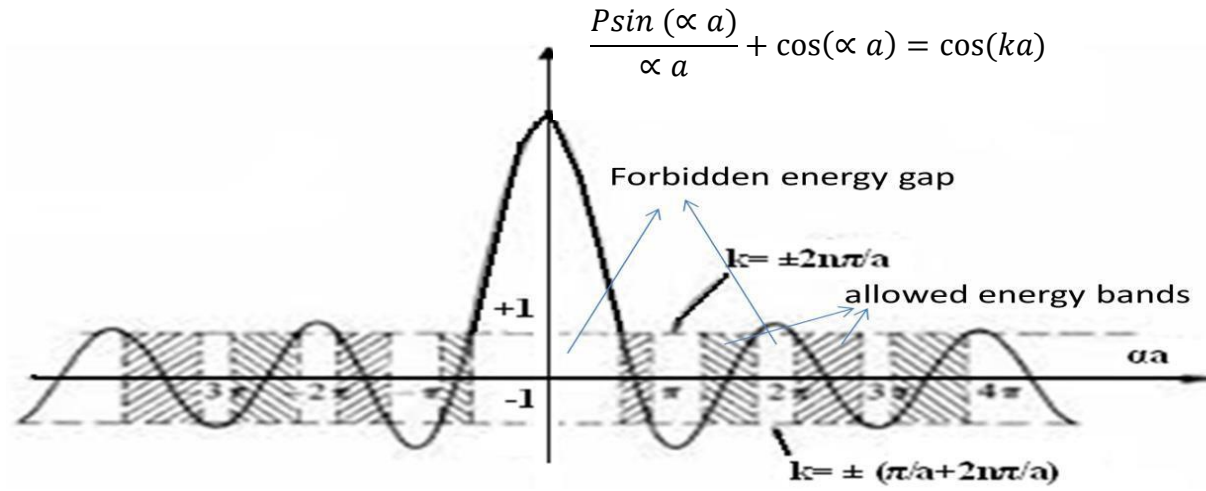
$$\left\| \frac{P \sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka) \right\|$$

P is called Potential barrier.

$$P = \frac{\beta^2 ab}{2} = \frac{mV_0 ab}{\hbar^2}$$

Case-1:

For $P \rightarrow \frac{3\pi}{2}$



As the value of α increases the width of allowed bands increases and width of forbidden bands decreases.

Case-2:

For $P \rightarrow \infty$

If $P \rightarrow \infty$, the allowed band reduces to a single (line) energy level, gives us steeper lines. So the energy spectrum becomes line spectrum.

We have,

$$\cos(ka) \left(\frac{\alpha a}{P} \right) = \sin(\alpha a) + \cos(\alpha a) \left(\frac{\alpha a}{P} \right)$$

$$P \rightarrow \infty, \frac{1}{\infty} = 0 \text{ Then } \sin(\alpha a) = 0$$

$$\sin(\alpha a) = \sin(n\pi)$$

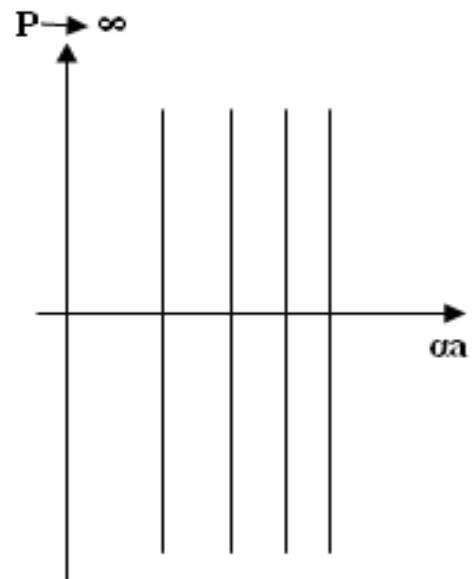
$$\alpha a = n\pi$$

$$\alpha^2 a^2 = n^2 \pi^2$$

$$\alpha^2 = \frac{n^2 \pi^2}{a^2}$$

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

$$\left[E = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \right], \text{ here } a \text{ is lattice constant}$$



Case-3:

