QUANTUM MECHANICS

The physical concept of a particle is characterized by mass and velocity. Experiments dealing with particles, usually interpreted in terms of mass and Velocity by using Newton's Laws of Motion. This classical approach is not sufficient to describe some experiments. The results of some of the experiments are contrary to Newton's Laws

The experiments like Photo Electric Effect, Black Body Radiation and Compton Effect confirmed the particle nature of Photons.

Interference, diffraction and Polarization of light confirmed that light is having wave nature.

Louis De Broglie extended the idea of dual nature of radiation to matter. According to De Broglie matter possesses wave as well as particle characteristics. The concept of dual nature of radiation can be understood by knowing relationship between particle as well as the wave and their characteristics.

Waves and Particles:

PARTICLES	WAVES
1. A particle occupies space. 2. A particle will have a definite mass. 3. The particle will have position. 4. Due to change in position of the particle, it will have velocity. 5. Due to Mass and Velocity , the particle posses momentum Momentum P= m X v 6. A Particle will have Energy.	1. The transmission of disturbance from one point to other point in a material medium is known as Wave. 2. A Wave will have amplitude. 3. It will have time period. 4. It will have frequency. 5. It will have wave length. 6. It will have phase. 7. It will have intensity $I \propto A^2$.

The particle and wave nature can be explained by using Planck's Quantum Theory. According to this theory emission of radiation is in the form of photons. A photon will have velocity of light and mass which is in motion. i.e., it will have both momentum and energy. Thus a photon behaves like a particle. The energy of a photon is given by (According to MaxPlank)

$E = nh\upsilon$ Where n=1, 2, 3… i.e., the energy of the photon is quantized.

h= Planck's constant, $\upsilon =$ Frequency of radiation.

Therefore in addition to frequency, the other parameters attribute wave nature to a photon. i.e., a photon will have dual nature.

The De Broglie Hypothesis:

The dual nature of light possessing both wave and particle properties was explained by combining plank's expression for the energy and Einstein's Mass – Energy relation.

The Energy of a photon according to Max Plank is given by

$$E = h\upsilon \quad \text{--------------------} \ (1)$$

Einstein's Mass – Energy relation is given by

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

Here h= Plank's constant

υ = Frequency of Radiation

m = Mass of Photon

c = Velocity of light

From equations (1) & (2)

$$h\upsilon = mc^2 \quad \text{------------------} \ (3)$$

Also the velocity of light is given by

$$c = \upsilon\lambda$$

$$\upsilon = \frac{c}{\lambda} \quad \text{------------------------} \ (4)$$

$\therefore$ From (3) & (4) we have

$$\frac{hc}{\lambda} = mc^2$$

$$\Rightarrow \lambda = \frac{h}{mc}$$

$$\lambda = \frac{h}{p} \quad \text{------------------------------} \ (5)$$

Where λ = wave length of the Photon

p = Momentum of Photon = mc

Using this concept, De Broglie proposed the concept of matter waves.

According to this the material particle of mass 'm' moving with a velocity 'v' should have an associated wave length λ .

This wave length λ is called the De Broglie wave length.

$$\text{Now } \lambda = \frac{h}{momentum}$$

$$\lambda = \frac{h}{mv} = \frac{h}{p} \qquad \text{------------------ (6)}$$

Where h = Plank's constant, p=momentum

Equation (6) is known as De Broglie wave equation and λ is called De Broglie wave length.

If the particle is moving with a velocity comparable to the velocity of light then the mass of the particle is always changes. The mass 'm' according to theory of relativity is not an invariable entity as in Newtonian Physics. The relativistic mass 'm ' is given by

Here m_0= rest mass of the electron

$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$$

c = Velocity of Light

From equation (6) it is found that if the particles are accelerated to various velocities, we can produce waves of various wave lengths.

Higher the electron velocity, smaller the De Broglie wave length and vice versa.

RalationbetweenDeBroglie Wavelength λ and KiniticEnergyEof the particle

Let us assume m is the mass of the particle. Now the particle is moving with velocity 'v'.

Kinetic Energy of the particle , $E = \frac{1}{2}mv^2$ since $E = \frac{1}{2m}m^2v^2 = \frac{(mv)^2}{2m}$

$$\Rightarrow \quad E = \frac{p^2}{2m}$$

$$\Rightarrow \quad p^2 = 2mE$$

$$\Rightarrow \quad p = \sqrt{2mE} \qquad \text{---------------------------- (1)}$$

But according to De Broglie hypothesis $\lambda = \frac{h}{p}$ ---------------------- (2)

From (1) & (2) $\lambda = \frac{h}{\sqrt{2mE}}$ ----------------------------(3)

Where h = Plank's constant

m = Mass of the particle and E = Kinetic energy of the particle

Relation between de Broglie wave length and the applied potential difference:

(De Broglie wave length of electrons)

Let m be the mass of the electron. This electron is applied with a potential difference of V volt.

Here the work done (energy) on the electron is given by eV.

Here e = charge on the electron

V= applied potential difference in volts.

The work done is converted into Kinetic Energy of the electron.

i.e. $\frac{1}{2}mv^2 = eV$

Here v = velocity acquired by the electron .

Now $\frac{p^2}{2m} = eV$

$$p^2 = 2meV$$

Momentum, $p = \sqrt{2meV}$ ---------------------------- (1)

Now the De Broglie wave length associated with the electron is given by

$$\lambda = \frac{h}{p} \qquad \text{---------------------------- (2)}$$

From (1) & (2) $\lambda = \frac{h}{\sqrt{2meV}}$ ----------------------------(3)

Ignoring the relativistic considerations, m = rest mass of the electron

$$\lambda = \frac{h}{\sqrt{2meV}}$$

$$\lambda = \frac{6.625X10^{-34}}{\sqrt{2X9.1X10^{-31}X1.602X10^{-19}V}} = \frac{12.26X10^{-10}}{\sqrt{V}} \text{ meter}$$

$\lambda = \frac{12.26}{\sqrt{V}} A^0$ V = Applied Voltage in Volts.

Matter Waves:

According to Debroglie concept that a moving particle is associated with wave nature. This can be explained by Bohr's atomic model.

According to Bhors concept the angular momentum (L) of a moving electron in an Atomic orbit of radius ‘r’ is quantized.

$$\text{i.e.} \quad L = \frac{nh}{2\pi} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \; (1)$$

$$n = 1, 2, 3, 4 \ldots\ldots\ldots\ldots$$

Now Angular momentum L= m v r ……….. (2)

Here m=mass of an electron

v=linear Velocity of Electron

r=Radius of the orbit

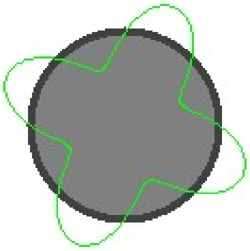
form (1)&(2) ,now we have

$$L = mvr = \frac{nh}{2\pi} \quad \ldots\ldots\ldots(3)$$

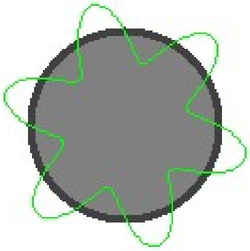
$$\Rightarrow 2\pi r = \frac{nh}{mv}$$

$$\Rightarrow 2\pi r = \frac{nh}{p} \quad \ldots\ldots\ldots\ldots\ldots(4)$$

$p = mv$, momentum of electron.



n=4 orbit



n=6 orbit

Figure (1) Bohr’s orbit and deBroglie Waves of an electron in the orbit

In the equation (4), $2\pi r$ is the circumference length of the orbit in which the electron is revolving.

This circumference is equal to the ‘n’ times the wave length of the associated wave of a moving electron in the orbit.

$$\text{i.e} \quad 2\pi r = n\lambda \ \ldots\ldots\ldots\ldots\ldots(5), \text{ since } \lambda = \frac{h}{p}$$

This is shown diagrammatically for n=4 and n=6 in figure (1).

According to the deBroglie, a moving particle will have both particle and wave nature. The waves associated with a moving material particle are called matter waves or deBroglie waves. The deBroglie waves are associated with materialistic particles such as electrons, protons, neutrons etc.

<u>Properties of Matter Waves</u>:

1. DeBroglie waves are not electromagnetic waves.

They are called pilot waves.

The waves that guide the particles are called matter waves or pilot waves.

2. Matter waves consist of a group of waves or a wave packet associated with a particle. The group has the velocity of particle.
3. Each wave of the group travel with a velocity known as phase velocity given by $V_{ph} = \frac{\omega}{K}$ where ω = Angular frequency, K = Wave vector. or wave Number.
4. These waves cannot be observed.
5. The wave length of matter waves is given by

   $\lambda = \frac{h}{p}$ Where h = Planck's constant, p = momentum of the particle

   $$\lambda = \frac{h}{mv}$$
6. Lighter the particle, greater will be the wave length associated with it.
7. Smaller the velocity of the particle, longer will be the wave length.
8. When $V = 0, \lambda = \infty$. Also if $V = \infty, \lambda = 0$
9. Matter waves can be produced whenever the particles in motion are charged or uncharged.
10. Matter waves travel faster than velocity of light.
11. The wave nature of the matter introduces uncertainty in the location of the position of the particle.

HeisenBerg's Uncertainty Principle:

Usually the moving particle must be regarded as a deBroglie wave group rather than a localized particle.

This suggests that there is a fundamental limit to the accuracy with which we can measure its particle properties.

According to classical Mechanics, a moving particle at any instant has a fixed position in space and a definite momentum which can be determined simultaneously with accuracy.

But we know that a moving particle is similar to a wave, we cannot determine the position and momentum simultaneously, accurately.

The measurement of position and moment of a moving particle is impossible

Let Δx denotes the error in the measurements of the position of the particle along x-axis and Δp represents the error in the measurement of momentum, then

$$(\Delta x)(\Delta p) = \frac{h}{2\pi}$$ Here h=Planks Constant.

If we locate the particle exactly $(\Delta x \to 0)$ only at the expense of imparting to it an infinite momentum $(\Delta p \to \infty)$

The uncertainty principle can also be written as $(\Delta E)(\Delta t) = \frac{h}{2\pi}$

Applications:

1. It explains the absence of electrons in the nucleus.
2. It gives proof for the existence of protons and neutrons inside the nucleus
3. Explains uncertainty in the frequency of highest emitted radiation by an Atom
4. Energy of an electron in an Atom

Differences Between Matter waves and Electromagnetic Waves:

Matter Waves	Electromagnetic waves
1. These waves are associated with the moving particles.	1.Oscillating charged particles gives electromagnetic radiation. (electromagnetic waves)
2.wavelength depends upon mass of the particle $\lambda = \frac{h}{P} = \frac{h}{mv}$	2. Wavelength depends upon the energy of the photon. $E = h\upsilon$, $E = \frac{hc}{\lambda}, \because c = \upsilon\lambda, \upsilon = \frac{c}{\lambda}$ $\therefore \lambda = \frac{hc}{E}$
3. Can travel with a velocity greater than velocity of light.	3. These waves travel with a velocity of light.

4. These waves are not electromagnetic waves.	C=$3\times10^8 m/s$ 4. In this wave electric and magnetic fields oscillate perpendicular to each other.

Note on Simple Harmonic Motion :

If a particle executing simple Harmonic motion, then its motion is periodic, acceleration is directed towards an equilibrium point and acceleration is proportional to displacement. ($a \propto$ -x)

The general equation of motion for SHM is given by

$$y = A\,\text{Sin}\,(\omega t - \phi) \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

Here y = displacement of the particle executing simple harmonic motion

A = Amplitude of the particle executing simple harmonic motion

ω = Angular frequency

Φ = Phase difference

Now Phase difference $=\frac{2\pi}{\lambda}$ X Path difference

$$\phi = \frac{2\pi}{\lambda}x \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

From equations (1) & (2) we get

$$y = ASin(\omega t - \frac{2\pi}{\lambda}x)$$

$$y = ASin(2\pi\upsilon t - \frac{2\pi}{\lambda}x)$$

$$y = ASin2\pi\upsilon(t - \frac{x}{\upsilon\lambda})$$

Since we have to solve problems by Schrödinger’s time independent Wave Equation, we choose wave equation involving no time.

$$y = ASin2\pi\upsilon(-\frac{x}{\upsilon\lambda})$$

$$y = ASin2\pi(-\frac{x}{\lambda})$$

$$y = -ASin2\pi(\frac{x}{\lambda}).$$

Schrodinger’s Wave equation(Time independent)

Let us consider a particle of mass m, moving with a velocity v along the positive X-direction.

The wave function ψ for a particle moving freely in the positive x-direction has the same form as the wave equation for simple harmonic motion and simple harmonic waves in the positive x-direction.

$$\therefore \psi = -ASin2\pi(\frac{x}{\lambda}) \quad \text{……………………(1)}$$

Here ψ is a function of x only.

Differentiating equation (1) with respect to x once and two times, we get

$$\frac{d\psi}{dx} = -A\frac{2\pi}{\lambda}\cos\frac{2\pi x}{\lambda}$$

Again differentiating, we get

$$\frac{d^2\psi}{dx^2} = A\frac{4\pi^2}{\lambda^2}\sin\frac{2\pi x}{\lambda}$$

$$\frac{d^2\psi}{dx^2} = \frac{4\pi^2}{\lambda^2}A\sin\frac{2\pi x}{\lambda}$$

But $\psi = -A\sin\frac{2\pi x}{\lambda}$

$$\therefore \frac{d^2\psi}{dx^2} = -\frac{4\pi^2}{\lambda^2}\psi \quad \text{……………………………..(2)}$$

DeBroglie wavelength associated with the particle is

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

$$\frac{1}{\lambda} = \frac{m\,v}{h}$$

$$\frac{1}{\lambda^2} = \frac{m^2v^2}{h^2} = \frac{2m(\frac{1}{2}mv^2)}{h^2} \quad \text{………………….(3)}$$

Let E be the total energy of the particle and V be the potential energy of the particle and T be the kinetic energy.

Then total energy ,E=T+V

T, KE = $\frac{1}{2}mv^2$ = E – V ……………………………….(4)

Substituting the above value of K.E. in Equation (3), we get

$$\frac{1}{\lambda^2} = \frac{2m(E-V)}{h^2} \quad \text{……………………………(5)}$$

From equations (5) and (2), we get

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

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

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\frac{h^2}{4\pi^2}}(E-V)\psi = 0$$

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

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad (\because \hbar = (\frac{h}{2\pi})) \text{ ....(6)}$$

This is the Schrödinger's time independent one dimensional wave equation.

Wave number:

In Spectroscopy	In wave mechanics
wave Number of an Electromagnetic wave is given by $K = \bar{\upsilon} = \frac{1}{\lambda}$, But $\lambda = \frac{h}{p}$ $\Rightarrow K = \frac{1}{(\frac{h}{P})} = \frac{P}{h}$ $\Rightarrow K = \frac{\sqrt{2mE}}{h} m^{-1}$	For the special case of an electromagnetic wave, $K = \frac{2\pi}{\lambda}$. $E = h\upsilon \Rightarrow \frac{hC}{\lambda}$ $\Rightarrow \lambda = \frac{hC}{E}$ $\therefore K = \frac{2\pi E}{hC}$ $\therefore K = \frac{E}{\hbar C}$

Wave velocity:

Wave velocity is defined as the velocity with which a particular crest or trough or a particular phase of a wave advances in a medium.

The wave Velocity u of the matter waves can be obtained from the energy of photon.

Now $E = h\upsilon$ ……………………………….(1)

Or frequency, $\upsilon = \frac{E}{h} = \frac{(\frac{1}{2})mv^2}{h} = \frac{p^2}{2m} X \frac{1}{h}$

Multiplying and dividing the numerator and the denominator by h, we get

Frequency, $\upsilon = \frac{h}{2m} X \frac{p^2}{h^2} = \frac{h}{2m} X \frac{1}{\lambda^2}$ ……………..(2)

There fore, the wave velocity,

u = frequency X wave length

$$u = \frac{h}{2m} X \frac{1}{\lambda^2} X\lambda$$

The wave velocity of the electron

$$u = \frac{h}{2m\lambda} \text{ ……………………………(3)}$$

Physical Significance of Wave Function

The wave function is a Complex function. This does not have a direct physical meaning. The square of its absolute magnitude $|\psi|^2$ can be taken as definite meaning by considering the case of an electromagnetic wave.

The intensity of a light wave is proportional to the square of the amplitude. $(I\alpha A^2)$

$|\psi|^2$ Is the probability density of the particle associated with the deBroglie wave described by the wave function ψ.

That is the probability of finding a particle is proportional to $|\psi|^2$ at the point x, and at any instant of time t.

The wave function is given by

$\psi(x,t) = a + ib$, ψ^* is its complex conjugate, $\psi^* = a - ib$

Now $\psi\ \psi^* = (a + ib)\ (a - ib\ ).= [a^2 - i^2b^2]$

$\psi\ \psi^* = a^2 + b^2$, $\psi\ \psi^*$ is denoted by P

$|\psi|^2$ is called the probability density.

The probability of finding a particle is real.

The probability of a particle being present in a volume dv=dx dy dz is

$|\psi|^2$ dx dy dz.

The total probability of finding the particle some where is unity.
Since the probability of finding a particle some where in the space is certain.

$$\iiint |\psi|^2 dxdydz = 1$$

Or $$\iiint \psi\psi^* dxdydz = 1$$

The triple integral extends over all possible values of x, y and z.
A wave function ψ satisfying the above relation is known as normalized wave function.This Condition is called condion of Normalization.

Particle in a One-Dimensional Potential Box:

(OR Electron in a Potential Well):

Consider an electron of mass 'm' this is bound to move in a one dimensional crystal of length L.
The electron is prevented from leaving the crystal by the presence of a large potential energy barrier at its surface.
Though the barriers extend over a few atomic layers near the surface, these are taken infinitely large for the sake of simplicity. The problem is similar to that of an electron moving in a one-dimensional potential Box.
This is represented by a line and is bounded by infinite potential energy as shown in figure (2).

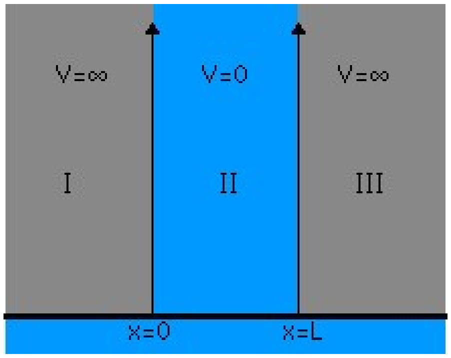


Fig (2) Electron in a one dimensional Potential well.

The potential energy within the crystal or box is assumed to be zero
Thus we have
$V(x) = 0$ for $0<x<L$ ………………… (1)
$V(x) = \infty$ for $x \leq 0 and x \geq L$

The wave function ψ_n of the electron occupying the nth state is given by

$$\frac{d^2\psi_n}{dx^2} + \frac{2m}{\hbar^2}(E_n - V)\,\psi_n = 0 \quad \ldots\ldots\ldots\ldots\ldots (2)$$

Here also E_n= Total energy of the electron in the nth state.
V= Potential energy.

Inside the box, v=o

$$\frac{d^2\psi_n}{dx^2} + \frac{2m}{\hbar^2} E_n\psi_n = 0 \text{-------------------------} (3)$$

$$\frac{d^2\psi_n}{dx^2} + k^2\psi_n = 0 \text{-------------------------------} (4)$$

Where $k^2 = \frac{2m}{\hbar^2} E_n \Rightarrow k = \frac{\sqrt{2m\,E_n}}{\hbar}$ --------------(5)

Equation (4) is a differential equation. The general solution of the equation (4) is given by

$$\psi_n(x) = A Sinkx + B Coskx \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (6)$$

In equation (6), A and B are arbitrary constants,
These constants are to be determined from the boundary conditions.
Since the electron is constrained by infinitely high potential barriers at x=0 and x=L, $v \to \infty$. We assume that $\psi_n(0) = 0 and \psi_n(L) = 0$

The product V(x) ψ_n (x) in equation (2) also approaches infinity.

Thus in order that the wave function ψ_n (x) may be continuous, the kinetic energy must also become infinite which is not feasible.

Hence ψ_n (x) must vanish for x=0 and x=L.
For x=0 equation (6) gives B=0

ψ_n (0) =0=A SinK (0) +B CosK (0)
0=A (0) +B (1)
$\Rightarrow$B=0
Now equation (6) becomes

ψ_n (x)=A SinK(x) -------------------------------- (8)

Also since ψ_n (L) =0, equation (8) becomes

A SinKL=ψ_n (L)=0
$A \neq 0$ But SinKL=0$\Rightarrow KL = n\pi$
Or K=$\frac{n\pi}{L}$ ……………………………………(9)
Where n=1, 2, 3…
Thus the expression for the allowed wave function becomes.

ψ_n (x)=A Sin ($\frac{n\pi}{L}$) x ……………………. (10)

Eigen Energy Values:

The allowed energy values can be obtained from equations (5) & (9) as

$$k = \frac{\sqrt{2m\,E_n}}{\hbar}$$

$$k = \frac{\sqrt{2m\,E_n}}{\hbar} = \frac{n\pi}{L}$$

$$\frac{2m\,E_n}{\hbar^2} = \left(\frac{n\pi}{L}\right)^2$$

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

$$E_n = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{L^2}$$

$$E_n = \frac{h^2}{4\pi^2 2m}\;\frac{n^2\pi^2}{L^2} \quad , (\text{Since}\, \hbar = \frac{h}{2\pi})$$

$$E_n = \frac{n^2h^2}{8mL^2} \qquad ……………………. (11)$$

Here h= Planck's constant

m= Mass of Electron.

L= Length of One dimensional crystal, are constants.

i.e $E_n \alpha\, n^2$

Some Features:

1. The lowest energy of the particle is given putting n=1

$$E_1 = \frac{h^2}{8mL^2}$$

$$E_n = n^2E_1$$

This known as zero point energy.

2. For n=1, 2, 3…We get discrete energy values of the particle in the one dimensional box.

$$n_1 = E_1 = \frac{h^2}{8mL^2}$$

$$n_2 = E_2 = 2^2\frac{h^2}{8mL^2} = 4E_1$$

$$n_3 = E_3 = 3^2\frac{h^2}{8mL^2} = 9E_1$$

……………………..

3. It is apparent from equations (10) and (11) that the allowed wave functions ψ_n (x) and the allowed energy values E_n exist only for integral values of n. The number n is called principal quantum number.