If $P \rightarrow 0$, then

$$\cos(\alpha a) = \cos(ka)$$

$$\alpha a = ka$$

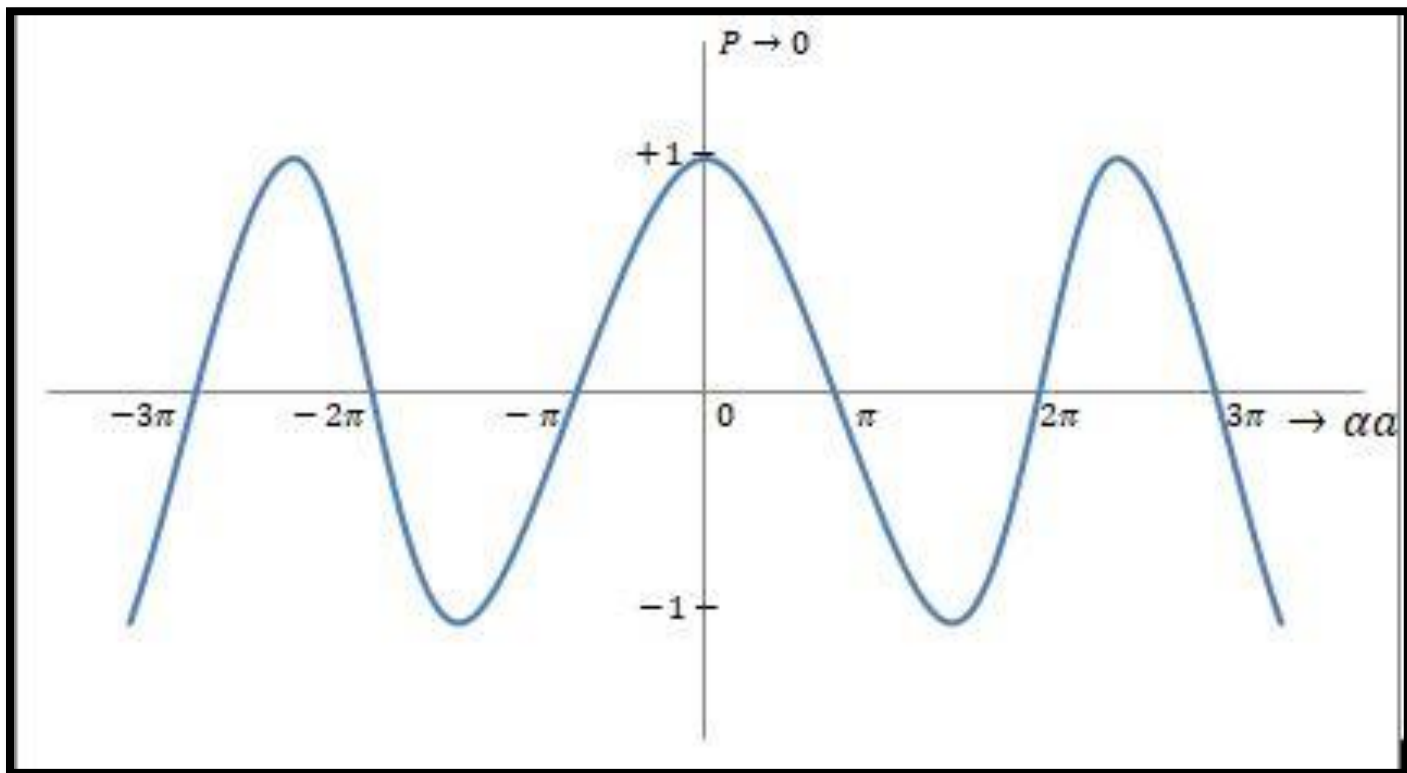
$$\alpha^2 = k^2$$

$$\frac{2mE}{\hbar^2} = k^2 = \frac{4\pi^2}{\lambda^2}$$

$$E = \frac{4\pi^2 \hbar^2}{2m\lambda^2} = \frac{4\pi^2 \hbar^2 p^2}{2m h^2}$$

$$E = \frac{4\pi^2 \hbar^2 p^2}{2m h^2 (4\pi^2)} = \frac{p^2}{2m}$$

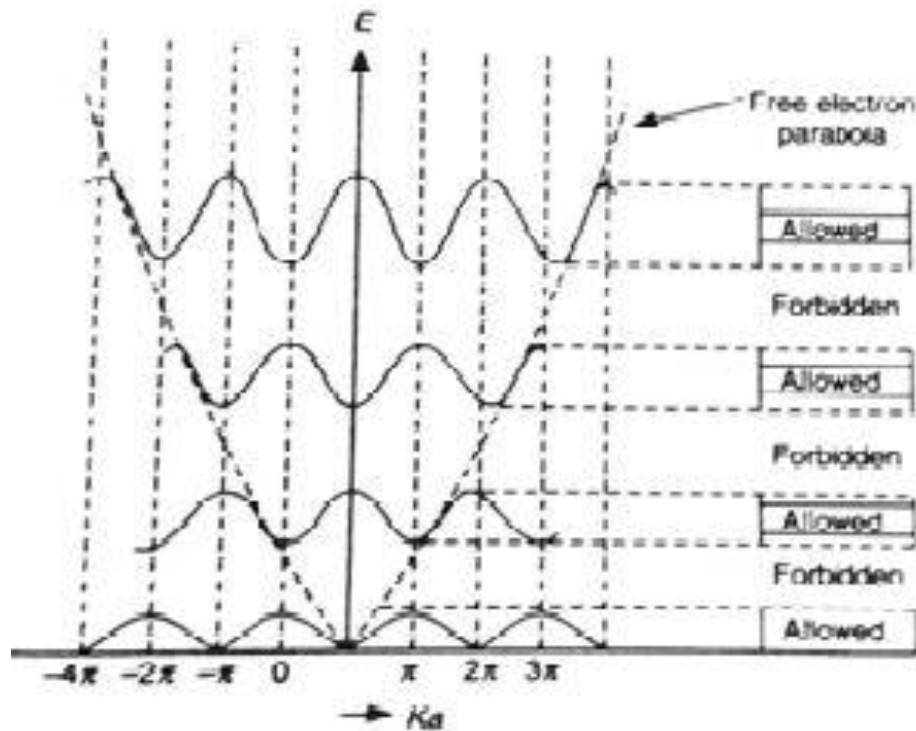
This shows that the particle is free and no energy exists.