4. The spacing between the nth energy level and next highest energy level [n+1] th level is given by

$$E_{n+1} = \frac{(n+1)^2 h^2}{8mL^2} = (n+1)^2 E_1$$

$$E_n = \frac{n^2 h^2}{8mL^2} = n^2 E_1$$

$$E_{n+1} - E_n = (n+1)^2 E_1 - n^2 E_1$$

$$E_{n+1} - E_n = (n^2 + 1 + 2n)\ E_1 - n^2 E_1$$

$$E_{n+1} - E_n = (2n+1)\ E_1$$

5. The energy spectrum consists of discrete energy levels. The spacing between the levels is determined by the values of n and L.

The Spacing decreases with increase in L.

If L is of the order of a few centimeters, the energy level form almost a continuum.

But if L has atomic dimensions, the spacing between the levels becomes appreciable.

The energy levels corresponding to n=1, 2, 3 and 4 are shown in fig (3).

Fig (3) First four energy levels of an electron in a one dimensional Box.

Determination of constant A in ψ_n (x)=A Sin ($\frac{n\pi}{L}$)x (Normalization of the wave function):

The constant A in ψ_n **(x) =A Sin (**$\frac{n\pi}{L}$ **)x** is determined by using the condition that the probability of finding an electron some where on the line **is unity**

$$i.e. \int_0^L \psi_n^*(x)\ \psi_n(x)\ dx = 1$$

$$\int_0^L |\psi_n(x)|^2 dx = 1$$

$$\int_0^L A^2 Sin^2\left(\frac{n\pi}{L}\right)x\ dx = 1$$

$$A^2\int_0^L Sin^2\left(\frac{n\pi}{L}\right)x\ dx = 1$$

$$A^2\int_0^L \frac{1-Cos\left(\frac{2n\pi}{L}\right)x}{2}\,dx = 1$$

$$\frac{A^2}{2}\int_0^L dx - \frac{A^2}{2}\int_0^L Cos\left(\frac{2n\pi}{L}\right)x\ dx = 1$$

Now $\int_0^L Cos\left(\frac{2n\pi}{L}\right)x\ dx = 0$

$$\therefore\ \frac{A^2}{2}\int_0^L dx = 1 \Rightarrow \frac{A^2}{2}[x]_0^L = \frac{A^2L}{2} = 1$$

$$\therefore\ A^2 = \frac{2}{L} \Rightarrow \therefore\ A = \sqrt{\frac{2}{L}}$$

Now from the equation $\psi_n(x) = A\ Sin\left(\frac{n\pi}{L}\right)x$

$$\psi_n(x) = \left(\sqrt{\frac{2}{L}}\right) Sin\left(\frac{n\pi}{L}\right)x \quad \text{..............} \ \textbf{(1)}$$

This is the normalized wave function. The first four wave functions and the wave functions of the electron in a one dimensional Box are shown in the figure (4)

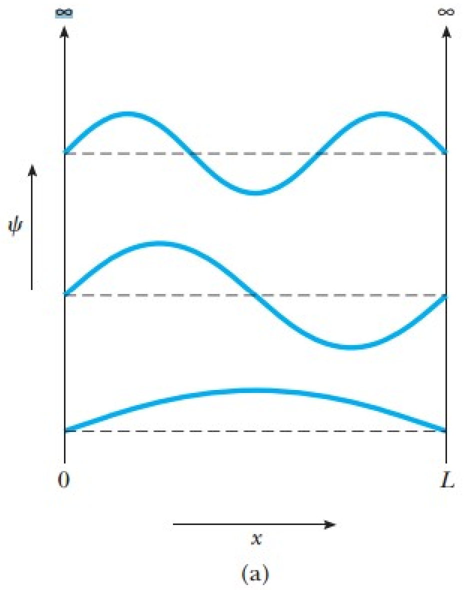


Fig (4) First three wave functions of an electron in a one dimensional box

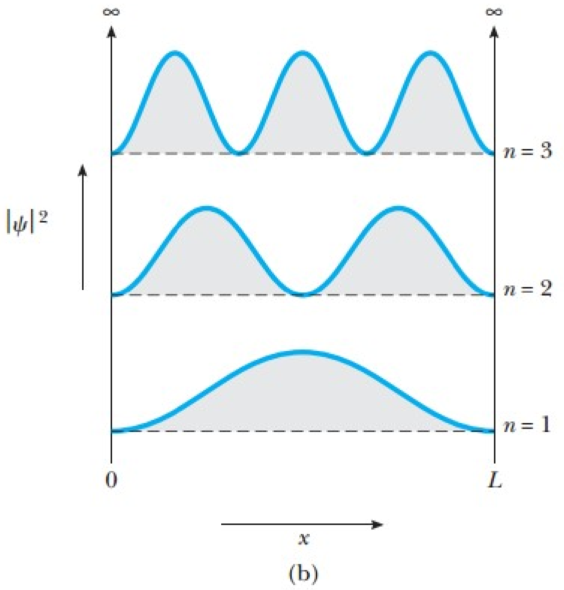


Fig.(5) the probability density of an electron in a one dimensional

The probability density of the particle in the one dimensional Box.

The probability of finding the particle in a small length dx along x is given by $P_n(x)dx = A\,|\psi_n|^2\,dx \Rightarrow P_n(x)dx = \frac{2}{L}\,Sin^2\left(\frac{n\pi}{L}\right)x\,dx$

Also Probability Density $$P_n(x) = \frac{2}{L}\,Sin^2\frac{n\pi}{L}x$$

This is maximum when $$\frac{n\pi}{L}x = \frac{\pi}{2},\frac{3\pi}{2},\frac{5\pi}{2},- - -$$

$$or\ \ x = \frac{L}{2n},\frac{3L}{2n},\frac{5L}{2n},- - -$$

For n=1, the most probable positions of the particle is at x=$\frac{L}{2}$

For n=2, the most probable positions are at x=$\frac{L}{4}$ and $\frac{3L}{4}$

The probability density of the particle in the one dimensional Box is shown for various values of 'n' in the figure (5).

Fermi-Dirac Distribution:

According to free electron theory, Electrons in a solid move in all possible directions like gas molecules in a container. These free electrons contribute for electrical conduction.

The free electron model of a metal has survived to the actual situation in metals, particularly the monovalent atoms such as Alkali metals.

Quantum mechanics requires that all valence or free electrons should be specified by the three quantum numbers n_x , n_y , n_z together with the spin.

The spin can have either $+\frac{1}{2}$ or $-\frac{1}{2}$

The Pauli Exclusion Principle does not permit more than one electron to have same four quantum numbers.

Many of the occupied states in a metal containing 10^{23} free electrons must be described with fairly large quantum numbers.

Now it is most convenient to discuss the metallic state with statistical mechanics.

The probability that a particular quantum state having an energy E is occupied is given by Fermi-Dirac function.

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - Ef}{K_B T}\right)}$$

Here f (E) is called probability of occupying a state

EF is the energy of the Fermi level.

E is the energy of the state in which the electron is occupied at $T\,^0K$.

K_B is the Boltzmann constant.

Properties:

1. The Fermi-Dirac function also valid for semiconductors. In a semiconductor, the probability of occupancy of states by electrons is given by the F-D distribution function.

   $$P_e(E) = f(E) = \frac{1}{1 + \exp\left(\frac{E - Ef}{K_B T}\right)}$$

2. The distribution function is valid only in equilibrium.
3. The Fermi level is absolutely valid in equilibrium only.
4. Fermi-Dirac distribution function is valid for all the particles obeying Pauli's exclusion principle. This is equally applicable regardless of the type of the solid, doping of the semiconductor, etc.

   Any particle obeying F-D distribution function is called Fermions.

   The Fermi-Dirac distribution function considers statistically the entire collection of fermions in the volume.

   Thus it considers all electrons in the semi conducting solid and not merely electrons in a Band.
5. An empty electron state is called a HOLE. The Fermi-Dirac distribution function for holes in the solid would correspond to the statistical distribution of vacant sites.

   The hole distribution function is denoted as

$$P_h(E) = 1 - P_{FD}(E)$$

$$P_h(E) = \frac{1}{1 + \exp\left(\frac{E_f - E}{K_B T}\right)}$$

6. AT $E = E_f$,

   $$P_h(E) = P_e(E) = \frac{1}{1+1} = \frac{1}{2}$$

   i.e. the probability of occupancy of the electron or hole is $\frac{1}{2}$

   This also gives a definition for the Fermi level.

7. Fermi level is the energy level where the probability of occupation is $\frac{1}{2}$

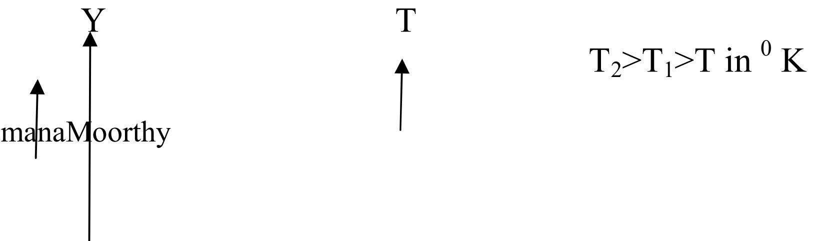
8. At 0^0 K, Pe (E) =1 for $E \leq E_f$

   And Pe (E) = 0 for $E > E_f$

   This implies that at 0^0 K all states up to the Fermi level are completely occupied by the electrons. All the states above the Fermi level are empty.

9. The distribution function is a strong function of temperature only at energies close to E_f.

Plots of P_e (E) and E at different temperatures are shown in figure (6).



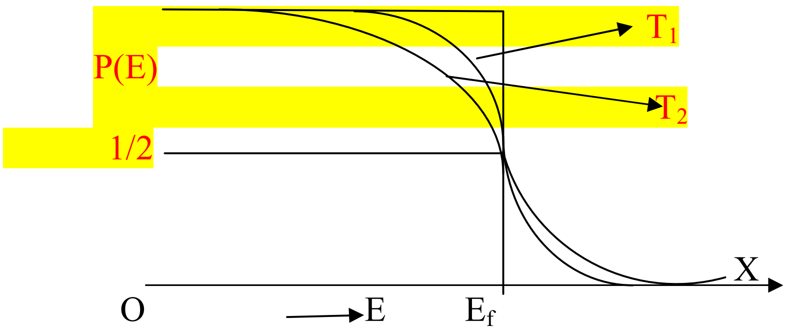


Fig (6). P_e (E) versus E for various T values. At all temperatures, the curves passes through the point $\left[E_f, \frac{1}{2}\right]$.

Note on Fermi-Dirac Distribution function: The Fermi-Dirac distribution for Electrons is given by

$$P_e(E) = f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{K_B T}\right)}$$

Now at the Absolute zero ($T = 0^0 K$), there are two situations

(i) For $E < E_F$,

$$P_e(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{K_B T}\right)}$$

$$P_e(E) = \frac{1}{1 + e^{-\frac{X}{K_B(0)}}}$$

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

$$P_e(E) = \frac{1}{1 + \frac{1}{e^{\infty}}} \qquad \text{But } e^{\infty} = \infty \Rightarrow \frac{1}{\infty} = 0$$

P_e (E) = 1, for $E < E_F$ at $T = 0^0$

(ii) For $E > E_F$

$$P_e(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{K_B T}\right)}$$

$$P_e(E) = \frac{1}{1 + \exp\left(\frac{+X}{K_B(o)}\right)}$$

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

$$P_e(E) = \frac{1}{1+\infty}$$

$$P_e(E) = \frac{1}{\infty}$$

$$P_e(E) = 0$$

This means that no electrons have energy greater than E_F at 0^0 K.
i.e the Fermi energy E_F is the maximum energy that a free electron in the metal can have at absolute zero.

Schrodinger's Wave equation(Time independent)

Let us consider a particle of mass m, moving with a velocity v along the positive X-direction.

The wave function ψ for a particle moving freely in the positive x-direction is given by a complex function

$$\Psi(x,t) = Ae^{i(kx-\omega t)}. \qquad \text{……………………(1)}$$

Here ψ is a function of x and t only.
A= amplitude.
k= Wave vector.
x= position.
ω=Angular frequency.
t=time

Differentiating equation (1) with respect to x once and two times, we get

$$\frac{d\psi}{dx} = iKAe^{i(kx-\omega t)}$$

Again differentiating, we get

$$\frac{d^2\psi}{dx^2} = i^2k^2Ae^{i(kx-\omega t)}$$

$$\frac{d^2\psi}{dx^2} = i^2k^2\psi$$. ,Here $i=\sqrt{-1}$, Also $k=\frac{2\pi}{\lambda}$, k= wave number

But $i^2=-1$

$$\therefore \frac{d^2\psi}{dx^2} = -\frac{4\pi^2}{\lambda^2}\psi \qquad \text{……………………………..(2)}$$

DeBroglie wavelength associated with the particle is

$$\lambda = \frac{h}{p} = \frac{h}{mv}, \; p = momentum$$

$$\frac{1}{\lambda} = \frac{mv}{h}$$

$$\frac{1}{\lambda^2} = \frac{m^2v^2}{h^2} = \frac{2m(\frac{1}{2}mv^2)}{h^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(3)$$

Let E be the total energy of the particle and V be the potential energy of the particle and T be the kinetic energy.
Then total energy ,E=T+V

$$\text{T, KE} = \frac{1}{2}mv^2 = \text{E} - \text{V} \quad \ldots\ldots\ldots\ldots\ldots\ldots(4)$$

Substituting the above value of K.E. in Equation (3), we get

$$\frac{1}{\lambda^2} = \frac{2m(E-V)}{h^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(5)$$

From equations (5) and (2), we get

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

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

$$\frac{d^2\psi}{dx^2} + \frac{2m}{(\frac{h^2}{4\pi^2})}(E-V)\psi = 0$$

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

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad (\because \hbar = (\frac{h}{2\pi})) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(6)$$

This is the Schrödinger’s time independent one dimensional wave equation.

Schrödinger Wave Equation Derivation (Time-Dependent)

Considering a complex plane wave for particle

$\psi(x,t) = Ae^{i(kx-\omega t)}$ --------------(1)

Here ψ is a function of x and t only.
A= amplitude.
k= Wave vector.
x= position.
ω=Angular frequency.
t=time.

Now the Total energy of a system is

E=T+ V, [(K.E)+(P.E)]

Where ‘V’ is the potential energy and ‘T’ is the kinetic energy.

T= $\frac{1}{2}mv^2$= $\frac{p^2}{2m}$

And V= A function of x only. (v= mgx or v= mgh)
As we already know that E is the total energy, we can rewrite the equation as:

$$E = \frac{p^2}{2m} + V(x)$$

Differentiating equation (1) with repect to t ,we get

$$\frac{d\psi}{dt} = -i\omega Ae^{i(kx-\omega t)} = -i\omega\psi(x,t)$$

$$\frac{d\psi}{dt} = -i(2\pi\upsilon)\psi(x,t)$$

$$\frac{d\psi}{dt} = -i(2\pi\upsilon)\psi, \psi isafunctionofx, t$$

But according to MaxPlanck, E=hυ , $\Rightarrow \upsilon = \frac{E}{h}$

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$$\frac{d\psi}{dt} = -i(\frac{2\pi E}{h})\psi$$

$$\frac{d\psi}{dt} = -i(\frac{E}{\frac{h}{2\pi}})\psi$$

$$\frac{d\psi}{dt} = -\frac{iE}{\hbar}\psi$$

$$E\psi = -\frac{\hbar}{i}\frac{d\psi}{dt} ---------(2)$$

Also the time independent wave equation is given by

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

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}V\psi = -\frac{2m}{\hbar^2}E\psi -----(3)$$

From equations (2) and(3) we get

$$\frac{d^2\psi}{dx^2}-\frac{2m}{\hbar^2}V\psi=\frac{2m}{\hbar^2}\frac{\hbar}{i}\frac{d\psi}{dt}---------(4)$$

$$\frac{d^2\psi}{dx^2}-\frac{2m}{\hbar^2}V\psi=\frac{2m}{\hbar i}\frac{d\psi}{dt}---------(5)$$

This is time dependent Shroedingers wave equation.

Schrodinger's Wave equation

Let us consider a particle of mass m, moving with a velocity v along the positive X-direction.

The wave function ψ for a particle moving freely in the positive x-direction has the same form as the wave equation for simple harmonic motion and simple harmonic waves in the positive x-direction.

$$\Psi(x,t)=Ae^{i(kx-\omega t)}. \qquad \text{……………………(1)}$$

Here ψ is a function of x only.

Differentiating equation (1) with respect to x once and two times, we get

$$\frac{d\psi}{dx}=iKAe^{i(kx-\omega t)}$$

Again differentiating, we ge

$$\frac{d^2\psi}{dx^2}=i^2k^2Ae^{i(kx-\omega t)}$$

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Let E be the total energy of the particle and V be the potential energy of the particle and T be the kinetic energy.

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$$\text{T, KE} = \frac{1}{2}mv^2 = E - V \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4)$$

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

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This is the Schrödinger’s time independent one dimensional wave equation.

Schrödinger Wave Equation Derivation (Time-Dependent)

Considering a complex plane wave:

$$\Psi(x,t) = Ae^{i(kx-\omega t)}.$$

Now the Hamiltonian of a system is

$$H = T + V$$

Where ‘V’ is the potential energy and ‘T’ is the kinetic energy. As we already know that ‘H’ is the total energy, we can rewrite the equation as:

$$E = \frac{p^2}{2m} + V(x).$$

Now taking the derivatives,

$$\frac{\partial \Psi}{\partial t} = -i\omega A e^{i(kx-\omega t)} = -i\omega \Psi(x,t)$$
$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 A e^{i(kx-\omega t)} = -k^2 \Psi(x,t)$$

We know that,

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

where ‘λ’ is the wavelength and ‘k’ is the wave number.

We have

$$k = \frac{p}{\hbar}.$$

Therefore,

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\Psi(x,t).$$

Now multiplying Ψ (x, t) to the Hamiltonian we get,

$$E\Psi(x,t) = \frac{p^2}{2m}\Psi(x,t) + V(x)\Psi(x,t).$$

The above expression can be written as:

$$E\Psi(x,t) = \frac{-\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi(x,t).$$

We already know that the energy wave of a matter wave is written as

$$E = \hbar\omega,$$

So we can say that

$$E\Psi(x,t) = \frac{\hbar\omega}{-i\omega}\,\Psi(x,t).$$

Now combining the right parts, we can get the Schrodinger Wave Equation.

$$i\hbar\,\frac{\partial\Psi}{\partial t} = \frac{-\hbar^2}{2m}\,\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi(x,t).$$

This is the derivation of Schrödinger Wave Equation (time-dependent).

FREE ELECTRON THEORY & BAND THEORY OF SOLIDS

FREE ELECTRON THEORY

Introduction:

In solids, electrons in outer most orbits of atoms determine its electrical properties. Electron theory is applicable to all solids, both metals and non metals. In addition, it explains the electrical, thermal and magnetic properties of solids. The structure and properties of solids are explained employing their electronic structure by the electron theory of solids. It has been developed in three main stages.

1. Classical free electron theory.
2. Quantum Free Electron Theory.
3. Zone Theory.

1. **Classical free electron theory:** The first theory was developed by Drude and Lorentz in 1900. According to this theory, metal contains free electrons which are responsible for the electrical conductivity. Also electrons obey the laws of classical mechanics.

2. **Quantum Free Electron Theory**: In 1928 Sommerfeld developed the quantum free electron theory. According to Sommerfeld, the free electrons move with a constant potential. This theory obeys quantum laws.

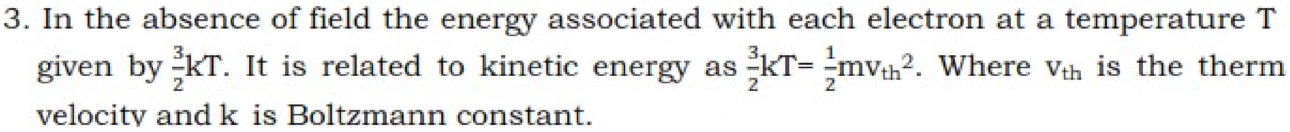
3. **Zone Theory:** Bloch introduced the band theory in 1928. According to this theory, free electrons move in a periodic potential provided by the lattice. This theory is also called “Band Theory of Solids”. It gives complete information regarding electrons.

Classical free electron theory of metals (Drude – Lorentz theory of metals):

Drude and Lorentz proposed this theory in 1900. According to this theory, the metals containing the free electrons obey the laws of classical mechanics.

Assumptions (or) Salient features in classical free electron theory

1. In metals there are a large number of free electrons moving freely in all possibledirections.
2. These free electrons behave like gas molecules in a container obeying the laws of kinetic theory of gases.

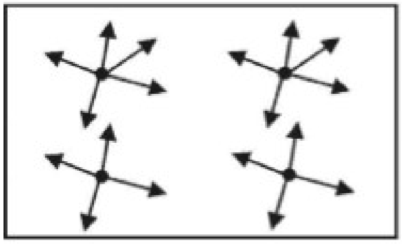


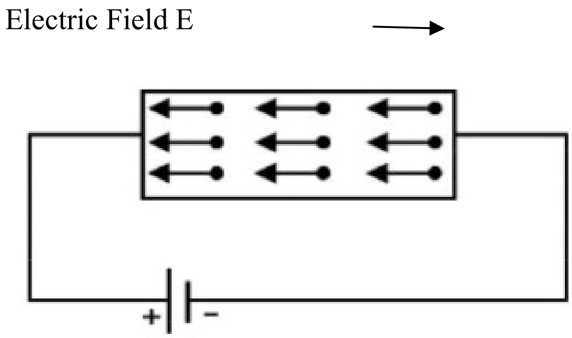
3. In the absence of field the energy associated with each electron at a temperature T given by $\frac{3}{2}kT$. It is related to kinetic energy as $\frac{3}{2}kT= \frac{1}{2}mv_{th}^2$. Where v_{th} is the therm velocity and k is Boltzmann constant.

4. In metals, the positive ion cores are at fixed positions and the free electrons move randomly and collide either with positive ion cores or with other free electrons or with boundaries. Hence these collisions are elastic. Therefore the electric conduction is dueto free electrons only.