This indicates that the particle is completely free and no energy level exists.

Brillouin Zone OR E-K diagram:

The Brillouin zone are the boundaries that are marked by the values of wave vector ' k ' in which electrons can have allowed energy values. These represent the allowed values of k of the electrons in 1D, 2D&3D.



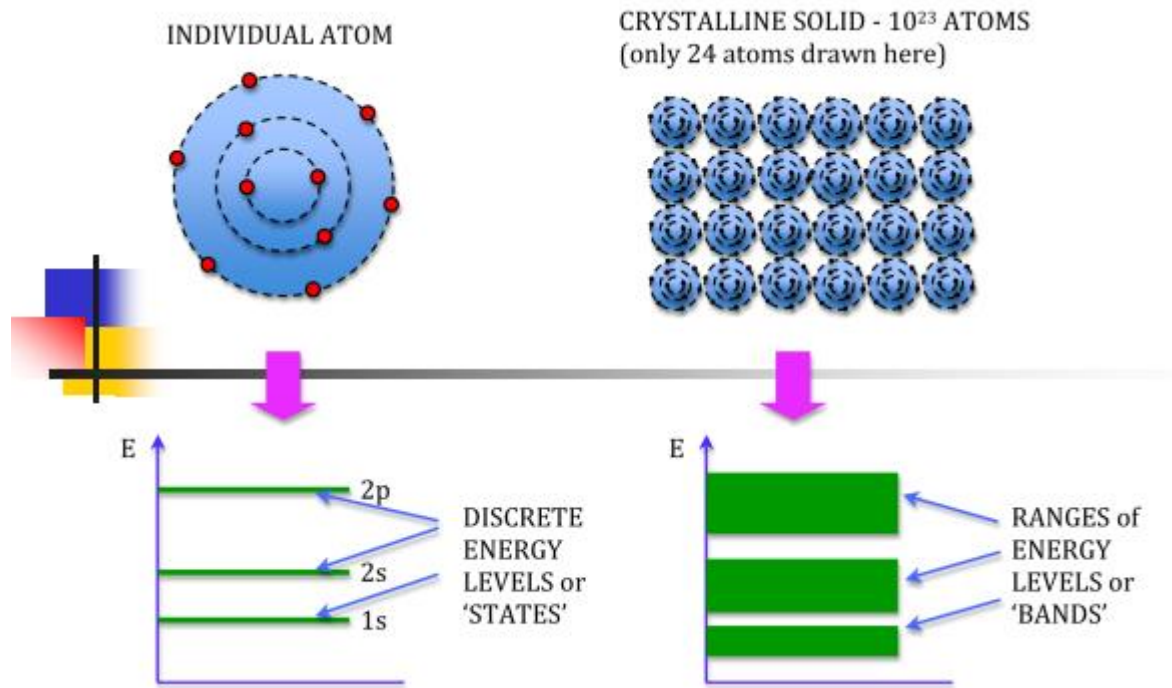
Allowed energy values lie in the region $k = -\pi/a$ to $k = +\pi/a$. This zone is called the first Brillouin zone. After a break in the energy values, called forbidden energy band, we have another allowed zone spread from $k = -\pi/a$ to $-2\pi/a$ and $+\pi/a$ to $+2\pi/a$. This zone is called the second Brillouin zone. Similarly, higher Brillouin zones are formed.

Energy Bands in Crystalline Solids

The band theory of solids explains the formation of energy bands and determines whether a solid is a conductor, semiconductor or insulator. The electrons of a single isolated atom occupy atomic orbitals, which form a discrete set of energy levels.

When two identical atoms are brought closer, the outermost orbits of these atoms overlap and interact. When the wave functions of the electrons of different atoms begin to overlap considerably, the energy levels corresponding to those wave functions split.

If more atoms are brought together more levels are formed and these energy levels are so close that they form an almost continuous band. The width of the band depends upon the degree of overlap of electrons of adjacent atoms.

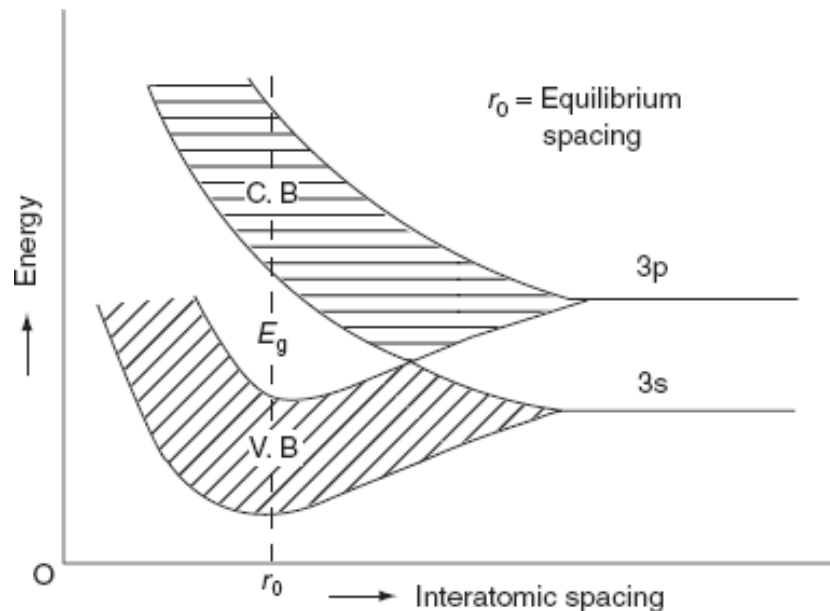


As a result of the finite width of the energy bands, gaps are essentially leftover between the bands called **forbidden energy gap**.