5. Electron velocities in a metal obey Maxwell-Boltzmann distribution of velocities.

6. The free electrons move in a constant potential field. Hence the potential energy of the electrons is constant.





7. When an electric field is applied to a metal, free electrons are accelerated in the direction opposite to the direction of applied electric field with a velocity called drift velocity represented as V_d.

Advantages or Merits classical free electron theory

1) It verifies ohm's law.
2) It explains electrical and thermal conductivities of metals.
3) It derives Widemann-Franz law.
4) It explains optical properties of metals.

Drawbacks or Demerits classical free electron theory

1) Failed to explain the electrical conductivity of semiconductors and insulators.
2) Failed to explain the temperature variation of electrical conductivity at low temperatures.
3) Failed to explain the concept of specific heat of metals.
4) Failed to explain the mean free path of the electrons.
5) The phenomenon like photo electric effect, Compton effect and black body radiationcould not be explained by classical free electron theory.
6) Failed to explain temperature dependence of paramagnetic susceptibility and ferromagnetism.

Quantum Free Electron Theory:

Quantum free electron theory was proposed by Sommerfeld in 1928. It overcomes many of the drawbacks of classical theory. Sommerfeld explained them by choosing Fermi- Dirac statistics instead of Maxwell-Boltzmann statistics. He developed this theory by applying the principles of quantum mechanics.

Assumptions of Quantum Free Electron Theory

1) Valence electrons move freely in a constant potential within the boundaries

of metal and is prevented from escaping the metal at the boundaries (high potential). Hence the electron is trapped in a potential well.

2) The distribution of electrons in various allowed energy levels occurs as per Pauli Exclusion Principle.

3) The attraction between the free electrons and lattice ions and the repulsion betweenelectrons themselves are ignored.

4) The distribution of energy among the free electrons is according to Fermi-Dirac statistics.

5) The energy values of free electrons are quantized.

6.)To find the possible energy values of electron Schrodinger time independent wave equation is applied. The problem is similar to that of particle present in a potential box.

Energy of the electron is given by $E_n = \dfrac{n^2h^2}{8mL^2}$

Merits of quantum free electron theory

1. Successfully explained the electrical and thermal conductivities of metals.
2. Explained the phenomenon of Thermionic emission.
3. It explains temperature dependence of conductivity of metals.
4. It can explain the specific heat of metals.
5. Explained magnetic susceptibility of metals.
6. Explained photo electric effect, Compton Effect and black body radiation etc.
7. It gives the correct mathematical expression for the thermal conductivity and electrical conductivity of metals.

Demerits of quantum free electron theory

1. It is unable to explain the metallic properties exhibited by only certain crystals.
2. It is unable to explain why the atomic arrays in metallic crystals should prefer certainstructures only.
3. This theory fails to distinguish between metals, semiconductors and Insulators.
4. It also fails to explain the positive value of Hall Co-efficient.
5. According to this theory, only two electrons are present in the Fermi level and theyare responsible for conduction which is not true.

Fermi-Dirac Distribution:

According to free electron theory, Electrons in a solid move in all possible directions like gas molecules in a container. These free electrons contribute for electrical conduction.

The free electron model of a metal has survived to the actual situation in metals, particularly the mono valent atoms such as Alkali metals.

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E_F is the energy of the Fermi level.

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$$P_e(E) = f(E) = \frac{1}{1 + \exp\left(\frac{E - Ef}{K_B T}\right)}$$

7. The distribution function is valid only in equilibrium.
8. The Fermi level is absolutely valid in equilibrium only.
9. Fermi-Dirac distribution function is valid for all the particles obeying Pauli's exclusion principle. This is equally applicable regardless of the type of the solid, doping of the semiconductor, etc.

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   The Fermi-Dirac distribution function considers statistically the entire collection of fermions in the volume.

   Thus it considers all electrons in the semi conducting solid and not merely electrons in a Band.
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    The hole distribution function is denoted as

$$P_h(E) = 1 - P_{FD}(E)$$

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6. AT $E = E_f$,

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8. At 0^0K, Pe (E) =1 for E < E_f

   And Pe (E) = 0 for E > E_f

   This implies that at 0^0 K all states up to the Fermi level are completely occupied by the electrons. All the states above the Fermi level are empty.
9. The distribution function is a strong function of temperature only at energies close to E_f.

Plots of P_e (E) and E at different temperatures are shown in figure (6).

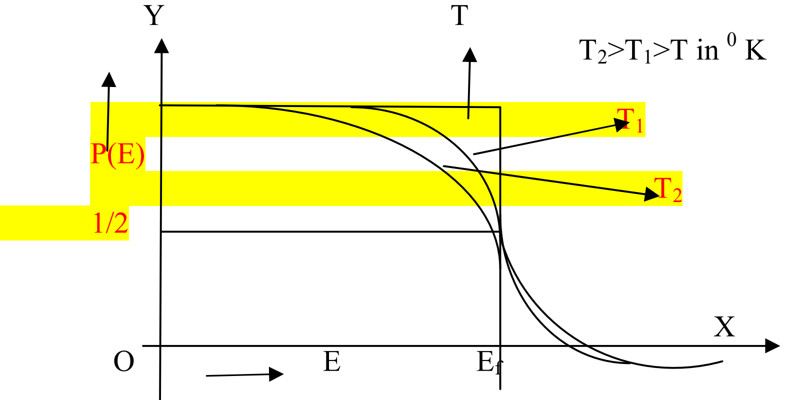

Fig (6). P_e (E) versus E for various T values. At all temperatures, the curves passes through the point $\left[E_f, \frac{1}{2}\right]$.

<u>Note on Fermi-Dirac Distribution function</u>: The Fermi-Dirac distribution for Electrons is given by

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Now at the Absolute zero (T = 0^0 K), there are two situations

(ii) For E < E_F ,

$$P_e(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{K_B T}\right)}$$

$$P_e(E) = \frac{1}{1 + e^{[-\frac{X}{K_B(0)}]}}$$

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

$$P_e(E) = \frac{1}{1 + \frac{1}{e^{\infty}}} \qquad \text{But } e^{\infty} = \infty \Rightarrow \frac{1}{\infty} = 0$$

P_e (E) = 1, for E < E_F at T = 0^0

(ii) For E > E_F

$$P_e(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{K_B T}\right)}$$

$$P_e(E) = \frac{1}{1 + \exp\left(\frac{+X}{K_B(o)}\right)}$$

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

$$P_e(E) = \frac{1}{1 + \infty}$$

$$P_e(E) = \frac{1}{\infty}$$

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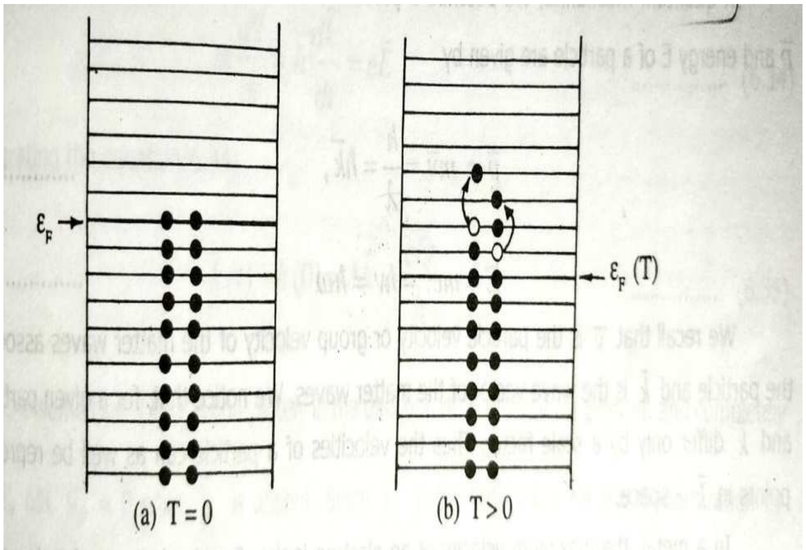
P_e (E) = 0, for E > E_F at T = 0^0

This means that no electrons have energy greater than E_F at 0^0 K.
i.e the Fermi energy E_F is the maximum energy that a free electron in the metal can have at absolute zero.



(a) T = 0 (b) T > 0

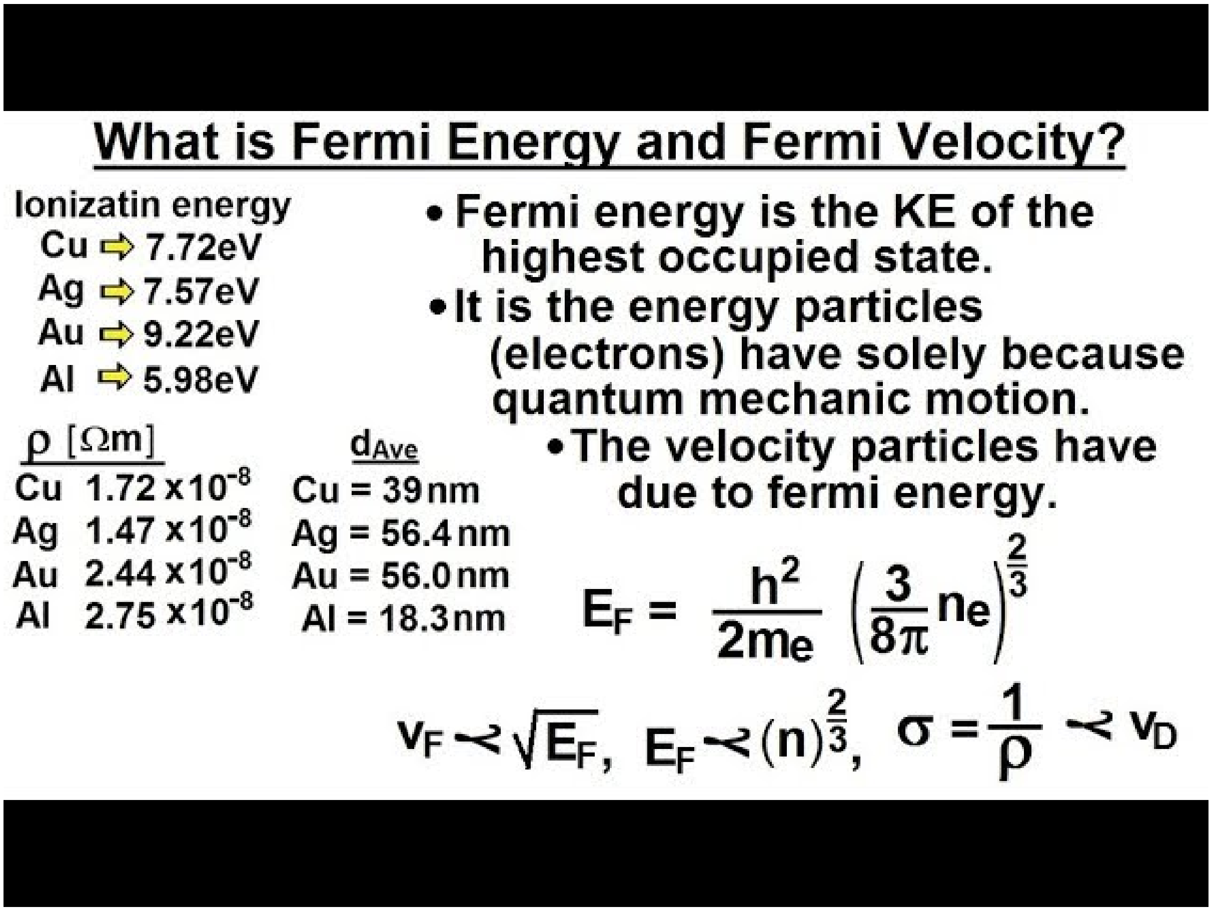
: The effect of temperature on the occupation of energy levels of electrons in a crystal.

Fermi Energy Level (E_f):

Fermi Energy level is the top most occupied energy level.
The level above which all the energy levels are empty and below which all the energy levels are occupied.

Fermi Energy:

The Fermi energy is only defined at absolute zero, while the Fermi level is defined for any temperature.
Fermi Energy is the energy of highest occupied level. That is kinetic energy of highest occupied state.



What is Fermi Energy and Fermi Velocity?

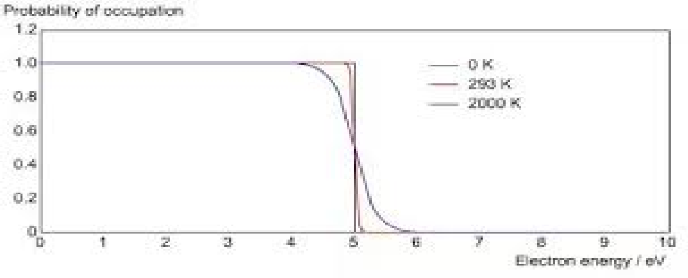
Ionizatin energy
Cu ⇨ 7.72eV
Ag ⇨ 7.57eV
Au ⇨ 9.22eV
Al ⇨ 5.98eV

	ρ [Ωm]	d_{Ave}
Cu	1.72×10^{-8}	Cu = 39nm
Ag	1.47×10^{-8}	Ag = 56.4nm
Au	2.44×10^{-8}	Au = 56.0nm
Al	2.75×10^{-8}	Al = 18.3nm

- Fermi energy is the KE of the highest occupied state.
- It is the energy particles (electrons) have solely because quantum mechanic motion.
- The velocity particles have due to fermi energy.

$$E_F = \frac{h^2}{2m_e}\left(\frac{3}{8\pi}n_e\right)^{\frac{2}{3}}$$

$$v_F \propto \sqrt{E_F},\ \ E_F \propto (n)^{\frac{2}{3}},\ \ \sigma = \frac{1}{\rho} \propto v_D$$



Fermi-Dirac distribution for several temperatures

Prepared By

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Expression for electrical Conductivity:

Let us suppose, we have an electron of mass 'm'. when an electric field is applied, the force on the electron is givenby

$$F = -eE \quad \text{———} \quad ①$$

where e = charge on electron
E = Intensity of the electric field.

Also force F is given by rate of change of momentum.

$$\therefore \quad F = \frac{dP}{dt} \quad \text{———} \quad ②$$

From equations ① and ②, we get

$$-eE = \frac{dP}{dt} \quad \text{———} \quad ③$$

where P = momentum of electron.

Now according to debroglie hypothesis, we have

$$\lambda = \frac{h}{P}$$, λ = debroglie wavelength
h = planck's constant.

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

$$P = \left(\frac{h}{2\pi}\right)\left(\frac{2\pi}{\lambda}\right)$$

$$\text{Now} \quad P = \hbar K \quad \text{———} \quad ④$$

where $\hbar = \frac{h}{2\pi}$ and $K = \frac{2\pi}{\lambda}$

K = Wave Vector.

Now differentiating equation ④, with respect to t, we get.

$$\frac{dp}{dt} = \hbar \frac{dk}{dt} \quad \text{———} \quad ⑤$$

From Equations ③, and ⑤. we get

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

$$\Rightarrow dk = -eE \frac{dt}{\hbar}$$

$$\Rightarrow dk = \frac{-eE}{\hbar} dt \text{ ———— } ⑥$$

That is the origin of k space moves through a distance dk in a time dt

Now the displacement in the average collision time τ is given by

$$\Delta K = -\frac{eE\tau}{\hbar} \text{ ———— } ⑦$$

Also Momentum $P = mv = \hbar k$

$$\Rightarrow m\Delta v = \hbar \Delta k$$

$$\Rightarrow \Delta K = \frac{m\Delta v}{\hbar} \text{ ———— } ⑧$$

From Equations ⑦ and ⑧, we get

$$m\frac{\Delta v}{\hbar} = -\frac{eE\tau}{\hbar}$$

$$\Delta v = -\frac{eE\tau}{m} \text{ ———— } ⑨$$

Now Also expression for Current density is given by $J = -ne\delta v$ ———— ⑩

From equations ⑨ and ⑩, current density J is given by $J = -ne\left(-\frac{eE\tau}{m}\right)$

$$\therefore \; J = \frac{ne^2 E \tau}{m} \quad \text{———} \quad ⑪$$

where: n = Electron concentration.

Also we know that $J = \sigma E$ —— ⑫

Comparing the equations ⑪ and ⑫, we get

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

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

Density of States:

The number of electrons present per unit volume in an energy level at a given temperature is equal to the product of density of states and Fermi Dirac distribution function.

Density of States is the number of energy levels per unit volume.

To calculate the number of electrons in an energy level per unit volume at a given temperature, it is important to know the number of energy states per unit volume.

The number of energy states with a particular energy value E is depending on how many combinations of the quantum numbers resulting in the same value. Usually the energy levels appear continuum inside the space of Atom.

Let n_x, n_y and n_z are the coordinates representing an energy level.

Let us consider a spherical system of radius n. This 'n' represents a vector to a point n_x, n_y and n_z in the three dimensional space.

i.e $n = n_x^2 + n_y^2 + n_z^2$

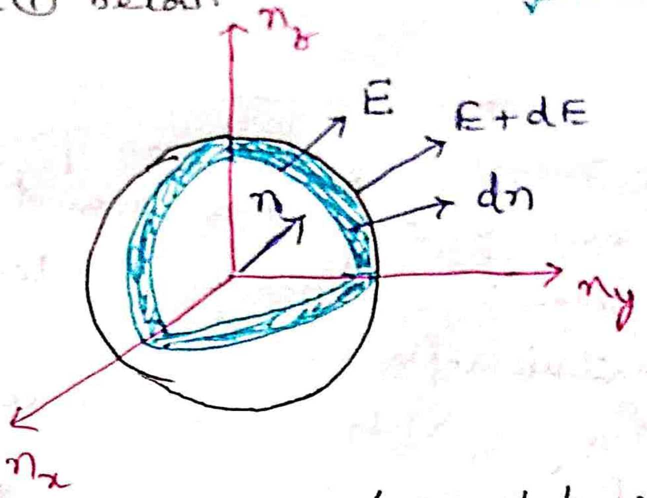
In this space every integer specifies an energy level. i.e Each unit cube contains exactly one state. Hence the number of energy states in any volume is in units of cubes of lattice parameters.

Consider a sphere of radius n and another sphere of radius $(n+dn)$ in which energy values are E and $E+dE$ respectively.

This is shown in figure ① below.

The number of energy states available in the sphere of radius 'n' is given by

$$\frac{1}{8}\left(\frac{4}{3}\pi n^3\right) \text{ —— } ①$$



Figure① Density of states in "dn" region..

Also the number of energy states in the sphere of radius (n+dn) is given by

$$\frac{1}{8}\left[\frac{4}{3}\pi (n+dn)^3\right] \text{ —— } ②$$

E and dE are the energy values of two regions with radius n and (n+dn)

From equations ① and ②, the number of energy states available in dn or dE region is given by

$$g'(E)\,dE = \frac{1}{8}\left[\frac{4}{3}\pi (n+dn)^3\right] - \frac{1}{8}\left[\frac{4}{3}\pi n^3\right]$$

$$g'(E)\,dE = \left[\frac{\pi}{6}(n+dn)^3\right] - \frac{\pi}{6}n^3$$

$$g'(E)\,dE = \frac{\pi}{6}\left[(n+dn)^3 - n^3\right]$$

$$g'(E)\,dE = \frac{\pi}{6}\left(n^3 + (dn)^3 + 3n^2(dn) + 3n(dn)^2 - n^3\right]$$

Neglecting higher order terms,

$$g'(E)\,dE = \frac{\pi}{6}\left[3n^2\,dn\right]$$

$$g'(E)\,dE = \frac{\pi}{2}\left[n(n\,dn)\right] \text{ —— } ③$$

The expression for nth energy level can be written as

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

$$\Rightarrow n^2 = \frac{8ma^2}{h^2}E \quad \text{———} \ ④$$

$$\Rightarrow n = \left[\frac{8ma^2}{h^2}E\right]^{1/2} \quad \text{———} \ ⑤$$

Now differentiating equation ④, taking n and E as variables, we get

$$2n\,dn = \frac{8ma^2}{h^2}dE$$

$$\Rightarrow n\,dn = \frac{1}{2}\left(\frac{8ma^2}{h^2}\right)dE \quad \text{———} \ ⑥$$

From equations ③, ⑤ and ⑥, substituting the values of 'n' and 'ndn' in Equation ③, we get

$$g'(E)\,dE = \frac{\pi}{2}\left(\frac{8ma^2}{h^2}\right)^{1/2}E^{1/2} \cdot \frac{1}{2}\left(\frac{8ma^2}{h^2}\right)dE$$

$$g'(E)\,dE = \frac{\pi}{4}\left(\frac{8ma^2}{h^2}\right)^{3/2}E^{1/2}\,dE \quad \text{———} \ ⑦$$

According to paulis exclusion principle each energy level contains two electrons. That means each energy level will have two sub energy levels.

∴ Equation ⑦ should be multiplied with '2'.

$$\therefore g'(E)\,dE = 2\times\frac{\pi}{4}\left(\frac{8ma^2}{h^2}\right)^{3/2}E^{1/2}\,dE$$

$$\Rightarrow g'(E)\,dE = \frac{\pi}{2}\left(\frac{8ma^2}{h^2}\right)^{3/2}E^{1/2}\,dE$$

$$\Rightarrow g'(E)\,dE = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{3/2}a^3\,E^{1/2}\,dE \quad \text{———} \ ⑧$$

Now Density of states is given by

$$g(E)\,dE = \frac{g'(E)}{V}dE \quad \text{———} \ ⑨$$

If length of energy level is 'a' then its Volume $V = a^3$

Hence ⑨ $\Rightarrow g(E)\,dE = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{3/2} \frac{a^3}{a^3} E^{1/2}\,dE$

$$\Rightarrow g(E)\,dE = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{3/2} E^{1/2}\,dE \quad \text{———} ⑩$$

Equation ⑩ gives the expression for density of states.

Bloch theorem:

When ever an electron moves in a periodic potential, it can be represented as shown in figure ①.

Here the potential is periodic, with a period 'a'. This is like an electron moving in a one dimensional periodic lattice.

Since the electron is moving in a periodic potential, having period 'a',

potential $V(x) = V(x+a)$

where x = distance of the electron from the Core.

Bloch's theorem states that, for a particle moving in a periodic potential, the eigen functions for a conduction electron are of the form

$$\psi(x) = U(x) \cos kx$$

Where $U(x) = U(x+a)$

The eigen functions are the plane waves modulated by the function $U(x)$

the function $U(x)$ has the same periodicity as the potential energy of the electron..