The band corresponding to outermost orbit is called Conduction band and next inner band is called Valence band.

Concept of hole

1. The negative effective mass of electron is called hole.
2. Holes can be seen on the top of the energy bands.
3. In semiconductors, missing of electron in valence band is defined as hole.
4. Holes can be obtained in valence band in semiconductors.
5. The charge of hole is assumed to be positive.



Classification of Crystalline Solids

The electrical properties of a solid depends upon its energy band structure and they occupied by the electrons. So solids can be classified into conductors, semiconductors and insulators. The metals are good conductors of electricity and insulators are bad conductor of electricity.

The electrical conductivity of semiconductors lies between metal and insulator. The completely filled bands and completely empty bands don't contribute to the electrical conduction. The valence band and conduction band energies are important for electrical properties of a solid.

Based on the energy band diagram materials of solids are classified as follows:

Conductors:

In this kind of materials, there is no forbidden gap between the valence band and conduction band. It is observed that the valence band overlaps with the conduction band in metals as shown in figure. There are sufficient numbers of free electrons, available for electrical conduction and due to the overlapping of the two bands there is an easy transition of electrons from one band to another band takes place, and there no chance for the presence of holes. Resistivity of conductors is very small and it is very *few milliohm meters. (Ωm)*.

Examples: All metals (Na, Mg, Al, Cu, Ni Cu, Ag, Li, and Ar etc.)

Semiconductors:

In semiconductors, there is a band gap exists between the valence band and conduction band and it is very less and it is the order of -1 to 2 eV are known as semiconductors. It will conduct electricity partially at normal conditions. The electrical resistivity values are 0.5 to 10^3 ohm meter. Due to thermal vibrations within the solid, some electrons gain enough energy to overcome the band gap (or barrier) and behave as conduction electrons. Conductivity exists here due to electronics and holes.

Examples: Silicon, Germanium, Ga As.

Insulators:

In insulators, the width of forbidden energy gap between the valence band and conduction band is very large. Due to large energy gap, electrons cannot jump from V.B to C.B. Energy gap is of the order of ~ 10 eV and higher than semiconductors. Resistivity values of insulators are 10^7 to 10^{12} ohm-m. Electrons are tightly bound to the nucleus, no valence electrons are available.

Examples: Wood, rubber, glass.

Semiconductor Physics

Introduction

SEMICONDUCTORS: The substances whose conductivity lies in between conductors and insulators are called as *semiconductors*.

Properties:

1. The conductivity of semiconductors depends on its temperature and it is increased with increase in temperature.
2. The energy gap of a semiconductor decreases with rise in temperature.
3. At 0K a semiconductor becomes an insulator.
4. The absence of an electron in the VB of a semiconductor is called hole. Hole occur only in the VB. Or an empty electron state is called a hole.
5. Like electrons, the hole in the VB also conducts electricity in case of a semiconductor.
6. The electric current in a semiconductor is the sum of the currents due to electron and hole.
7. Hole is a positive charge carrier of current.

Depending on the relative concentration of holes and electrons the semiconductors are classified into two types:

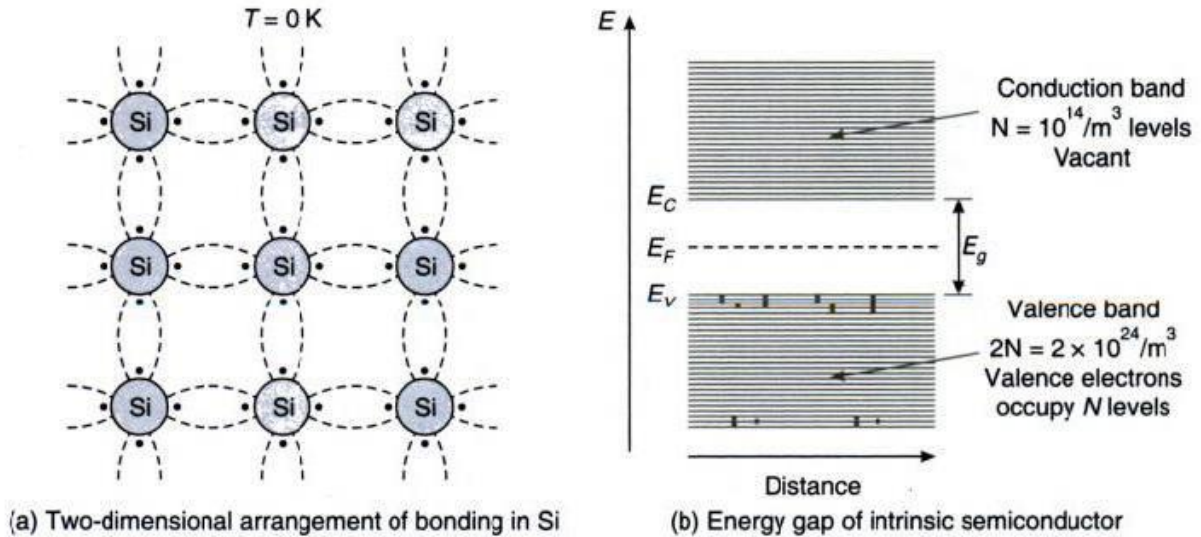
1. Intrinsic Semiconductors
2. Extrinsic Semiconductor

Bond Formation in Intrinsic Semiconductors and Extrinsic Semiconductors (P-type and N-type)

Intrinsic Semiconductor

The semiconductor which is pure and having the number of electrons in CB equal to number of holes in VB is called as *intrinsic semiconductor*.

Examples: Pure silicon and pure germanium crystals



When a covalent bond is broken, one electron becomes free and leaves the atom and becomes a positive ion known as hole. On applying electric field, the holes move in a direction opposite to valence band.

The fermi-level is middle of valence and condition bands.

$$E_g = E_C - E_V$$

Fermi energy,

$$E_F = \frac{E_C + E_V}{2}$$

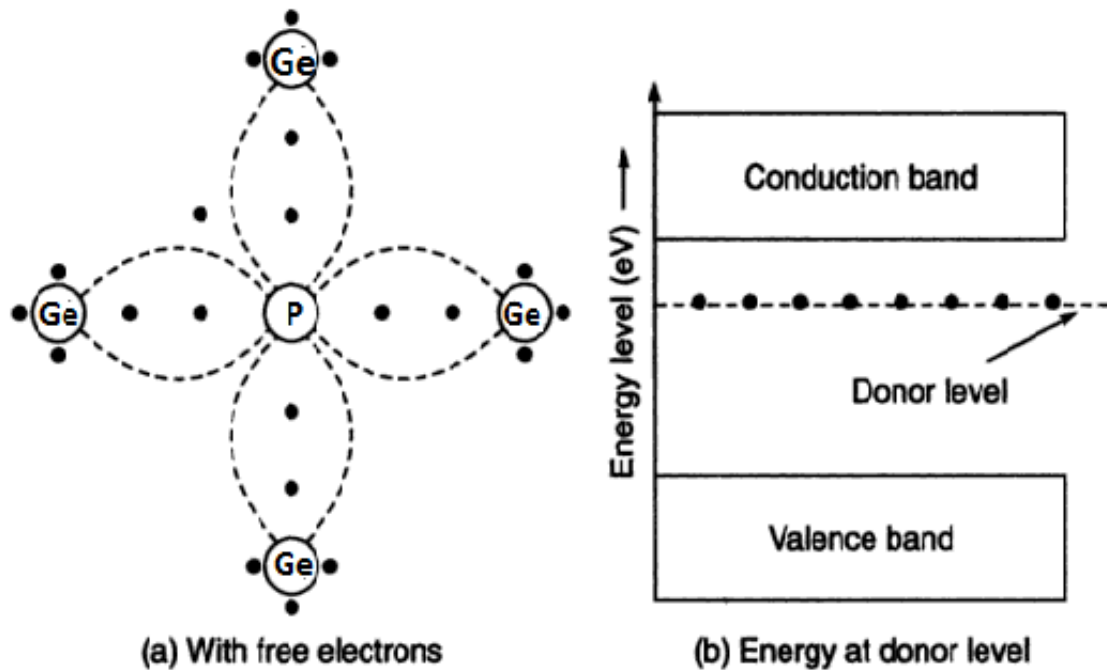
Extrinsic Semiconductors

When small quantities of selected impurities are added to an intrinsic semiconductor it becomes an extrinsic semiconductor. Depending upon the type of impurity extrinsic semiconductors is of two types:

1. N – Type semiconductor.
2. P – Type semiconductor.

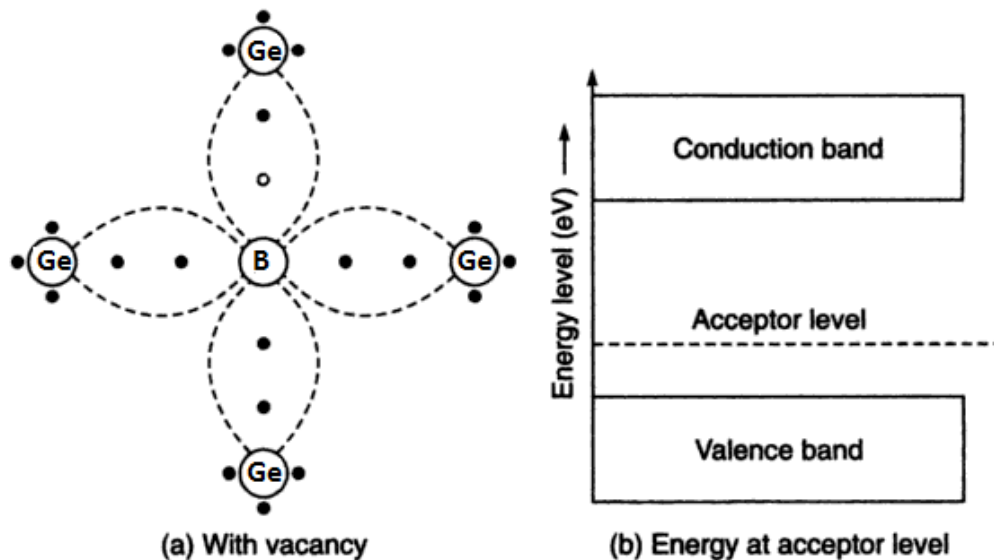
N-Type Semiconductor

A semiconductor doped with pentavalent impurities is called n-type semiconductor. Pentavalent impurities are Arsenic, Antimony etc. When pentavalent impurities like P or Sb is added to any semiconductor like Ge then the 4 electrons of Ge bond with 4 electrons of P and one extra electron is left out alone, i.e. it is ready to *donate* this electron. Such type of semiconductor is called *DONOR*.



P-Type Semiconductor

A semiconductor doped with trivalent impurity is called *p-type semiconductor*. Trivalent impurities are *Ga* and *In*. When a trivalent impure atoms (which have three valence electrons) like Gallium (*Ga*) or Boron (*B*) is added to any semiconductor like *Ge* then the 3 electrons of *Ge* bond with 3 electrons of *B* and the 4th electron doesn't have a pair, so a 'hole' is created. This means that it is ready to *accept* an electron to fill the hole. Thus a small amount of trivalent impurity creates *majority of holes*, which are positive, and are called as *Acceptors*.



Doping in p-type semiconductors

Intrinsic Electrical Conductivity

The electrical conductivity σ is given by,

$$\sigma = ne\mu_e + pe\mu_h$$

But $n = p = n_i$

$$\sigma = n_i(\mu_e e + \mu_h e)$$

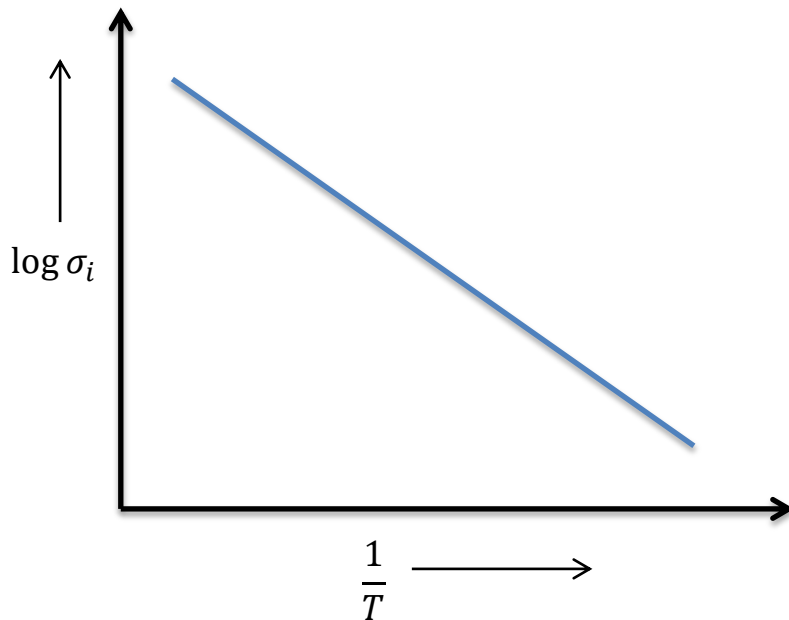
$$\sigma = n_i e(\mu_e + \mu_h)$$

$$\sigma = 2e(\mu_e + \mu_h) \left[\frac{2\pi K_B T}{h^2} \right]^{\frac{3}{2}} (m_e^* m_h^*)^{\frac{3}{4}} \times \exp \left[\frac{-E_g}{2K_B T} \right]$$