This $U(x)$ is called modulati- function.

For Solving the problem, we have to solve Schroedinger's equation. Hence it is difficult to solve the problem.

Kronig- penney adopted a model for simplification.

The Kronig-penney Model

The motion of an electron in a Crystal is described by the motion of an electron in a periodic potential. The periodic potential will have a periodicity equal to that of the lattice constant of the crystal.

According to Bloch, the periodic potential will be having the form as shown in figure ①

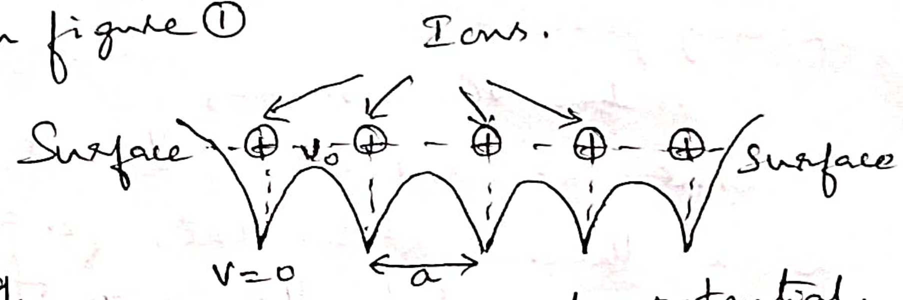


Figure ① A periodic potential.

This is a one dimensional crystal of lattice constant 'a'.

The potential energy of the electron V(x) is periodic with period 'a' as shown in figure①. The periodic potential arises from the periodic distribution of the positive charge associated with the ion cores situated on the lattice sites.

The periodic potential also arises due to constant distribution of other free electrons in the crystal.

When the electron approaches +ve ion, the potential of the electron is zero.

When the electron is inbetween the two +ve ions, then its potential is V_0.

Since the potential is periodic with period equal to the lattice constant 'a', we have $V(x) = V(x+a)$

When ever the electron moves in a potential of such type, its potential energy varies.

To study the behaviour of electron in such a varying potential fields, Kronig-penney modified the periodic potential to a rectangular square well potential wells. They are also periodic as shown in figure ②

This is the for the motion of an electron, in a one dimensional perfect crystal.

Here period of the periodic potential $= (a+b)$

Width of the potential $= W = b$; Height of the potential $= V_0$.

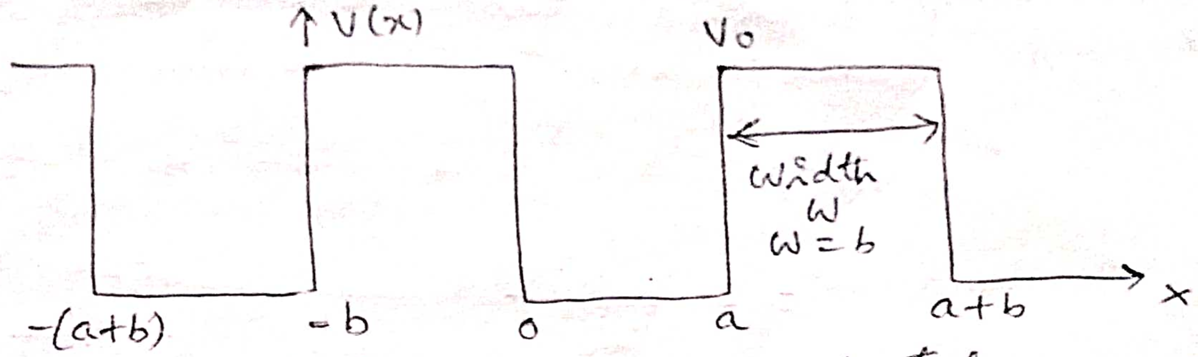


Figure ② A periodic Square well potential.

$V_0 b$ is called the Barrier strength. As V_0 increases the width of potential barrier 'W' decreases. However $V_0 b$ remains constant.

The region $0<x<a$, is like a potential well. In this region $0<x<a$, the potential energy $V=0$. In the regions such as $-b<x<0$, the potential energy is V_0. Each of the potential energy walls may be considered as a rough approximation for the potential in the vicinity of the Atom. This is an artificial model. This is the model for which the Schrodinger equation can be solved in terms of elementary functions.

The Schrodinger wave equation for one dimensional periodic potential field denoted by $V(x)$ is given by

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0. \quad \text{———} \quad ①$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{8\pi^2 m}{h^2}\left[E - V(x)\right]\psi(x) = 0$$

The Schrodinger equation for the two regions can be written as

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} E\,\psi(x) = 0 \quad \text{for } 0<x<a \quad \text{———} \quad ②$$

Here $V(x) = 0$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left[E - V_0\right]\psi(x) = 0 \quad \text{for } -b<x<0 \quad \text{———} \quad ③$$

Here $V(x) = V_0$.

Now we will consider that the energy E of the electrons under consideration is smaller than V_0.

Now let $\alpha^2 = \frac{2mE}{\hbar^2}$ ———— ④

and $\beta^2 = \frac{2m(V_0 - E)}{\hbar^2}$ ———— ⑤

Now substituting these values of α^2 and β^2 from ④ and ⑤ in ② and ③, we get

$$\frac{d^2\psi(x)}{dx^2} + \alpha^2\psi(x) = 0 \quad \text{———— ⑥}$$

$$\frac{d^2\psi(x)}{dx^2} - \beta^2\psi(x) = 0 \quad \text{———— ⑦}$$

$\psi(x)$ is the wave function.

The wave function for the electron is given by

$$\psi(x) = e^{\pm ikx} u_K(x) \quad \text{———— ⑧}$$

Here $u_K(x)$ is the periodic function in x with periodicity of $(a+b)$.

By solving the equations ⑥ and ⑦ and applying the condition that the wave function $\psi(x)$ and its derivative $\frac{d\psi(x)}{dx}$ and hence $u_K(x)$ and $\frac{du_K(x)}{dx}$ must be continuous, we get

$$\frac{P\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ka \quad \text{———— ⑨}$$

This is the condition that has to be satisfied for the solutions to Schrodinger wave equation to exist.

Here $P = \frac{mV_0ba}{\hbar^2}$

P gives a measure of the area V_0b of the potential Barrier.

The increasing P has the physical meaning of binding an electron more strongly to a particular potential well.

Now a plot of αa on x-axis and $P\frac{\sin \alpha a}{\alpha a} + \cos \alpha a$ on y-axis is shown in figure ③, for a P value $\frac{3\pi}{2}$.

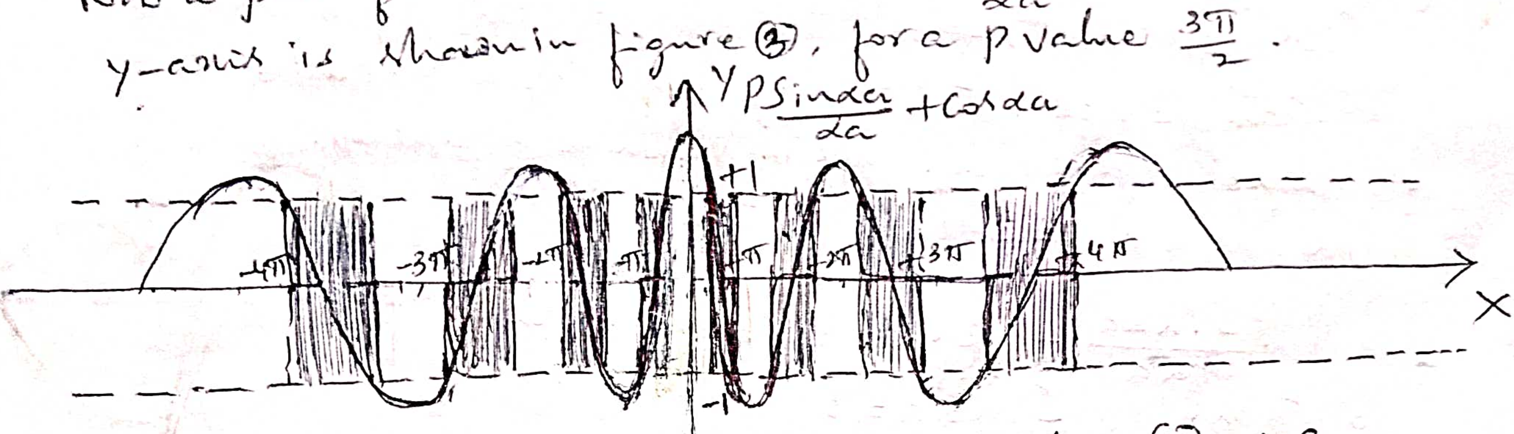


Fig ③ plot of left hand side of equation ⑨ as a function of αa using $P = \frac{3\pi}{2}$.

The right hand side of equation ⑨ is a cosine term. Since $\cos ka$ lies between +1 and −1, the left hand side can vary only between these limits.

ie The LHS assumes only those values of αa for which its value lies between +1 and −1

Such values of αa, therefore represent wave like solutions of the type $\psi(x) = e^{\pm ikx} u_k(x)$

These type of solutions are allowed. The other values of αa are not allowed.

The vertical axis lying between −1 and +1, as indicated by the horizontal lines, represents the values acceptable to the left hand side.

Also α^2 is proportional to the energy E, therefore the abscissa is a measure of the energy.

The following conclusions may be drawn from figure ③.

1. The diagram is known as Energy Spectrum.
2. The energy spectrum of the electrons consists of alternate regions of allowed energy bands (shaded area) and forbidden energy bands (unshaded area)
3. The width of the allowed energy bands increases with αa or the energy.

4. The width of particular allowed energy bands decreases with increase in the value of P.

Case(ii): As $P \to \infty$, the allowed energy bands are compressed into energy levels and results in a line spectrum. This is shown in figure (2).

In such a case the equation

$$\frac{P\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ka,$$

will have solutions if $\sin\alpha a = 0$

or $\alpha a = \pm n\pi$

where n is an integer, $n = 1, 2, 3, \ldots$

But $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$

$$\therefore \alpha^2 = \frac{2mE}{\hbar^2}$$

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

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

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

$$\Rightarrow E = \frac{n^2\pi^2\left(\frac{h}{2\pi}\right)^2}{2ma^2}$$

$$\Rightarrow E = \frac{n^2h^2}{8ma^2} \qquad \text{———} \qquad ⑩$$

This expression gives the energy levels of a particle in a constant potential box of atomic dimensions.

For larger values of P, the tunneling through the barrier becomes difficult.

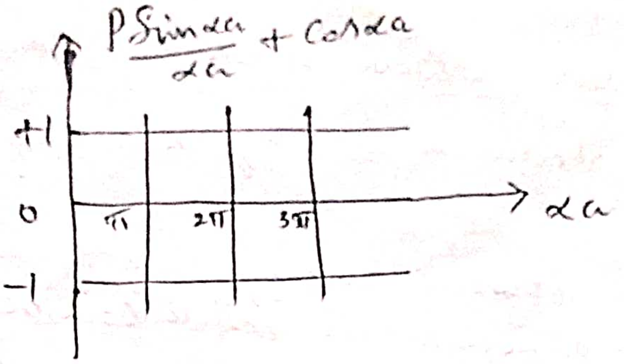


figure ④ line Spectrum.

If P is large, the function described by the right hand side of the equation crosses +1 and -1 region at a steeper angle. Thus the allowed bands become narrower.

Case(ii) when $P \to 0$, from equation (9),

i.e $\frac{P\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ka$

$\Rightarrow \cos\alpha a = \cos ka$

$\Rightarrow \alpha a = ka$

$\Rightarrow \alpha = k$

Now $\alpha^2 = k^2$

$\therefore \frac{2mE}{\hbar^2} = k^2$

$\Rightarrow E = \frac{\hbar^2 k^2}{2m}$ ——— ⑪

This is applicable to completely for free electrons, for which all the energies are allowed.

when $P \to 0$, then the left side of equation ⑨ will not cross ±1 lines. This is shown in figure ⑤.

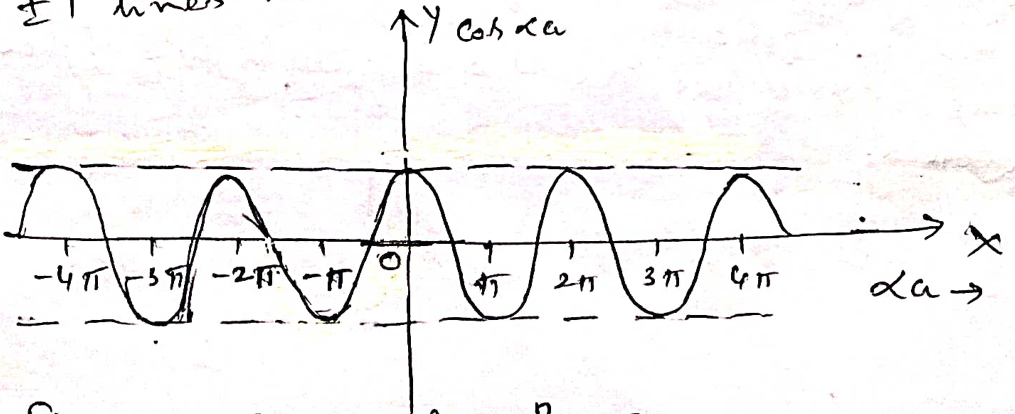


Figure (5) Graph when $P \to 0$.

Energy versus wave vector (E-K diagram)

The free electrons moving in a crystal will have allowed energies.

The relation between energy and wave vector for an electron in a one-dimensional lattice can be studied by using equation

$$\frac{P\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ka \quad \text{———} \quad ①$$

The righthand side of equation ① becomes ±1 for values of

$$K = \pm \frac{n\pi}{a}$$

These values actually define the boundaries of the allowed regions. It is possible to plot the total energy of free electrons versus the wave vector K as shown in figure ⑥. The We obreeve that the curve is not continuous. The discontinuities in E-K curve occur at $K = \pm \frac{n\pi}{a}$.

Here $n = 1, 2, 3, ---$

The dotted parabolic curve, indicates E-K relation for completely free electrons.

$$\text{ie } E = \frac{\hbar^2 K^2}{2m}$$

It is noted from the graph that, the allowed energy values extending from $K = -\frac{\pi}{a}$ to $+\frac{\pi}{a}$, is called first allowed region OR first Brillonin zone.

After a break in the energy values, called the forbidden energy band, we have second allowed region spreading from $K = -\frac{\pi}{a}$ to $-\frac{2\pi}{a}$ and $K = +\frac{\pi}{a}$ to $+\frac{2\pi}{a}$.

This is called second allowed region or second allowed zone or second Brillonin zone.

In the same manner we can also define higher order Brillonin zones.

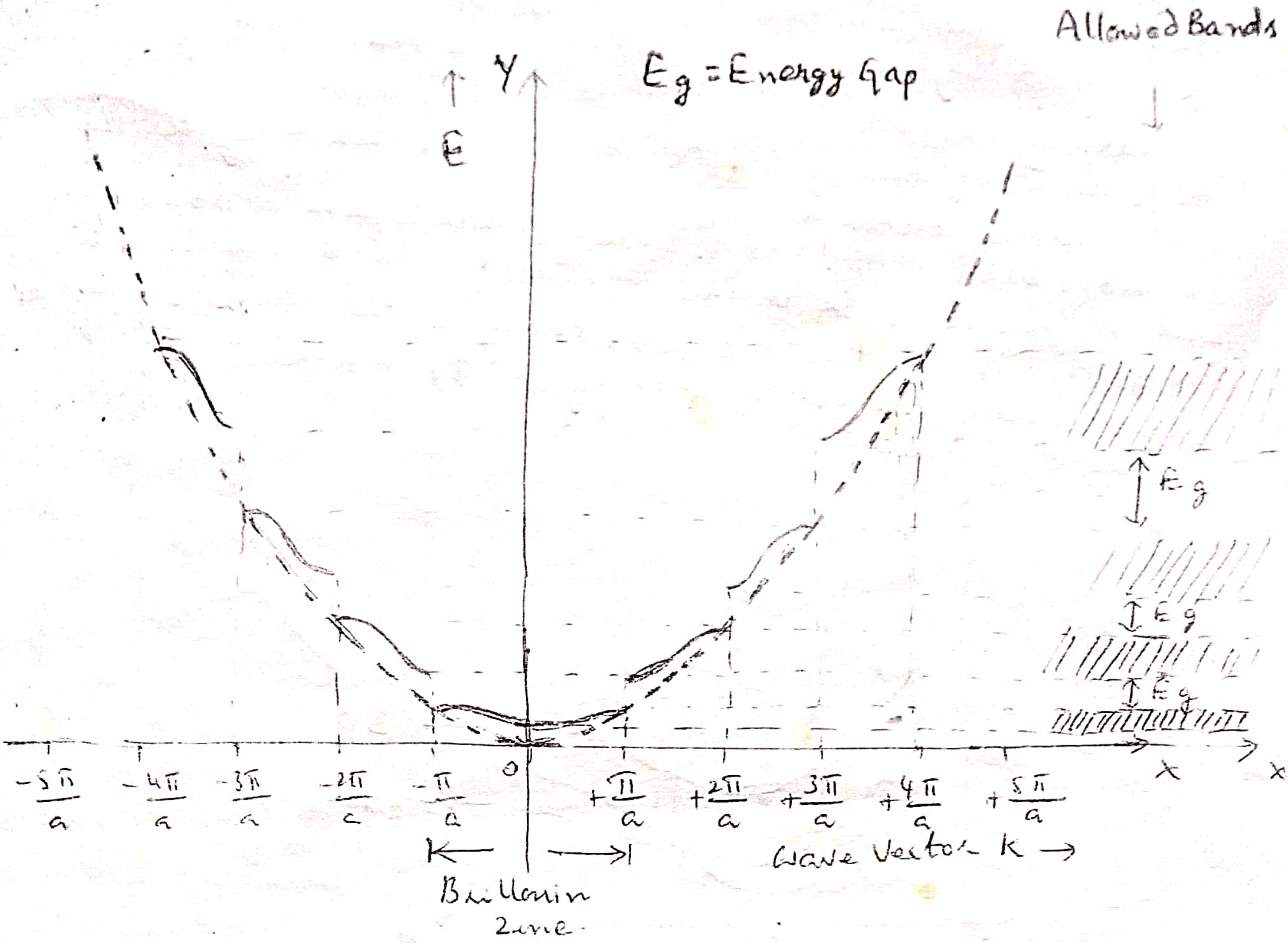


Fig ⑤ The relation between energy and wave vector for a one-dimensional lattice

Origin of Energy Bands Formation in Solids:

An isolated atom posses discrete energies for different electrons. When two isolated atoms are brought to close proximity, then the electrons in the orbits of two atoms interact. Now in the combined system the energies of electrons will not be same, but they slightly differ from the original value. So at the place of each energy level, a closely spaced two energy levels will exist.

If 'N' number of atoms are brought together to form a solid and if the electrons present in these atoms interact. Here they will give 'N' number of closely spaced energy levels in the place of discrete energy levels. These closely spaced energy levels are called allowed energy bands.

In between the allowed energy bands, there are empty regions called forbidden energy bands. Kronig-penney model supports the existence of these energy bands.

The formation of energy bands has been explained by taking Sodium as an example. when isolated atoms are brought together to form a Solid then the energy levels of the Valence electrons spread into Bands. The 3S and 3P orbitals electrons energies are shown in figure ⑦. These bands will overlap strongly at the interatomic spacing of Sodium.

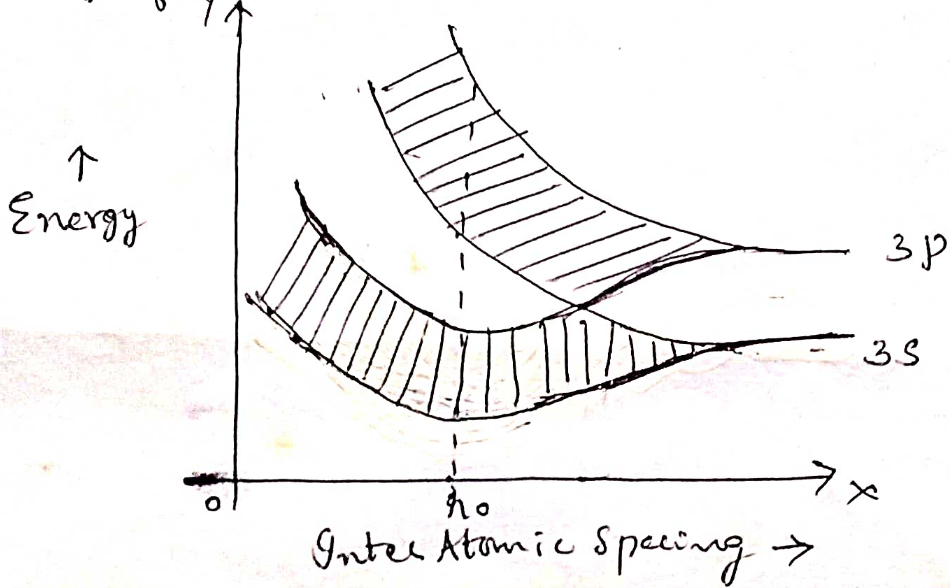


Figure ⑦ Spreading of energy levels into energy bands in Sodium Metal.

In the case of metals, the 3S and 3P Bands overlap at r_0.

Velocity of an Electron

Usually the Velocity of an electron is described by a wave Vector 'K'. According to wave mechanical theory of particles, a particle moving with a Velocity 'v' is equivalent to a wavepacket moving with a group Velocity v_g. ie $v = v_g$. Also group Velocity of the waves representing the particles is given by

$$v_g = \frac{d\omega}{dk}.$$

$$\therefore v = v_g = \frac{d\omega}{dk} \qquad \text{———} \qquad ①$$

Where ω = Angular frequency

$\omega = 2\pi\nu$

K = wave vector , $K = \frac{2\pi}{\lambda}$

usually energy $E = h\nu$

But $\omega = 2\pi\nu$, ν = frequency

$$E = \frac{h.\omega}{2\pi}$$

$$E = \hbar\omega \quad \text{———} \quad ②, \text{ where } \hbar = \frac{h}{2\pi}$$

Differentiating Equation ②, with respect to 'k',

We get

$$\frac{dE}{dk} = \hbar\frac{d\omega}{dk}$$

$$\Rightarrow \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{dE}{dk} \quad \text{———} \quad ③$$

From Equations ① and ③, we get

$$v = \frac{1}{\hbar}\frac{dE}{dk} \quad \text{———} \quad ④$$

Equation ④, gives the expression for velocity of electron.