The electrical conductivity for intrinsic semiconductor

$$\log \sigma_i = A \exp \left[\frac{-E_g}{2K_B T} \right]$$

$$\log \sigma_i = \log A + \left[\frac{-E_g}{2K_B T} \right]$$



Band Gap

We know that,

$$\log \sigma_i = A \exp \left[\frac{-E_g}{2K_B T} \right]$$

Resistivity,

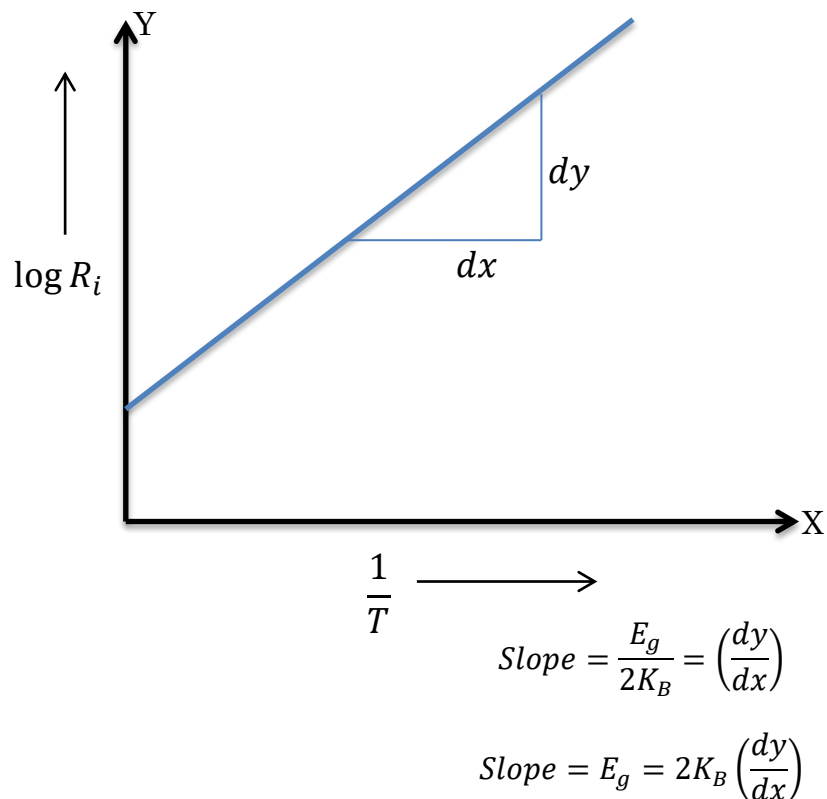
$$\rho = \frac{1}{\sigma_i} = \frac{1}{A} e^{\frac{E_g}{2K_B T}}$$

$$\frac{R_i a}{L} = \frac{1}{A} e^{\frac{E_g}{2K_B T}}$$

$$R_i = \frac{L}{Aa} e^{\frac{E_g}{2K_B T}}$$

$$\log R_i = \log c + \frac{E_g}{2K_B T}$$

The graph between $\frac{1}{T}$ and $\log R_i$ is



Drift & Diffusion

DRIFT CURRENT: The current that flows through the diode due to the applied electric field is called drift current.

$$J = V_d n e$$

But $V_d \propto E \Rightarrow V_d = \mu E$

$$J = \mu E n e$$

$$J_n = n e \mu_e E$$

$$J_p = p e \mu_h E$$

$$J_{drift} = J_n + J_p = e E [n \mu_e + p \mu_h]$$

But $n = p = n_i$

$$\|J_{drift} = E e n_i [\mu_e + \mu_h]\|$$

DIFFUSION CURRENT: The current that flows across the junction of a diode due to the difference in the concentration of holes or conduction electrons on its either side is called diffusion current.

OR

The motion of charge carriers from region of higher concentration to the region of lower concentration leads to a current called *diffusion current*.

The rate of flow of electrons is proportional to $-\frac{dn}{dx}$ and $\frac{dp}{dx}$

$$J_n = +e D_n \frac{dn}{dx}$$

$$J_p = -e D_p \frac{dp}{dx}$$

D_n And D_p are diffusion coefficients of electrons and holes

$$J_{diffusion} = J_n + J_p$$

$$\|J_{diffusion} = e D_n \frac{dn}{dx} - e D_p \frac{dp}{dx}\|$$

$$Total\ current\ flow = J_{drift} + J_{diffusion} = E e n [\mu_e + \mu_h] + e D_n \frac{dn}{dx} - e D_p \frac{dp}{dx}$$

$$\|J = e \left[E n \mu_e + E n \mu_h + D_n \frac{dn}{dx} - D_p \frac{dp}{dx} \right]\|$$

Einstein's equation

Since we know under equilibrium conditions, the drift and diffusion currents are equal.

$$(dn)eE\mu_e = e D_n \frac{dn}{dx}$$

$$(dn)eE = \frac{e D_n}{\mu_e} \frac{dn}{dx}$$

$$F = \frac{e D_n}{\mu_e} \frac{dn}{dx} \dots\dots \textcircled{1}$$

But force corresponding to pressure gradient is:-

$$F = K_B T \frac{dn}{dx} \dots\dots \textcircled{2}$$

So, from equation $\textcircled{1}$ & $\textcircled{2}$, we get

$$K_B T \frac{dn}{dx} = \frac{e D_n}{\mu_e} \frac{dn}{dx}$$

$$K_B T = \frac{e D_n}{\mu_e}$$

$$\frac{D_n}{\mu_e} = \frac{K_B T}{e}$$

For holes,

$$\frac{D_p}{\mu_h} = \frac{K_B T}{e}$$

Therefore,

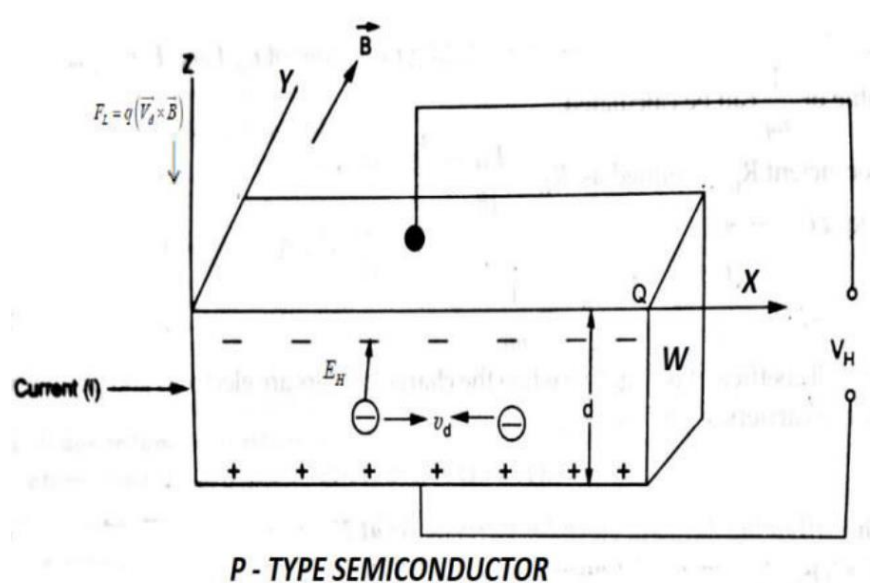
$$\left[\frac{D_n}{\mu_e} = \frac{D_p}{\mu_h} = \frac{K_B T}{e} \right]$$

The ratio between diffusion constant and mobility of charge carriers is directly proportional to absolute temperature.

Hall Effect in semiconductors

When magnetic field is applied perpendicular to a current carrying conductor (metal or semiconductor) then a voltage is developed in the material perpendicular to both magnetic field and current in the conductor. This effect is known as **Hall Effect** and the voltage is developed is known as **Hall voltage (V_H)**.

Consider a rectangular block of extrinsic semiconductor. Let a current ' I ' is passed in the conductor along **X -direction** and magnetic field (\vec{B}) is established along **Y -direction**, then the charge carrier experiences a Lorentz force (F_L) along the **Z -direction**. The direction of this force is noted by Fleming left hand rule. As a result of this force (downward), the charge carriers are forced down into the bottom surface.



If the specimen is a ***P-type*** semiconductor, since the holes are the charge carriers, they are forced down into the bottom surface and hence the upper surface is occupied by the electrons. Therefore, a potential difference is developed between the upper and bottom surface. This Hall potential V_H can be measured by connecting two surfaces to a voltmeter.

This separation of charge carriers creates an electric field (E_H) in the upward direction (positive Z -direction).

These charge carrier are moving in a magnetic field in the semiconductor, they experience *Lorentz force*

$$F_L = q(\vec{V_d} \times \vec{B}) \quad (V_d = \text{drift velocity of the carriers})$$

$$F_L = qV_d B \sin \theta$$

$$F_L = qV_d B \sin 90$$

($\theta = 90$ because the force is acting on charge perpendicularly)

$$F_L = qV_d B \quad (\because q = -e)$$

$$[F_L = -eV_d B]$$

Since, the electric force due to electric field created by the surface charges.

$$F_H = qE$$

$$[F_H = -eE_H]$$

Where, E_H is the hall electrical field.

After some time both forces become equal in magnitude and act in opposite direction, this situation is said to be under equilibrium.

At equilibrium,

$$\mathbf{F_H = F_L}$$

$$eE_H = eV_d B$$

$$E_H = V_d B \quad \dots \textcircled{1}$$

The current density is

$$J = -neV_d \quad \dots \textcircled{2}$$

Form equations $\textcircled{1}$ & $\textcircled{2}$, we get

$$E_H = -\frac{BJ}{ne} \quad \dots \textcircled{3}$$

But we know that the Hall Coefficient R_H

$$R_H = -\frac{1}{ne} \quad \dots \textcircled{4}$$

From equation $\textcircled{3}$ & $\textcircled{4}$, we get

$$E_H = R_H B J$$

$$\left[\left[R_H = \frac{E_H}{BJ} = -\frac{1}{ne} \right] \right]$$

For holes,

$$\left[\left[R_H = \frac{E_H}{BJ} = \frac{1}{pe} \right] \right]$$

Determination of Hall coefficient

Let 'w' is the width of sample then

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

$$R_H = \frac{E_H}{JB} = \frac{V_H}{JBw}$$

$$V_H = R_H(JBw) = R_H \times \frac{I}{A} \times Bw \quad (\because J = \frac{I}{A})$$

$$V_H = R_H \times \frac{I}{wt} \times Bw = \frac{R_H IB}{t}$$

$$R_H = \frac{V_H t}{IB}$$

Applications of Hall Effect

- It is used to find out whether the given semiconductor is N – type or P – type.
- It is used to measure carrier concentration, mobility and conductivity of a semiconducting material.
- Hall voltage is produced of two input quantities namely the current and the magnetic field. Using this principle, the Hall Effect device is used as a multiplier.
- It is used as a magnetic field sensor. Using the Hall Effect devices, the magnetic field ranging from **1μT** to **1T** is sensed.
- The sign of charge carriers can be determined.
- The carrier density can be estimated.
- Mobility of charge carriers can be measured.
- It can be used to determine the given material is a metal, insulator or semiconductor.