Note: In quantum theory, the momentum of an electron is given by

$P = \hbar K$ and energy $E = \frac{\hbar^2 k^2}{2m}$ ——— ⑤

Differentiating Equation ⑤ with respect to K,

$$\frac{dE}{dk} = \frac{\hbar^2}{\cancel{2}m}\cancel{2}K$$

$$\frac{dE}{dk} = \frac{\hbar^2 K}{m} \quad \text{———} \quad ⑥$$

Now from equations, ④ and ⑥,

We get

$$v = \frac{1}{\hbar}\frac{\hbar^2 K}{m}$$

$$v = \frac{\hbar K}{m}$$

$$v = \frac{h}{2\pi}\frac{2\pi}{\lambda}\frac{1}{m} \quad (\because \hbar = \frac{h}{2\pi} \ \& \ K = \frac{2\pi}{\lambda})$$

$$v = \frac{h}{\lambda m}$$

Also $\lambda = \frac{h}{P} \Rightarrow P = \frac{h}{P}$

$$\therefore v = \frac{P}{m}$$

$$\Rightarrow P = mv$$

⑤ $\Rightarrow E \propto K^2$ for a free electron.

Effective Mass of an Electron:

The mass of an Electron in the periodic potential of a Crystal is different from the free electron mass.
This mass is known as effective mass.
Let us assume that there is an electron present in state K in a Brillouin zone of one dimensional Crystal.
Now an external field $\mathcal{E}$ is applied on this electron for a time of dt
The electron is now accelerated and gains an amount of energy dE
This gain of energy dE = work done on the electron by the electric field.

Now work done dE = force x displacement

$$\Rightarrow dE = e\mathcal{E} \times dx$$

$$\Rightarrow dE = e\mathcal{E} v\, dt \quad \text{———} \quad ①$$

where dx = displacement in a time of dt.
Also v = Velocity

$$v = \frac{dx}{dt}$$

Also velocity of electron $v = \frac{1}{\hbar}\frac{dE}{dk}$ ——— ②

From Equations ① and ②, we get

$$dE = e\mathcal{E}\left[\frac{1}{\hbar}\frac{dE}{dk}\right] dt$$

$$\Rightarrow \frac{dk}{dt} = \frac{e\mathcal{E}}{\hbar} \quad \text{———} \quad ③$$

Also acceleration attained by the electron is given by

$$a = \frac{dv}{dt}$$

$$\Rightarrow a = \frac{d}{dt}\left[\frac{1}{\hbar}\frac{dE}{dk}\right]$$

$$a = \frac{1}{\hbar}\left(\frac{d^2E}{dk^2}\right)\left(\frac{dk}{dt}\right) \quad \text{———} \quad ④$$

From the equation ③ and ④, we get

$$a = \frac{1}{\hbar}\left(\frac{d^2E}{dk^2}\right)\frac{e\mathcal{E}}{\hbar}$$

$$a = \frac{e\mathcal{E}}{\hbar^2}\left(\frac{d^2E}{dk^2}\right) \quad \text{———} \quad ⑤$$

The acceleration of an electron in free state, having mass 'm' in an electric field is given by

$$a = \frac{e\mathcal{E}}{m} \quad \text{——} \quad ⑥ \quad \left(\because F = ma \Rightarrow a = \frac{F}{m} \Rightarrow a = \frac{e\mathcal{E}}{m}\right)$$

In band theory the mass of electron is represented by m^*

m^* = effective mass

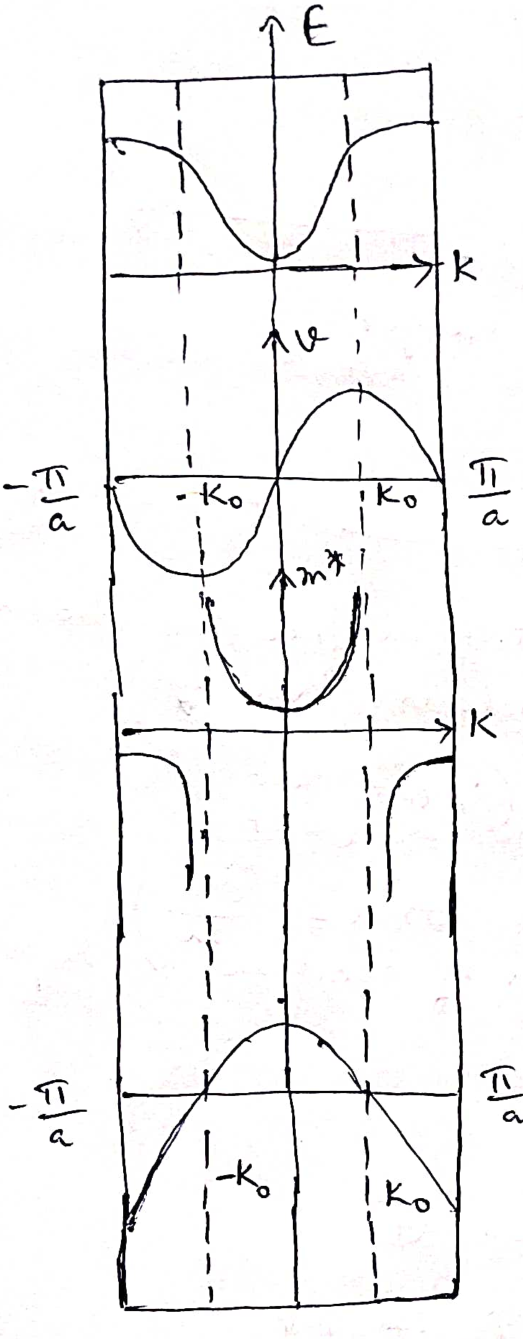
$$\therefore a = \frac{e\mathcal{E}}{m^*} \quad \text{———} \quad ⑦$$

From Equations ⑤ and ⑦, we get

$$\frac{e\mathcal{E}}{m^*} = \frac{e\mathcal{E}}{\hbar^2}\left(\frac{d^2E}{dk^2}\right)$$

$$\Rightarrow m^* = \frac{\hbar^2}{\left(\frac{d^2E}{dk^2}\right)} \quad \text{———} \quad ⑧$$

The variation of effective mass m^* with respect to k is shown in the figure below.



①a E-K Diagram

①b Velocity Versus K diagram

①c Effective mass m^* Versus K.

fig ①d f_k Versus K.

Variation of m^* with k is shown in fig ①c.

In the lower portion of E-K curve, $\frac{d^2E}{dk^2}$ is +ve, so m^* is +ve.

It increases with k and attains a maximum value at the point of inflection k_0.

For further higher values of K, $\frac{d^2E}{dK^2}$ is $-ve$.

Hence m^* is negative.

As $K \to \frac{\pi}{a}$, $m^* \to$ Smaller $-ve$ value

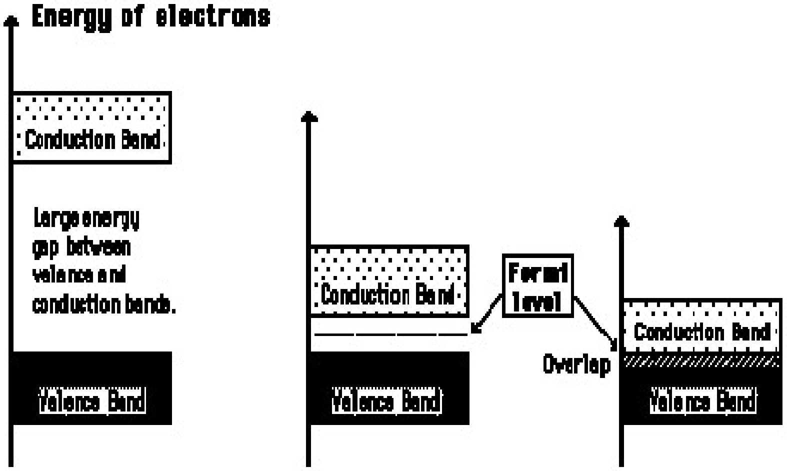
At the point of inflection $\left[\left(\frac{d^2E}{dK^2}\right) = 0\right]$, m^* becomes ∞.

i.e. In the upper of the Band, the particles behave like +ve charges, ie Holes.

In the lower part of the Band the particles behave like $-ve$ charges i.e electrons.

Classification of crystalline solids:

Based on the width of forbidden band, solids are classified into insulators, Semiconductors and conductors.



a. Insulator b. Semiconductor c. Conductor

Conductors: The valence band and conduction bands are overlapped with each other and the energy gap E_g is zero. At room temperatures, free electrons already exist in huge number at conduction band. Hence these solids are good electrical conductors as well as good thermal conductors. The electrical resistivity increases at high temperature by collisions among the free electrons.

Ex: Al, Cu, Ag, Au etc.,

Semiconductors: The valence band and conduction bands are separated with a small energy band gap $E_g \approx 1$ eV. At low temperatures (0 K), free electrons are not available in conduction band. Hence they behave like insulators at low temperatures. The electrical conductivity increases at high temperatures by the transition of free electrons from valence band to conduction band. Thus these solids behave like electrical conductors at high temperatures.

Ex: Silicon $E_g = 1.1$ ev, Germanium $E_g = 0.7$ev

Insulators: The valance band and conduction bands are separated by a very large energy gap $E_g \geq 3$ eV. At room temperatures conduction band is empty and valance band is full of electrons. Hence they these solids are electrical insulators. Even at high temperatures valence electrons are unable to jump in to conduction band. Ex: Glass, Mica, Ebonite, Rubber etc.,

Semiconductors exhibit negative temperature coefficient of Resistance.

SEMICONDUCTORS

Semiconductors are classified basing on their conductivities and resistivity's.

Electrical resistivity of semi conductors lies in between those of conductors and insulators.

In semiconductors, there are two types of carriers namely electrons and holes.

Hence semiconductors are bipolar materials.

The current in semiconductors is due to two types of carriers namely electros and holes.

Pure semi conductors are known as intrinsic semiconductors.

Example : Silicon and Germanium.

The electrical conductivity can be enhanced by a process called doping. i.e. the number of carriers can be increased by a process called doping. Doping is the process of adding an impurity to a pure semi conductor. By adding a suitable impurity to an intrinsic semi conductor, it will become an extrinsic semi conductor.
The transportation of charge carriers (movement) takes place due to drift and diffusion.

The extrinsic semi conductors are widely used in solid state electronic devices and semi conductor electronic devices.

To study electronic devices, it is important to study the fundamental electronic transportation properties in semi conductors.

Intrinsic semiconductors

Usually pure semiconductors are known as intrinsic semiconductors. Examples are Silicon (Si) and Germanium (Ge) .Silicon (Si) and Germanium belongs to **IV group** of periodic table.

Atomic Number of Silicon is 14.

Electronic configuration $1s^2\ 2s^2\ 2p^6\ \mathbf{3s^2\ 3p^2}$

Atomic number of Germanium is 32.

.Electronic configuration is

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ \mathbf{4s^2\ 4p^2}$

In Silicon and Germanium, there are four valence electrons. Bonding in these semiconductors is covalent bonding.

Each silicon Atom forms four covalent bonds with the surrounding electrons from neighboring Silicon atoms in the silicon Semiconductor crystal.

Here no electrons are available freely for conduction and the semi conductor acts like an insulator.

The conduction process can be understood with the help of energy band diagram.

In the energy band diagram, we have conduction band and valence band.

The conduction band and valence band are separated by a forbidden energy gap Eg., known as energy band gap. The covalent bond representation and the energy band structure is shown in figure (1) at O^0K.

At O^0K, all valence electrons are tightly bound to their atoms and are taking part in covalent bond formation.

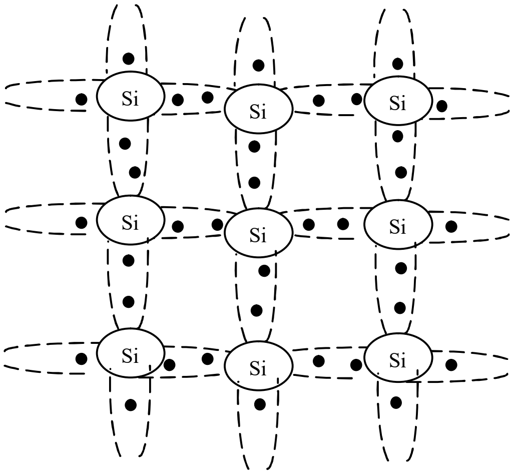


Fig. (1)a: Intrinsic silicon at O^0k – Two dimensional Representation.

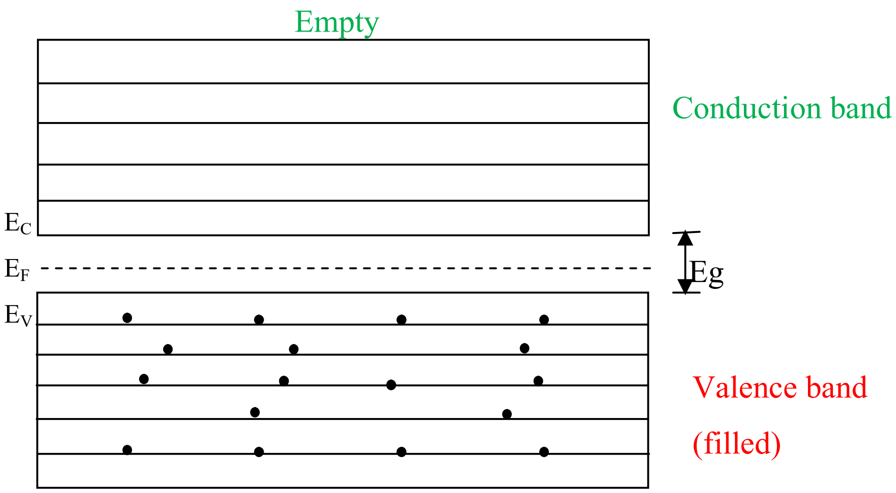


Fig (1)b: Energy band structure of Intrinsic Semiconductor Silicon at O^0k.

For Silicon Eg = 1.12 ev.
Germanium Eg = 0.69 ev.

In the figure (1) b E_c**= Energy level corresponding to Bottom of the conduction band.**
E_v **= Energy of the energy level corresponding to the top of the Valence band.**
E_f **= Fermi energy level.**

At O^0K, the semiconductors behave like insulators.
At O^0K, the valence band is completely filled and the conduction band is empty.

Above O^0K (i.e. At Room temperature), the valence electrons acquire sufficient amount of thermal energy. Due to this they break the covalent bonds and make themselves available as free electrons. Against to creation one free electron, a vacancy is created in its initial position in the crystal structure. This vacancy is known as a hole.

The hole is a virtual positive charge, having the magnitude of charge of the electron.

The free electrons after acquiring sufficient thermal energy, and crosses the energy gap.

These electrons will enter into the conduction band from valence band and occupy energy levels in the conduction band.

The electrons leaving the valence band create holes in its original place.

Now the valence band will have holes and the conduction band contains electrons.

The crystal structure and energy band structure above O^0K is shown in figure (2).

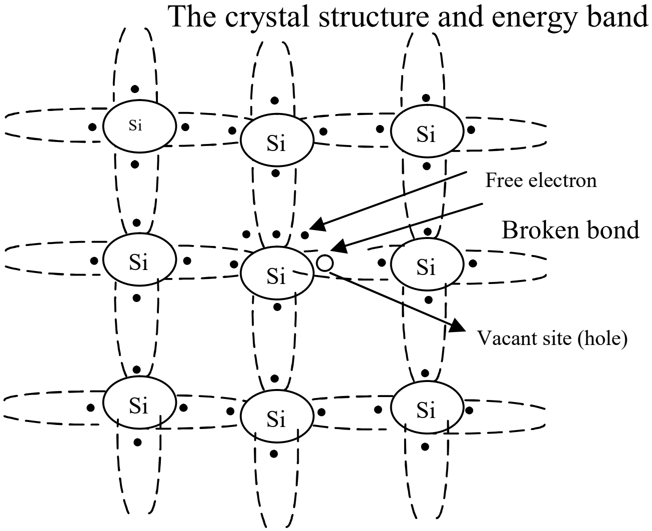


Figure (2) a: Two dimensional crystal structure of intrinsic semi conductor silicon above O^0K

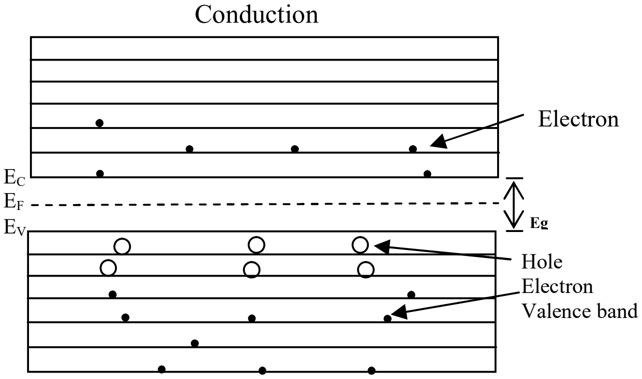


Figure (2) b: Intrinsic Silicon – Energy band structure above O^0K.

In an intrinsic semi conductor,

Number of holes = No. of electrons = n_i; $n=p=n_i$

n = Number of electrons per unit volume (or) electron concentration (or) electron density.

p = Number of holes per unit volume (or) hole concentration (or) hole density.

n_i = Intrinsic concentration.

Now $np = n_i^2$ (Law of mass action)

Intrinsic carrier concentration

Above O^0K, in an intrinsic semi conductor, each broken bond leads to generation of two carriers. They are electron and hole.

At any temperature T, the number of electrons generated will be therefore equal to the number of generated Holes.

Let n = Number of electrons per unit volume or electron concentration in the Conduction band.

P = Number of holes per unit volume or Hole concentration in the valence band.

For an intrinsic semiconductor;

$$n = p = n_i \qquad \text{--- (1)}$$

Where n_i = intrinsic carrier concentration.

Now the electron concentration in the conduction band is given by

$$n = N_c e^{-(E_c - E_F)/K_B T}$$

$$n = N_c e^{(E_F - E_C)/K_B T} \qquad \text{--- (2)}$$

The Hole concentration in the valence band is given by

$$P = N_v e^{-(E_F - E_V)/K_B T}$$

$$p = N_v e^{(E_V - E_F)/K_B T} \qquad \text{--- (3)}$$

Here N_c, N_V are known as **pseudo constants**, depends on temperature.

K_B = Boltzmann constant

T = Temperature in ^{0}K of the intrinsic semiconductor.

Now $n_i^2 = np$

$$n_i^2 = N_c e^{(E_F - E_C)/K_B T} N_V e^{(E_V - E_F)/K_B T}$$

$$n_i^2 = N_c N_v e^{\frac{(\cancel{E}_F - E_C + E_V - \cancel{E}_F)}{K_B T}}$$

$$n_i^2 = N_c N_V e^{\frac{(-E_c + E_v)}{K_B T}}$$

$$n_i^2 = N_c N_V e^{\frac{-(E_c - E_v)}{K_B T}}$$

$$n_i^2 = N_c N_V e^{\frac{-E_g}{K_B T}}$$

Where $E_c - E_v = Eg$, Energy Gap.

$$n_i = (N_c N_v)^{1/2} e^{(\frac{-[E_g]}{2 K_B T})} \qquad \text{-------------------- (4)}$$

From equation (4), It is clear that

i) Intrinsic carrier concentration is independent of Fermi level.

ii) Intrinsic carrier concentration n_i is a function of temperature T.

iii) Intrinsic carrier concentration n_i is a function of Energy gap E_g.

Fermi level expression

The **Fermi level is the top most occupied energy level**. The Fermi level indicates the probability of occupation of energy levels of the electrons in conduction and valence bands.

In intrinsic semiconductors, electron and hole concentrations are equal.

i.e. it indicates that the probability of occupation of energy levels in conduction band and valence band are equal.

Usually in an intrinsic semiconductor, the Fermi level lies in the middle of the energy gap Eg.

For an intrinsic semiconductors, n=p.

$$n = N_c e^{-(E_c - E_f)/K_B T}$$

Now

$$n = N_c e^{(E_f - E_c)/K_B T} \qquad \text{------------ (1)}$$

Hole concentration, $p = N_v e^{-(E_f - E_v)/K_B T}$

$$p = N_v e^{(E_V - E_f)/K_B T} \qquad \text{------------ (2)}$$

Equations (1) and (2) represent electron and hole concentrations for intrinsic semiconductors.

Since n=p.

$$N_c e^{(E_f - E_c)/K_B T} = N_V e^{(E_v - E_f)/K_B T}$$

$$\Rightarrow \frac{N_V}{N_C} = \frac{e^{(\frac{E_f - E_c}{K_B T})}}{e^{(\frac{E_v - E_f}{K_B T})}}$$

$$\Rightarrow \frac{N_V}{N_C} = \frac{e^{\frac{(E_f - E_c)}{K_B T}}}{} . e^{-\frac{(E_v - E_f)}{K_B T}}$$

$$\Rightarrow \frac{N_V}{N_C} = e^{\frac{(E_f - E_c - E_v + E_f)}{K_B T}}$$

$$\Rightarrow \frac{N_V}{N_C} = e^{[2E_f - (E_c + E_v)]/K_B T} \qquad \text{--------------------- (3)}$$

Taking Naparian Logarithm on both sides.

$$\log_e\left(\frac{N_V}{N_C}\right) = Log_e e^{[2E_F-(E_C+E_V)]/K_BT}$$

$$\log_e\left(\frac{N_V}{N_C}\right) = \frac{2E_F-(E_C+E_V)}{K_BT}$$

$$\Rightarrow 2E_F-(E_C+E_V) = K_BT\log_e\left(\frac{N_V}{N_C}\right)$$

$$\Rightarrow 2E_F = E_C+E_V+K_BT\log_e\left(\frac{N_V}{N_C}\right)$$

$$\Rightarrow E_F = \left(\frac{E_C+E_V}{2}\right)+\frac{K_BT}{2}\log_e\left(\frac{N_V}{N_C}\right)$$

For an intrinsic semiconductor $m_e^* = m_h^*$

Hence $N_V = N_c$

$$\therefore E_F = \left(\frac{E_C+E_V}{2}\right)+\frac{K_BT}{2}\log_e(1)$$

$$\therefore E_F = \frac{E_c+E_V}{2}$$

Therefore Fermi level lies exactly midway between conduction band and valence band.

Expression for intrinsic conductivity

Let us consider intrinsic semiconductors. This is applied with a potential difference of V volts.

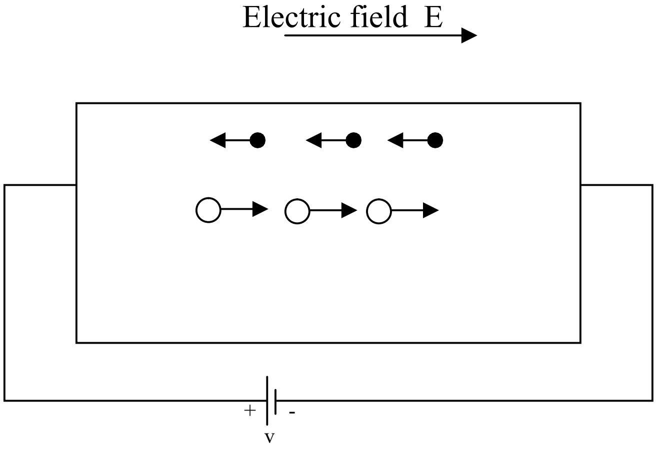


Fig. 3 Conduction in an intrinsic semiconductor

Due to the applied voltage an electric field E will be established as shown in the figure.
Now the charge carriers drift as indicated in figure (3).This constitutes an electric current I.
The drift velocity acquired by the charge carriers is given by.

$V_d = \mu E$ ----------------- (1)

Where μ = Mobility of charge carriers. E= Electric field

Also the current density due to drift of electrons is given by

$$J_n = nev_d \quad \text{-------------------- (2)}$$

Where n= electron concentration

e = charge on the electron.

v_d = drift velocity of the electrons.

From Equations (1) &(2), we get,

$$J_n = ne\mu_n E \quad \text{---------------------- (3)}$$

Where μ_n = Mobility of electrons.

Current density $\text{J}=\dfrac{\text{Current}}{\text{Area}}=\dfrac{\text{I}}{A}$

Also the holes will drift in a direction opposite to electrons, the hole current density is given by

$$\text{J}_\text{p} = pe\mu_P E \quad \text{------------------------- (4)}$$

Where p = Hole concentration.

e = charge on the hole.

μ_p = Mobility of holes.

Now the total current density is given by

$$J = J_n + J_p$$

$$J = ne\mu_n E + Pe\mu_p E \quad \text{------------------- (5)}$$

$$J = \left(n\mu_n + P\mu_p\right)eE$$

But according the classical theory, ohms law is given by

$$J = \sigma E \quad \text{------------------------------- (6)}$$

Where σ = Electrical conductivity

$\therefore$ From equations (5) and (6), we have

$$\sigma E = \left(n\mu_n + P\mu_p\right)eE$$

$$\sigma = \left(n\mu_n + P\mu_p\right)e$$

But according to law of mass Action, for an intrinsic semiconductors $n = p = n_i$

$$\therefore \sigma = \left(n_i\mu_n + n_i\mu_p\right)e$$

$$\sigma = n_i e\left(\mu_n + \mu_p\right) \quad \text{----------------------- (7)}$$

Where n_i = Intrinsic concentration.

But $n_i = \left(N_C N_V\right)^{1/2} e^{-Eg/2K_BT}$ ------------------- (8)

Substituting (8) in (7), we get

$$\sigma = \left(N_C N_V\right)^{1/2} e\left(\mu_n + \mu_p\right)e^{-Eg/2K_BT}$$

Electrical conductivity for intrinsic semi conductors is given by

$$\sigma = Ae^{-Eg/2K_BT} \quad \text{-------------------- (9)}$$

Where $A=\left(N_C N_V\right)^{1/2} e\left(\mu_n+\mu_p\right)$

A = a constant

In pure Semiconductors electrical conductivity is due to both electrons and holes.

Determination of Energy Gap (Eg) for intrinsic semiconductors

The energy gap between the conduction Band and the valence band is represented as band gap Eg. For intrinsic semi conductors, the energy gap is given by

$\sigma = Ae^{-Eg/2K_BT}$, σ = Electrical conductivity. ------- (1)

Where A = a constant

Eg= Energy band Gap.

K_B= Boltzmann constant.

T = Absolute scale of temperature.

Let ρ = Electrical Resistivity.

$$\rho=\frac{1}{\sigma}$$

$$\therefore \rho=\frac{1}{Ae^{-Eg/2K_BT}}$$

$$\rho=\frac{1}{A}e^{Eg/2K_BT}$$

$\rho = Be^{Eg/2K_BT}$ ------------------------ (2) , Where $B=\frac{1}{A}$, a new constant.

Taking Neparian logarithm on both sides,

$$\log_e \rho=\log_e\left(Be^{Eg/2K_BT}\right)$$

$$\log_e \rho=\log_e B+\log_e e^{(\frac{E_g}{2K_BT})}$$

$$\ln\rho=\ln B+\frac{Eg}{2K_BT}$$

$$\ln\rho=\frac{Eg}{2K_BT}+\ln B \qquad \text{--- (3)}$$

(3) is slope intercept form equation.

Where m = slope of the straight line

From figure (1), $m=\frac{Eg}{2K_B}=\frac{\Delta y}{\Delta x}$

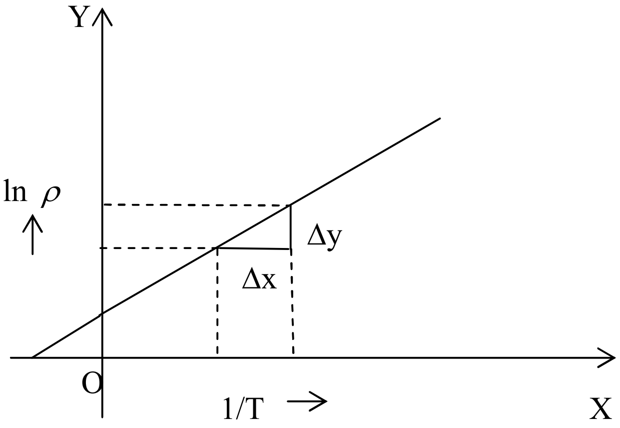


Fig 4: Plot of 1/T and ln ρ

$$\therefore Eg = \left(\frac{\Delta y}{\Delta x}\right) 2K_B \quad \text{---- (4)}$$

If a graph is plotted between $\frac{1}{T}$ on X-axis and $\ln \rho$ on y-axis, a straight line graph is obtained. The straight line graph is shown in figure (4).

Extrinsic Semiconductors

Extrinsic semi conductors are impure semiconductors. With the addition of impurities, a pure semi conductors becomes an extrinsic semiconductors.

An extrinsic semi conductor shows good conducting properties due to the presence of impurities.

Depending on the type of impurity present in the intrinsic semi conductors, extrinsic semi conductors are classified into two types.

1) N – type extrinsic semi conductors. 2) P - type extrinsic semi conductors.

N-Type semi conductors

For silicon if a small amount of pentavalent impurity such as phosphorous, arsenic or antimony or Bismuth is added, we get N-type semiconductors.

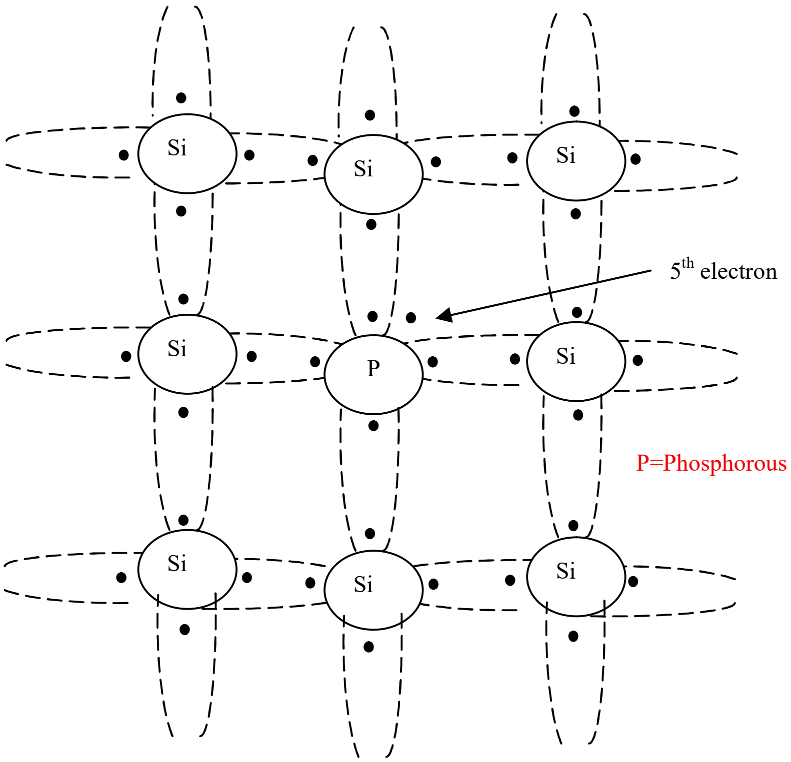
Four valence electrons of phosphorous form covalent bonds with the adjacent four silicon atoms. The fifth electron is left free. It cannot form bond with any other electron in the lattice structure. This is shown in figure (1).a.

At O^0k, this fifth electron is bound to phosphorous with 0.045 ev.

The corresponding energy Band diagram and lattice structure are shown in figure (1) at O^0k. At O^0k, the valence Band and the conduction band are separated by an Energy Gap Eg.

Pure Silicon+ Pentavalent impurity =N-type Semiconductor.

Pentavalent Impurities EX: Arsenic ,Antimony,Bismuth, Phosphorous.



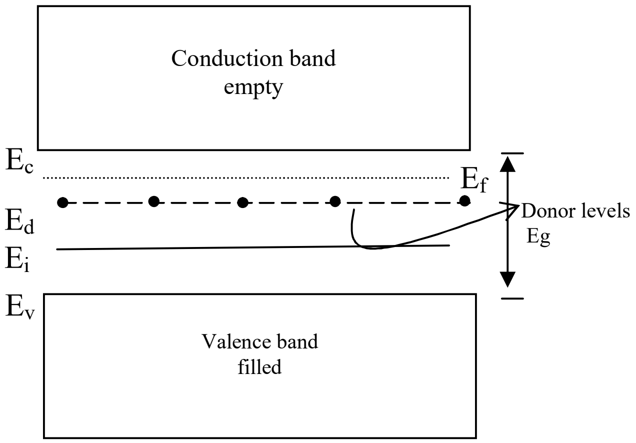


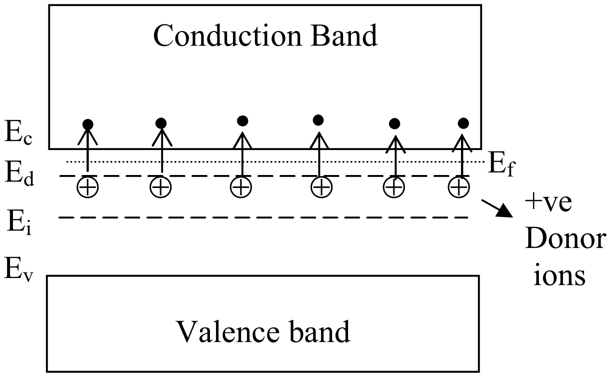
Figure (1) b: Energy band diagram of N-type semiconductor at O^0k

Figure (1)a: N-type silicon at O^0k

The donor energy level Ed lies below the bottom of conduction band. This donor energy level contains phosphorous atoms. Which denotes electrons at $T>O^0k$ The donor energy level in shown in the figure (1) b. Above O^0k, when temperature is increased. The 5th bond electron becomes a free electron. This free electron enters into the conduction band. Due to this the Donor Atoms will get ionized, by denoting an electron to the conduction band. When temperature is further increased, the covalent bonds will break down. Here electron hole pairs will be generated.

Electrons will move from valence bond to conduction bond, leaving holes in the valence bond. At higher temperatures, the energy band diagram of N-type silicon is shown in figure (2)

The Fermi level varies as shown in fig (2) b at 300^0k.



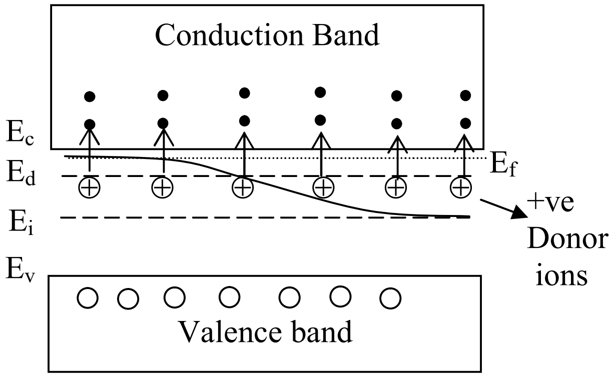


Figure (2)a: Energy band diagram of N-type semiconductor at $T>O^0k$

Figure (2)b: Energy band diagram of N-type silicon at $T=300^0K$ and above

Now the concentration of electrons increases in the conduction band when compared to holes. Hence the electrons become the majority charge carriers and holes the minority charge carriers.
The variation of Fermi level is also shown in figure 2(b).

P-type semi conductors

For silicon if a small amount of trivalent impurity such as indium, Gallium, Thallium or Aluminum or Boron is added, we get a P- Type semi conductors.Three valence electrons of Boron form covalent bonds with the adjacent three silicon Atoms. There is not fourth electron to form a covalent bond with the neighboring silicon atom. This is like a missing bond. This is represented as a missing electron or vacant site.
This is shown in figure (1)

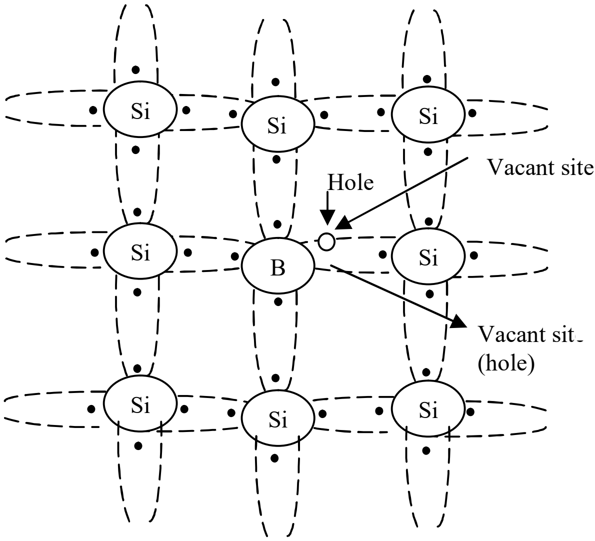


Fig. (1)a: P-type silicon at O^0K

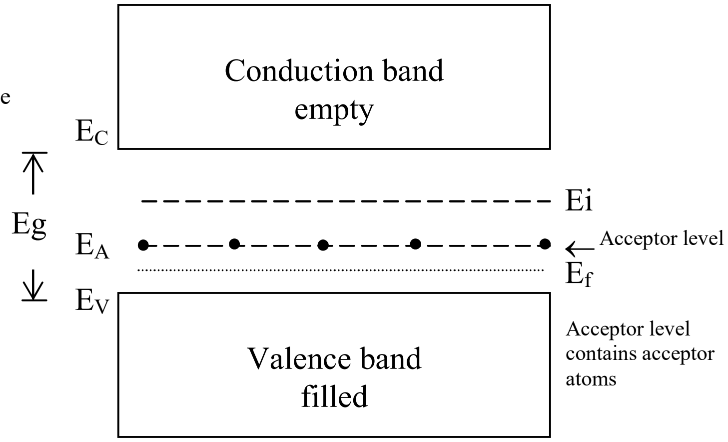


fig.(1)b: Energy band structure of P-type silicon at 0^0k

This missing electron is called Hole. The energy Band structure of P-type semi conductors is shown in figure (1) b.

At O^0k, the conduction Band is empty and the valence B and contains electrons.
The acceptor energy level E_A is just above the top of the valence Band.
Acceptor energy level E_A contains the acceptor atoms.

Here E_c = Bottom of the conduction band.

E_V = Top of the valence band.

E_i = Intrinsic energy level.

The Energy band structure of P-type silicon is shown in figure (2) a above O^0k.
When the temperature is above O^0k, the covalent bonds with the silicon are broken down.

E_A level contains acceptor negative ions.

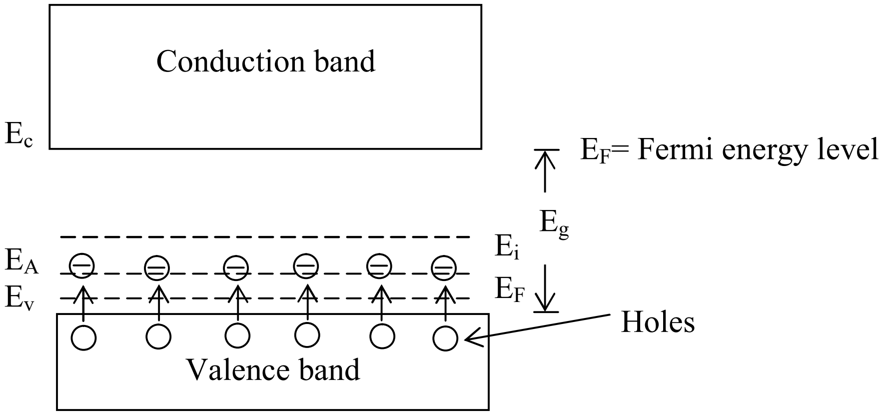


Fig.(2)a: Energy band structure of P-type silicon above O^0k

Here same electrons are released and the acceptor atoms accept three electrons and there by they become negatively charged ions. There are called negative acceptor ions. Here the Fermi energy level lies just above the top of the valence bond and below the acceptor level.

The energy band diagram of P-type semi conductors is shown in the figure (2) b. at T = 300^0k.At and above 300^0k, the bonds in silicon with further breakdown and the electrons will move from valence band to conduction band. Therefore electrons are available in the conduction band. At 300^0k the Fermi level varies as shown in the figure.

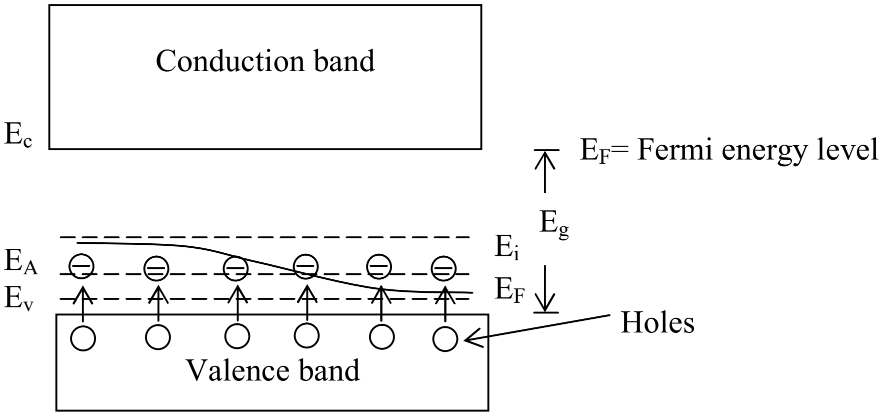


Fig.(2)b: Energy band diagram of P-type silicon at 300^0K & above

Pure Silicon+ Trivalent impurity =P-type Semiconductor.
Trivalent impurities EX: Indium, Gallium,Thallium, Aluminium,Boron.
Doping: It is the process of adding an impurity to a pure Semiconductor.

Law of Mass Action

The electron concentration in intrinsic semi conductors is given by

$$n = N_c e -^{\left(E_c - E_f\right)} / K_B T$$

$$n = N_c e^{\left(E_f - E_c\right)} / K_B T \qquad \text{---- (1)}$$

Similarly in an intrinsic semiconductors, the hole concentration is given by

$$P = N_v e^{\left(E_f - E_c\right)} / K_B T$$

$$P = N_v e^{\left(E_v - E_f\right)} / K_B T \qquad \text{---- (2)}$$

Where N_c and N_v are pseudo constants.

K_B is the Boltzmann constant.
T is temperature in ^{0}K.
E$_F$ is the energy of Fermi level.
E$_C$ is the bottom of the conduction band.
E$_v$ is the top of the valence band.

In an intrinsic semiconductors n=p=n$_i$

$$\therefore np = N_c e^{\left(E_f - E_c\right)/K_B T} . N_v e^{\left(E_v - E_f\right)/K_B T}$$

$$np = ni^2 = N_c e^{\left(E_f - E_c\right)/K_B T} . N_v e^{\left(E_v - E_f\right)/K_B T}$$

$$np = ni^2 = N_c N_V e^{-\left(E_f - E_c\right)/K_B T}$$

$$np = ni^2 = N_c N_V e^{-Eg/K_B T} \text{ Where } E_c - E_v = E_g$$

$$\Rightarrow n_i = \left(N_c N_v\right)^{1/2} e^{-Eg/2K_B T} \qquad \text{--- (3)}$$

The above relation shows that for any arbitrary value of E$_g$ the product of n and p is a constant.

This is known as Law of Mass Action

For an extrinsic semiconductors, the electrons and hole concentrations are given by expressions similar to Equations (1) and (2)

For an N-type semiconductor

$$N_n = N_c e^{\left(E_f - E_c\right)/K_B T} \qquad \text{----- (4)}$$

$$P_n = N_v e^{\left(E_v - E_f\right)/K_B T} \qquad \text{----- (5)}$$

Where $n_n =$ Electron concentration. And $P_n =$ Hole concentration.

Now $N_n P_n = N_C N_V e^{\left(E_f E_c\right)/K_B T} . N_v e^{\left(E_v - E_f\right)/K_B T}$

$$n_n P_n = N_C N_V e^{-\left(E_f E_c\right)/K_B T}$$

$$n_n P_n = N_C N_V e^{-E_g / K_B T} \qquad \text{------ (6)}$$

Where $E_c - E_v = E_g$

$$n_n P_n = ni^2 \qquad \text{---- (7)}$$

The above expression (7) is known as Law of Mass action for N-type semi conductors. For P-type semi conductors, the law of mass action is given by

$$p_p n_p = n_i^2 \qquad \text{----- (8)}$$

Equations (7) and (8) imply that the product of majority and minority carrier concentrations in extrinsic semi conductors at a given temperature is equal to the square of Intrinsic carrier concentration at that temperature.

The law of mass action is very important in conjunction with charge neutrality condition.. This enables us to calculate minority carrier concentration. This law states that the addition of impurities to intrinsic semi conductors increases the concentration of one type of carrier, which consequently becomes majority carrier and simultaneously decreases the concentration of the other carriers, which is known as the minority carrier.

The minority carriers decrease in number below the intrinsic value.

This is because there is an increase of majority charge carriers Recombination rate.

According to the law of Mass action, the product of majority and minority carriers remains constant in an extrinsic semi conductors and it is independent of the amount of donor and acceptor impurity concentrations. When the doping concentration levels are high, the minority carrier concentration will be law and the majority carrier concentration will be high when the doping concentration levels are low, the majority carrier concentration is low and the minority carrier concentration is high.

Charge neutrality

Let us consider extrinsic semi conductors with both donor and Acceptor impurities.

At usual ambient temperatures, we may assume that impurity atoms are ionized and no charge carriers are created due to breaking of covalent bonds.

Now concentration of electrons n = concentration of positively ionized donor impurity atoms, N_d.

Concentrations of holes P = concentration of negatively ionized acceptor impurity atoms N_a.

Now the total charge neutrality of the material can be written as

$$P + N_d = n + N_a \qquad \text{--- (1)}$$

According to law of Mass action, in any semiconductor, under thermal equilibrium condition, the product of the number of electrons and number of holes is a constant.

$$np = ni^2 \qquad \text{----- (2)}$$

Where ni = intrinsic carrier concentration.

Also $n = \frac{ni^2}{p}$ and $p = \frac{ni^2}{n}$

Now from equation (1), we have

$$p = n + N_a - N_d$$

But $n = \frac{ni^2}{p}$

$$p = \frac{ni^2}{p} + \left(N_a - N_d\right)$$

$$\Rightarrow p^2 = ni^2 + P\left(N_a - N_d\right)$$

$$\Rightarrow p^2 - P\left(N_a - N_d\right) - ni^2 = 0$$

This is a quadratic equation of the type
$ax^2 + bx + c = 0$

$$\therefore P = \frac{N_a - N_d}{2} \pm \sqrt{\frac{\left(N_a - N_d\right)^2 + 4ni^2}{2}}$$

$$P = \frac{N_a - N_d}{2} \pm \left[\frac{\left(N_a - N_d\right)^2}{4} + ni^2\right]^{1/2} \qquad \text{---- (3)}$$

Similarly we can show that

$$n = \frac{N_d - N_a}{2} \pm \left[\frac{\left(N_d - N_a\right)^2}{4} + ni^2\right]^{1/2} \qquad \text{----- (4)}$$

Equations (3) and (4) represent the equations for charge densities.

Case I: For intrinsic semi conductors.

$$N_a = 0$$

Hence we get $n = p = ni$ ---- (5)

Case II: N – type semiconductors

Now $p = \frac{-Nd}{2} \pm \left[\frac{\left(-Nd\right)^2}{4} + ni^2\right]^{1/2}$

$$p = -\frac{Nd}{2} \pm \frac{\left(-Nd^2 + 4ni^2\right)^{1/2}}{2}$$

$$p = \frac{-Nd \pm \left(-Nd^2 + 4ni^2\right)^{1/2}}{2}$$

$$p = \frac{-Nd \pm Nd^2\left[1 + \frac{4ni^2}{Nd^2}\right]^{1/2}}{2}$$

Since p cannot be negative

$$p = -\frac{-Nd + Nd\left(1 + \frac{4ni^2}{Nd^2}\right)^{1/2}}{2}$$

Expanding using power series and neglecting higher power terms

$$P=-\frac{Nd}{2}+\frac{Nd}{2}\left[1+\frac{1}{2}\left(\frac{4ni^2}{Nd^2}\right)+.......\right]$$

$$P=-\frac{Nd}{2}+\frac{Nd}{2}\left(1+\frac{2ni^2}{Nd^2}\right)$$

$$P=-\cancel{\frac{Nd}{2}}+\cancel{\frac{Nd}{2}}+\frac{Nd^2}{2}\frac{2ni^2}{Nd^2}$$

$$P=\frac{ni^2}{Nd} \qquad \text{---- (6)}$$

Similarly electron concentration

$$n=\frac{Nd}{2}+\left(\frac{Nd^2+4ni^2}{4}\right)^{1/2}$$

$$n=\frac{Nd}{2}+\frac{Nd}{2}\left(1+\frac{4ni^2}{Nd^2}\right)^{1/2}$$

Expanding using power series and neglecting higher power terms

$$n=\frac{Nd}{2}+\frac{Nd}{2}\left[1++\frac{1}{2}\left(\frac{4ni^2}{Nd^2}\right)+.........\right]$$

$$n=\frac{Nd}{2}+\frac{Nd}{2}\left(1+\frac{2ni^2}{Nd^2}\right)$$

$$n=N_d+\frac{ni^2}{N_d}$$

At low temperatures $ni \approx 0$

Hence $n \approx N_d$ ----- (7)

Case III : P-type semi conductor

In this case $N_d=0$

Now $$n=-\frac{Na}{2}\pm\left[\frac{(-Na)^2}{4}+ni^2\right]^{1/2}$$

$$n=-\frac{Na}{2}\pm\left[\frac{4a^2}{4}+ni^2\right]^{1/2}$$

$$n=-\frac{Na}{2}\pm\left(\frac{Na^2+4ni^2}{4}\right)^{1/2}$$

$$n=-\frac{Na}{2}\pm\frac{\left(Na^2+4ni^2\right)^{1/2}}{2}$$

$$n = -\frac{Na \pm \left(Na^2 + 4ni^2\right)^{1/2}}{2}$$

$$n = \frac{-Na \pm Na\left(1 + \frac{4ni^2}{Na}\right)^{1/2}}{2}$$

Since n cannot be negative

$$n = \frac{-Na \pm Na\left(1 + \frac{4ni^2}{Na}\right)^{1/2}}{2}$$

Expanding using power series and neglecting higher power terms

$$n = -\frac{Na}{2} + \frac{Na}{2}\left[1 + \frac{1}{2}\left(\frac{4ni^2}{Na^2}\right) + ...\right]$$

$$n = -\frac{Na}{2} + \frac{Na}{2}\left(1 + \frac{2ni^2}{Na^2}\right)$$

$$n = -\cancel{\frac{Na}{2}} + \cancel{\frac{Na}{2}} + \frac{Na}{2}\frac{2ni^2}{Na^2}$$

$$\therefore n = \frac{ni^2}{Na} \qquad \text{--- (8)}$$

Similarly Hole concentration

$$P = \frac{Na}{2} \pm \left[\frac{Na^2}{4} + ni^2\right]^{1/2}$$

$$P = \frac{Na}{2} \pm \left(\frac{Na^2 + 4ni^2}{4}\right)^{1/2}$$

$$P = \frac{Na \pm \left(Na^2 + 4ni^2\right)^{1/2}}{2}$$

$$P = \frac{Na \pm Na\left(1 + \frac{4ni^2}{Na^2}\right)^{1/2}}{2}$$

$$P = \frac{Na}{2} + \frac{Na}{2}\left(1 + \frac{4ni^2}{Na^2}\right)^{1/2}$$

Expanding using power series and neglecting higher power terms.

$$P = \frac{Na}{2} + \frac{Na}{2}\left[1 + \frac{1}{2}\left(\frac{4ni^2}{Na^2}\right) + ...\right]$$

$$P = \frac{Na}{2} + \frac{Na}{2}\left(1 + \frac{4ni^2}{Na^2}\right)$$

$$P = \frac{Na}{2} + \frac{Na}{2} + \frac{Na}{2}\frac{2ni^2}{Na^2}$$

$$P = Na + \frac{ni^2}{Na}$$

At low temperature ni □ 0

Hence p □ Na ---- (9)

Equation of Continuity

This equation governs the behavior of charge carriers in a semi conductor.

This equation gives a condition of dynamic equilibrium for the density of charge carriers in any elementary volume of semiconductors.

This is based on the fact that charge can neither be created nor be destroyed.

When an N-type semiconductor is exposed to light, excess carriers are generated at the exposed surface.

The generated carriers are in the form of electron – hole pairs. Since the given semiconductors are N-type, here the excess carriers are holes.

These charge carriers diffuse throughout the material. Hence the carrier concentration in the semiconductor is a function of both time and distance.

Consider the infinitesimal volume element of are A and length dx as shown in figure (1).

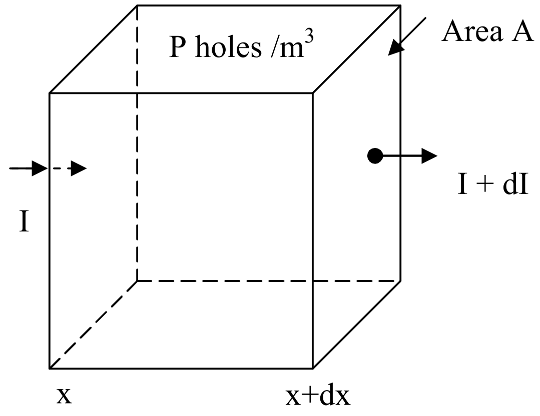


Figure (1) Conservation of charge carriers

Let P be the average hole concentration within this volume.

Let τ_p = Mean life of holes.

Now the holes lost per unit volume by recombination is $\frac{P}{\tau_p}$.

The rate of loss of charge within the volume under consideration = $eAdx\frac{P}{\tau_p}$ --------(1)

Recombination : *Electrons combining with holes is called recombination*

Let g = Thermal rate of generation of electron hole pairs per unit volume.

Now rate of increase of charge within the volume under consideration = $eAdxg$ ---- (2)

Let I = The current entering the volume at x.

I +d I = The current leaving the volume at x+dx.

It is found that the current leaving the sample has increased by an amount dI.

This means that these is a decrease of hole concentration. Now the decrease of holes (in coulombs) per second from the volume under consideration = dI.

Due to above stated three effects, the hole density changes with time.

Now increase in the number of holes per second

Within the given volume = $eA\dfrac{dp}{dt}dx$ ----------------------- (3)

According to conservation of charges, charge can neither be created nor be destroyed.

$\therefore$ Increase of Holes = generation of Holes – loss of Holes.

$$eA\,dx\frac{dp}{dt} = eAdxg - eAdx\frac{p}{\tau_P} - dI \qquad \text{-----------------------(4)}$$

Now total current due to excess carries (holes) in given by

Total current = Diffusion current + drift current

$$I = -Ae\,D_p\frac{dp}{dx} + Ape\mu pE \qquad \text{-------------------------- (5)}$$

Where E = Intensity of the electric field with in the given volume when there is no external field applied, then E = 0 under thermal equilibrium conditions the hole density attains a constant value P_0

Under these conditions dI=0 and $\dfrac{dp}{dt} = 0$

Now equation (4) becomes

$$O = eAdxg - eAdx\frac{P_0}{\tau_p}$$

$$\Rightarrow g = \frac{P_0}{\tau_p} \qquad \text{---------------------------- (6)}$$

Here g = generation rate.

This equation (6) indicated that, the rate of generation of holes is equal to the rate of loss due to recombination under equilibrium conditions.

Also (5) $\Rightarrow I = -AeD_p\dfrac{dp}{dx} + Ape\mu pE$

$$\text{Now } \frac{dI}{dx} = -AeD_p\frac{d^2p}{dx^2} + Ae\mu p\left(\frac{dp}{dx}\right)E \qquad \text{----------------------- (7)}$$

From equations (4), (6) and (7), we get

$$eADx\frac{dp}{dt} = eAdx\frac{P_0}{\tau_p} - eAdx\frac{p}{\tau_p}$$

$$-\left[-AeDp\frac{d^2p}{dx^2}dx + Ae\mu p\left(\frac{dp}{dx}\right)Edx\right]$$

$$\cancel{e}\,\cancel{A}\,\cancel{dx}\frac{dp}{dt} = -\cancel{e}\,\cancel{A}\,\cancel{dx}\left(\frac{P-P_0}{\tau_p}\right) + \cancel{A}\,\cancel{e}\,D_P\frac{d^2p}{dx^2}\cancel{dx} - \cancel{A}\,\cancel{e}\;\mu\,p\frac{dp}{dx}E\,\cancel{dx}$$

$$\Rightarrow \frac{dp}{dt} = -\left(\frac{P-P_0}{\tau_p}\right) + D_P\frac{d^2p}{dx^2} - \;\mu\,p\left(\frac{dp}{dx}\right)E \qquad \text{------------- (8)}$$

This equation (8), is called equation of continuity, since hole concentration P is a function of tome t and distance x, we have to use only partial derivatives.

$$\Rightarrow \frac{\partial p}{dt} = -\left(\frac{P-P_0}{\tau_p}\right) + D_P \frac{\partial^2 p}{dx^2} - \mu_p \left(\frac{\partial p}{dx}\right) E \quad \text{-------------} \ (9)$$

For holes in an n-type semiconductor

$$\therefore \frac{\partial p_n}{\partial t} = -\frac{(P_n - P_{on})}{\tau_p} + D_P \frac{\partial^2 p_n}{dx^2} - \mu_p E \frac{\partial p_n}{dx} \quad \text{----------------} \ (10)$$

For elections in a p-type semi conductor

$$\frac{\partial n_p}{\partial t} = -\frac{(n_p - n_{op})}{\tau_n} - D_n \frac{\partial^2 n_p}{dx^2} + \mu_n E \left(\frac{\partial n_p}{dx}\right) \quad \text{--------------} \ (11)$$

This sign difference between the above two equations in due to the different directions of drift of holes and electrons in an applied electric field.

Hall Effect:

Some times it is necessary to determine whether a material is n-type or p-type. Measured conductivity of a specimen will not give this information since it cannot distinguish between positive hole and electron conduction.

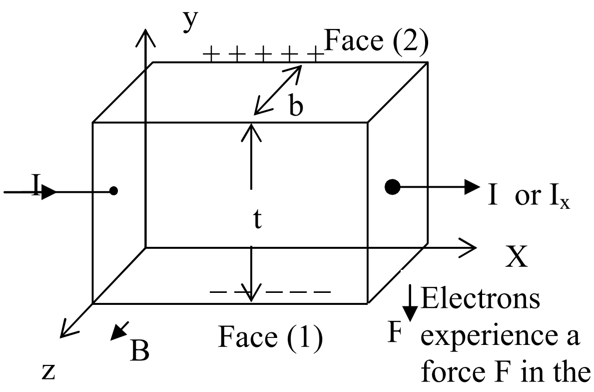
The Hall Effect can be utilized to distinguish between the two types of carriers, and it is also useful in the determination of density of charge carriers.

Hall Effect definition

"If a piece of conductor or Specimen (metal or semiconductor) carrying current is subjected to a transverse magnetic field, an electric field is generated inside the specimen in a direction normal to both the current and the magnetic field"

This phenomenon is known as Hall Effect. The generated voltage is known as Hall voltage. The corresponding electric field is known as Hall Electric field.

Let us consider a sample having thickness t and width b. the sample is a rectangle sample, as shown in the figure(1).



Electrons experience a force F in the down ward direction due to B

Figure (1) Hall effect

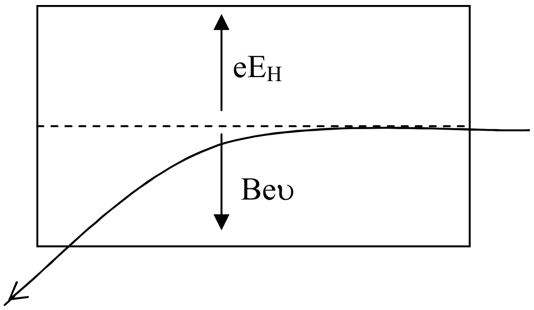


Fig (2) Motion of electrons in an n-type semiconductors

Assuming that the material is an n-type semiconductor, the current flow consists of almost due to electrons, moving from right to left.

This corresponds to the direction of conventional current from left to right as shown in figure (1).

Current I is in the positive X-direction and the magnetic field B is applied in the positive Z direction. According to Flemings, left hand Rule, The electrons experience a force, called Lorentz force. This Lorentz force acts in the negative Y-direction.

Now Lorentz force $F_L = B \times ev$ (cross product)

$F_L = Bev \sin\theta$ ----------(1)

Where v = velocity of electrons.

Since the velocity of electrons and B are perpendicular .$\theta=90^0$

$F_L=Bev$ -------------(1)a

Electrons experience a force downwards in the negative Y-direction and the positive charges drift upwards in the positive Y-direction. As a consequence, the lower surface collects negative charge and upper surface becomes positively charged. Due to this an electric field called Hall electric field will be established between upper and lower surface of the specimen.

This hall electric field E_H establishes a potential called the Hall Voltage V_H.

The hall field E_H exerts an upward force F_H on the electrons as shown in figure (2).

$\therefore F_H = eE_H$ ---------------- (2)

But total force on the electrons, is given by

$Bev + eE_H = 0$ ---------------- (3)

The above equation is called Lorentz equation. Under equilibrium conditions.

$\therefore E_H = -Bv$ ---------------------- (4)

Now the current density in the X-direction is given by

$J_x = nev$ ---------------------- (5)

Now (5) $\Rightarrow v = \frac{J_x}{ne}$ ---------------------- (6)

Here n = electron density (electron concentration)

e = charge on the electrons.

Now from (4) and (6),

$E_H = -\frac{BJ_x}{ne}$ -------------------------- (7)

Now the Hall coefficient R_H can be described as follows.

For a given semiconductor electron concentration n is constant and charge on the electron e is constant.

$\therefore E_H \alpha BJ_x$

$E_H = R_H BJ_x$ ------------------ (8)

Where R_H is a constant of proportionality.

$\therefore R_H = -\frac{1}{ne}$ ----------------------- (9)

Here E_H, B and J_x are measurable. Hence Hall coefficient R_H and carrier density ‘n’ can be found.

Determination of Hall coefficient

Let t be the thickness of the rectangular slab.
b be the width of the sample.

Now the Relation between E_H and V_H is given by

$V_H = E_H t$ ---------------------- (10)

Also (8)$\Rightarrow$ $E_H = R_H B J_x$ ---------------- (8)

Now from (8) and (10), we get

$V_H = R_H B J_x t$ ---------------------- (9)

But J_x = current density

$$J_x = \frac{I_x}{A} = \frac{current}{area}$$

$$J_x = \frac{I_x}{bt}$$

(Since A = Area of cross section
A = b t)

$\therefore$ Equation (9) becomes

$$V_H = R_H BX \frac{I_x}{b\cancel{t}}\cancel{t}$$

$$V_H = R_H \frac{I_x B}{b}$$

$\Rightarrow R_H = \dfrac{V_H b}{I_x B}$ -------------------------- (10)

V_H, b, I_x and B all are measurable and substituting them in equation (10), we can obtain the value of Hall coefficient R_H.

Note that the polarity of V_H will be opposite for n and p type semiconductors.

Carrier concentration and mobility

Hall coefficient $R_H = -\dfrac{1}{ne}$

$R_H = \dfrac{1}{ne}$ (Magnitude)

Electron concentration $n = \dfrac{1}{R_H e}$ can be determined.

Now electrical conductivity $\sigma = ne\mu$.

Where $\mu =$ mobility

Mobility $\mu = \dfrac{\sigma}{ne}$, $\mu = R_H \sigma$

For a P-type material Hall coefficient is positive.

$R_H = \frac{1}{pe}$, Where p= hole concentration. e= Charge on hole Which is +ve.

Application of the Hall Effect:

1. Useful in determining whether the given semiconductor is n-type or p-type.
2. Hall Effect can be used to find the carrier concentration and mobility of carriers.
3. Hall Effect is used to measure the magnetic field.
4. Hall Effect semi conducting devices are used as sensors to sense the magnetic fields.
5. The Hall Effect is used in magnetically activated electronic switches. They are used as non contacting key boards and panel switches.

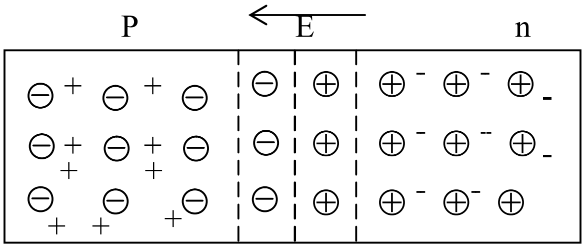
PN Junction

When a P type material is suitably joined with an N type material, a PN junction is formed. When an intrinsic semi conductors is simultaneously doped with P-type and n-type impurities, a PN junction is formed.

The PN junction may be formed by crystal growth or alloying or diffusion method.

The plane dividing the two zones is called PN Junction.

The PN junction is shown in figure (1) a



⊕ → + ve ionized Donors
⊖ → - ve ionized Acceptor
\+ → Hole
\- → Electron

Fig (1) a: a Pn junction

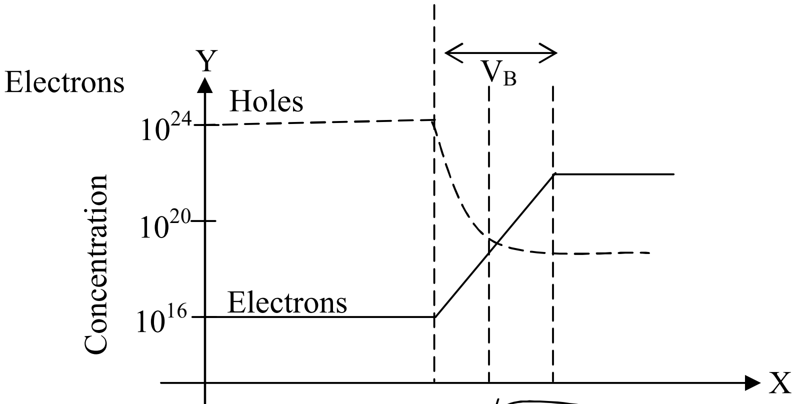


Fig (1) b: Diffraction of electrons and holes

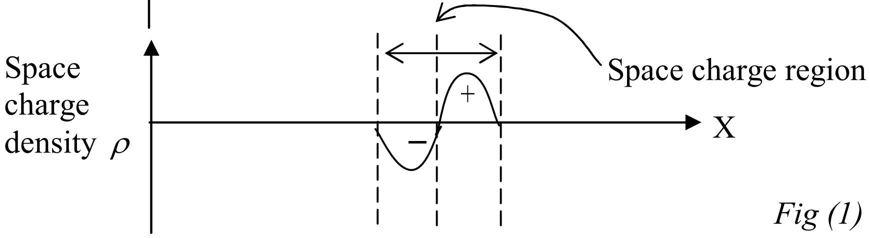


Fig (1) c: Space charge region for an alloy or abrupt junction

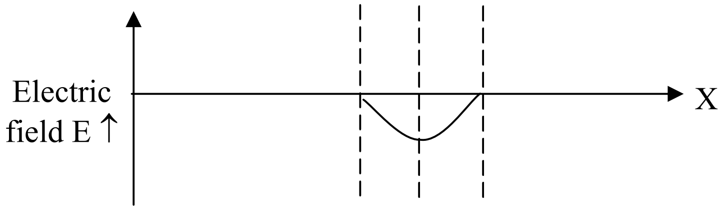


Fig (1) d: Electric field due to space charge region

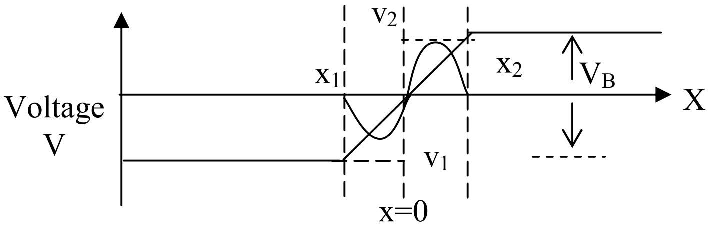


Fig (1) e: Barrier potential (or) contact potential

In the p side ‘+’ represents holes. In the n side ‘-’ represents electrons.

In the n-side there is a high concentration of electrons.

In the P- region there is a high concentration of holes.

Therefore, at the junction there is a tendency for the electrons to diffuse from n-region to p-region and holes from p-region to n-region. This process is called diffusion. When the free electrons move across the junction from n-side to p-side. The demotions become positively charged. Hence a not positive charge is built on the n-side of the junction.

The free electrons that cross the junction uncover the negative acceptor ions by combining with the holes.

Therefore a not negative charge is established on the p-side of the junction.

This not negative charge n the p-side prevents further diffusion of electrons from n-side to p-side.

Similarly the net positive charge on the n side prevents further diffusion of holes from p side to n side.

Due to this a barrier is set up near the junction.

This barrier prevents further movement of charge carriers i.e. electrons and holes. This barrier is called potential barrier.

It should be noted that outside this barrier an each side of the junction. The material is still neutral.

Only inside the barrier, there is positive charge on n side and negative charge on p-side.

This region is called depletion layer. This is so because mobile charge carriers are depleted in this region.

It is clear that a potential barrier V_O or V_B is set up.

As a consequence of this an electric field is established across the depletion layer.

The Barrier potential is about 0.3v for Germanium and 0.72V for silicon.

The depletion layer and the Barrier potential are shown in the fig (1)a and Fig (1)e.

The width of the depletion region is less than $1\,\mu m$ ($\sim 0.5\ \mu m$). Since the depletion region has immobile ions which are electrically charged it is known as space charge region. The space charge region is shown in figure (1) c. the established electric field is shown in figure (1) d.

Hence across the junction no current flows and the system is in equilibrium.

To the left of this depletion layer (in the P side), the carrier concentration is P ~ NA.

To the right of the depletion layer (in the n side), the carrier concentration is $n \sim N_D$.

Width of depletion layer

For a PN junction, the potential barrier is shown in the figure below.

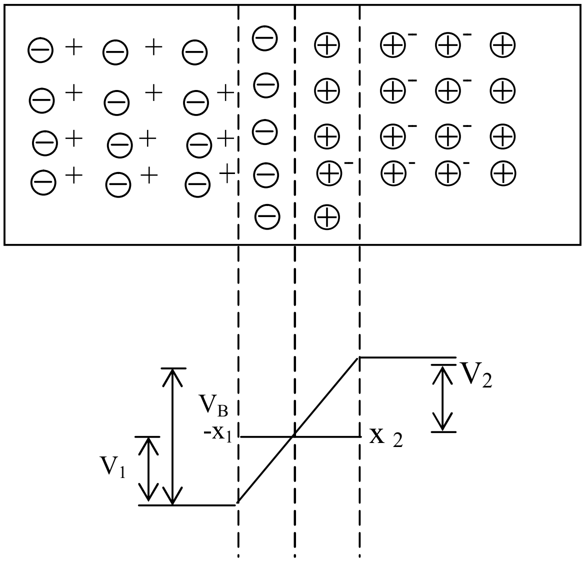


Figure (1) Potential Barrier in a Pn junction

This figure shows the space charge region in the two sides of the junction and the consequent potential variation.

Let $X_1 =$ width of the space charge region in the P side.

$X_2 =$ Width of the space charge region in the N side.

The area of the depletion layer in each region depends on the concentration of the impurities in the regions.

The effective areas of the depletion layer can be calculated using Poisson's equation.

According to Poisson's equation, the second derivative of the potential with respect to distance is proportional to the charge density.

In one dimension, the voltage varies only in the X-direction only. The length of the crystal.

Now the Poisson's equation may be written as

$$\frac{d^2V}{dx^2}\alpha - p$$

$$\frac{d^2V}{dx^2} = \frac{-p}{\in} \qquad \text{---- (1)}$$

Here V = voltage

P = volume charge density

E = Permittivity of the medium.

In the position of the depletion layers situated in the P-region near the junction the charge density may be given by

$$P = -eN_a \qquad \text{---- (2)}$$

Where N_a = Density of Acceptors Atoms.

e = charge on the electron.

Negative sign is used, since acceptors atoms are negatively ionized.

To find X_1 in the P-region, we use Poisson's equation.

i.e. from equations (1) and (2), we have

$$\frac{d^2v}{dx^2} = \frac{-p}{\in} = \frac{\in Na}{\in} \qquad \text{------ (3)}$$

On integrating the above equation, we get

$$\frac{d}{dx}\left(\frac{dv}{dx}\right) = \frac{eNa}{\in}$$

$$\Rightarrow d\left(\frac{dv}{dx}\right) = \frac{eNa}{\in}dx$$

$$\Rightarrow \int d\left(\frac{dv}{dx}\right) = \int \frac{eNa}{\in}dx + A$$

$$\Rightarrow \frac{dv}{dx} = \left[\frac{eNa}{\in}\right]x + A \qquad \text{----- (4)}$$

Again (4) $(4) \Rightarrow dv = \frac{eNa}{\in}xdx + Adx$

Integrating the above equation, again

$$\int dv = \int \frac{eNa}{\in}xdx + \int Adx + B$$

$$V = \frac{eNa}{\in}\frac{x^2}{2} + Ax + B \qquad \text{---- (5)}$$

Where A and B are the arbitrary constants. A and B can be determined by applying boundary conditions.

We assume that V = O Where X=0, so that all voltages are measured with respect to the potential at the boundary between P-type and N-type materials.

Using this boundary condition, we get

$$0 = 0 + 0 + B \Rightarrow B = 0$$

In the p-type semi conducting material, the potential is constant at the end of the depletion layer or depletion region.

Thus the depletion region may be assumed to end at a point $x = -X_1$ where $\frac{dv}{dx} = 0$

At this point the field strength is zero.

Using the condition in equation (4), we get

$$0 = \left(\frac{eNa}{\in}\right)(-x_1) + A$$

$$\therefore A = \frac{eNa}{\in}\times_1 \qquad \text{----- (6)}$$

Now substituting the values of the constants A and B in equation (5), we get

$$V = \frac{1}{2}\left(\frac{eNax^2}{\in}\right) + \frac{eNa}{\in}\times_1 x \qquad \text{----- (7)}$$

At $V = x_1$, we have $V = V_1$

$\therefore$ from (7), we have $V = V_1$

$$-V_1 = \frac{1}{2}\left(e\frac{Na \times 1^2}{\in}\right) - \left(e\frac{Na \times 1^2}{\in}\right)$$

$$\therefore -V_1 = -\frac{eNa \times 1^2}{\in}$$

$$V_1 = -\frac{eNa \times 1^2}{2\in} \qquad \text{----- (8)}$$

In the same manner the Poisson's equation may be applied for the position of the depletion layer situated in the n-region near the junction. Now the charge density in the n-region, of depletion layer is due to positively ionized donor atoms,
The charge density is given by

$$p = eN_d \qquad \text{----- (9)}$$

Now the Poisson's equation is given by

$$\frac{d^2}{dx^2} = \frac{-p}{\in_0} \qquad \text{----- (10)}$$

In equation (9), Nd = Density of Donor Atoms.
e = Charge on the electron.

From equations (9) and (10), we get

$$\frac{d^2v}{dx^2} = -\frac{eN_d}{\in} \qquad \text{----- (11)}$$

$$(11) \quad \Rightarrow \frac{d}{dx}\left(\frac{dv}{dx}\right) = -\frac{eNd}{\in}$$

$$\Rightarrow d\left(\frac{dv}{dx}\right) = -\frac{eNd}{\in}dx$$

On integrating the above equation

$$\int d\left(\frac{dv}{dx}\right) = -\int \frac{eNd}{\in}dx + c$$

$$\frac{dv}{dx} = -\frac{eN_d}{\in}x + c \qquad \text{---- (12)}$$

By integrating the equation (12), we get

$$dv = -\frac{eN_d}{\in}xdx + cdx$$

$$\int dv = -\int \frac{eN_d}{\in}xdx + \int cdx + D$$

$$V = -\frac{1}{2}\frac{eN_d x^2}{\in} + cx + D \qquad \text{---- (13)}$$

Where C and D are arbitrary constants. C and D are determined by applying the boundary conditions.

Where $x = 0$, $v = 0$

$\therefore$ from (13), We get D =0.

In the n-region, the potential in constant at $X = X_2$.

$\therefore$ At $X = X_2, \frac{dv}{dx} = 0$

$\therefore$ from equation (12), we get c = $\frac{eN_d X_2}{\in}$ ----- (14)

Thus $V = -\frac{1}{2}\frac{eN_d x^2}{\in} + \frac{eNd}{\in} xX_2$ ----- (15)

At $x = X_2, V = V_2$, now we get

$$V_2 = -\frac{1}{2}\left(\frac{eNd \times x_2^2}{\in}\right) + \left(\frac{eNd}{\in}\right) X_2^2$$

$$V_2 = \frac{eNd \times x_2^2}{\in} \qquad \text{----- (16)}$$

This V_2 is the potential at $x = X_2$. At $x = X_2$ the depletion layer in the n-region will ends.

Now the potential barrier at the junction is given by

$$V_B = V_2 - (V_1)$$

$$V_B = V_2 + V_1$$

$$V_B = \left(\frac{eN_d X_2^2}{\in}\right)\frac{1}{2} + \left(\frac{eN_d X_2^2}{\in}\right)\frac{1}{2}$$

$$V_B = \frac{e}{2\in}\left(NaX_1^2 + NdX_2^2\right) \qquad \text{---- (17)}$$

The equation of charge neutrality is given by

$$eN_a X_1 = eN_d X_2$$

$$X_2 = \frac{N_a X_1}{N_d} \qquad \text{---- (18)}$$

Now substituting the value of X_2 in equation (17)

$$V_B = \frac{e}{2\in}\left[\frac{N_d N_a^2 X_1^2}{Nd^2} + N_a X_1^2\right]$$

$$V_B = \frac{e}{2\in}\left[\frac{N_{a^2} X_{1^2}}{N_{d^2}} + N_a X_{1^2}\right]$$

$$X_{1^2} = \frac{2\in V_B}{eN_a\left(1 + \frac{N_a}{N_d}\right)}$$

$$X_1 = \left[\frac{2\in V_B}{eN_a\left(1 + \frac{N_a}{N_d}\right)}\right]^{1/2} \qquad \text{---- (19)}$$

From equation (18) and (19), we get

$$X_2 = \frac{N_a}{N_d}\left[\frac{2 \in V_B}{eN_a\left(1+\frac{N_a}{N_d}\right)}\right]^{1/2}$$

$$X_2 = \left[\frac{2 \in V_B}{e\frac{N_{d^2}}{N_{a^2}}N_a\left(1+\frac{N_a}{N_d}\right)}\right]^{1/2}$$

$$X_2 = \left[\frac{2 \in V_B}{e\frac{N_{d^2}}{N_a}\left(1+\frac{N_a}{N_d}\right)}\right]^{1/2}$$

$$X_2 = \left[\frac{2 \in V_B}{eN_d\left(1+\frac{N_a}{N_d}\right)}\right]^{1/2} \qquad \text{---- (20)}$$

Now the total width of the depletion layer is given by

$$X = X_1 + X_2$$

$$\therefore X = \left[\frac{2 \in V_B}{eN_a\left(1+\frac{N_a}{N_d}\right)}\right]^{1/2} + \left[\frac{2 \in V_B}{eN_d\left(1+\frac{N_d}{N_a}\right)}\right]^{1/2}$$

$$X = \left[\frac{2 \in V_B}{e\frac{N_a}{N_d}\left(N_a+N_d\right)}\right]^{1/2} + \left[\left(\frac{N_d}{N_a}\right)^{1/2} + \left(\frac{N_a}{N_d}\right)\right]^{1/2}$$

$$X = \left[\frac{2 \in V_B}{e\left(N_a+N_d\right)}\right]^{1/2} + \left[\frac{N_d+N_a}{\left(N_aN_d\right)^{1/2}}\right]$$

$$X = \left[\frac{2 \in V_B\left(N_a+N_d\right)}{eN_aN_d}\right]^{1/2} \qquad \text{---- (21)}$$

Diode Current Equations

The diode current pertaining to VI characteristics is given by

$$I = I_0\left[e^{\left(\frac{V}{\eta V_T}\right)} - 1\right]$$

Where I = Diode current

I_0 = Diode reverse saturation current at room temperature.

V = External voltage applied to the diode.

η = A constant

η=1 for Germanium

η=2 for Silicon

V_T = Volt equivalent temperature or thermal voltage.

$$V_T = \frac{K_B T}{q}$$

$K_B =$ Boltzmann constant

$K_B = 1.3806 \times 10^{-23} JK^{-1}$

q = Charge on the electron

q = 1.602×10^{-9} coulomb

T = Temperature of the junction in ^0K.

When the diode is reverse biased, the current equation is given by

$$I = I_0\left[e^{-\left(\frac{v}{\eta V_T}\right)} - 1\right]$$

Light Emitting Diode (LED)

Light Emitting diode (LED) is a PNjunction diode that emits light when forward biased.

The light is emitted by the forward biased junction by a phenomenon called Electroluminescence.

The materials that are used for fabricating LED are Galliumphosphide (GaP), Gallium Arsenide Phosphide (GaAsP) and Gallum Arsenide.

Usually direct B and Gap semiconductors are used for the fabrication of LEDs.

When an LED is forward biased, carrier recombination takes place i.e. electrons from the n-side cross the junction and recombine with the holes on the p-side.

In silicon and Germanium semiconducting P_n junctions greater percentage of energy is given out in the form of heat and the emitted light is not visible.

A forward biased LED and its symbol are shown in the figure (1)

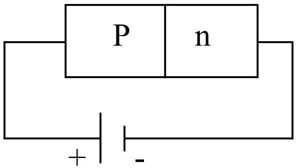


Fig (1) a: Forward biased LED

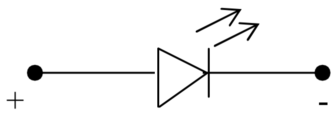
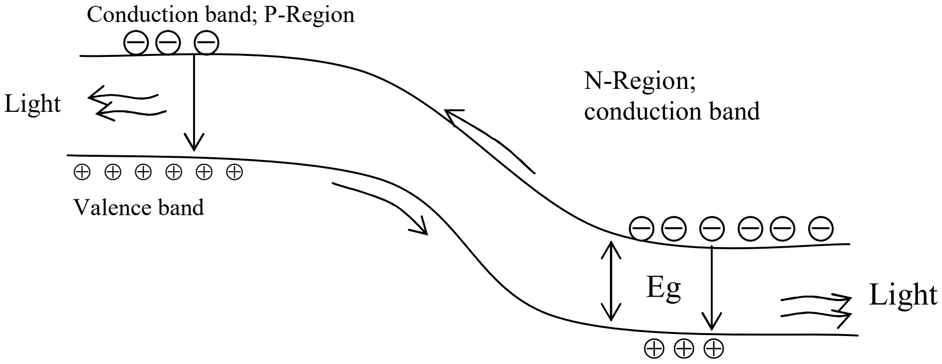


Fig (1) b: Symbol of LED

When an LED is forward biased, the electrons and holes move towards the junction and recombination takes place. As a result of recombination, the electrons present in the conduction band side of n-region fall into the holes present in the valence band side of P-region. When recombination takes place, energy emitted out in the form of light.
The emitted light will have energy equal to the energy difference between conduction band and the valence band. For every recombination light energy is emitted.
The excess energy in the process of recombination is given to the emitted photons.
The light emitted is directly proportional to the forward bias current in the LED.
The energy band diagram for the LED is shown in the figure (2)



Figure(2) Energy Band diagram of an LED

The basic structure of a LED is shown in the figure (3). Here an n-type layer is grown on a substrate and a p-type is deposited on it by diffusion.

Since carrier recombination takes place in the p-region, it is kept uppermost.

Metal contacts are made on the p-layer act like anodes.

Current is allowed through these anodes. A thin metal (gold) film at the bottom will act as a cathode. This also provides the reflection of light by the thin metal layer back into the medium.

LEDs are usually encased to protect their delicate metal contact wire.

The emission of light and its efficiency can be increased by increasing the junction current (injected current) LEDs are used to radiate different colors of light. The wavelength of light emitted depends on the energy gap of material.

The following table shows the colors emitted by different materials.

Material	Colors	Wavelength
GaAS	IR	9000
Gap	Green	5600
GaAsp	Yellow	5900

Usually a protective resistor of 1 k a or 1.5 ka is connected in series with the LED in a circuit. LEDs operate as a forward bias voltage of 1.5 volt to 3.3 V. Usually the current is in mill amperes.

The power requirement is 10 mw – 150 mw.

The switching time is around 1ms.

The wavelength of emmited light is given by

$$\lambda = \frac{hc}{Eg}$$

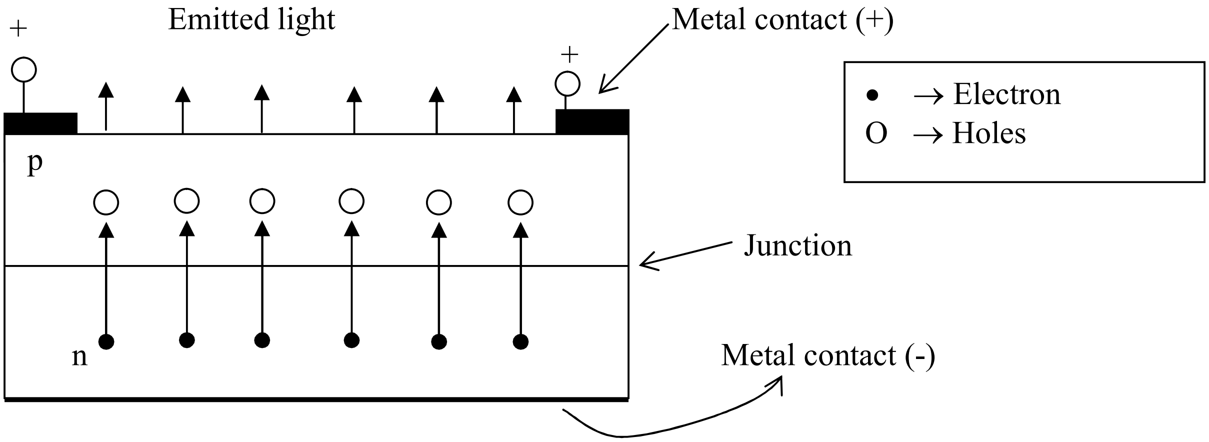


Figure (3) Structure and Recombination of electrons and holes in a LED.

Applications of LED

LEDs are used in

1. Intercoms
2. Digital clocks
3. Digital display systems
4. Instrument display systems

5. Power on/off indicating
6. Optical switching applications
7. Optical communication for energy coupling circuits
8. Opto isolation circuits
9. Solid state video-display system
10. used in computers
11. Calculators
12. Electronic panels

Photo diode

A Silicon photodiode is a light Sensitive Device. A photo diode is also known as photo detectors.

A photo diode converts light signals (optical signals) into electrical signals.

A photo diode must be always reverse biased. The reversed biased photodiode and its symbol are shown in figure (1)

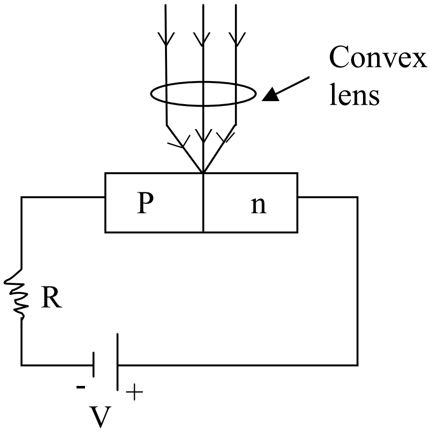


Figure (1) a: Photo diode and reverse bias

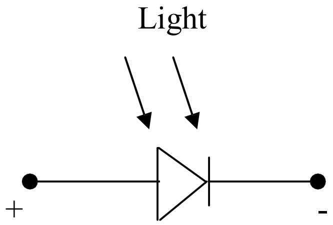


Figure (1)b: photo diode symbol

The photodiode is made of semiconductor PN junction kept in a sealed plastic or glass casing.

The casing is designed in such a manner that the light rays are allowed to fall on one surface across the junction.

The remaining sides of the casing are painted to restrict the penetration of light rays.

A convex lens permits the light rays to fall on the junction. When light falls on the reverse biased PN junction photodiode, electron – hole pairs are generated.

The movement of these electron hole pairs in a properly reverse biased circuit results in a current.

The energy band diagram of a photodiode is shown in figure (2)

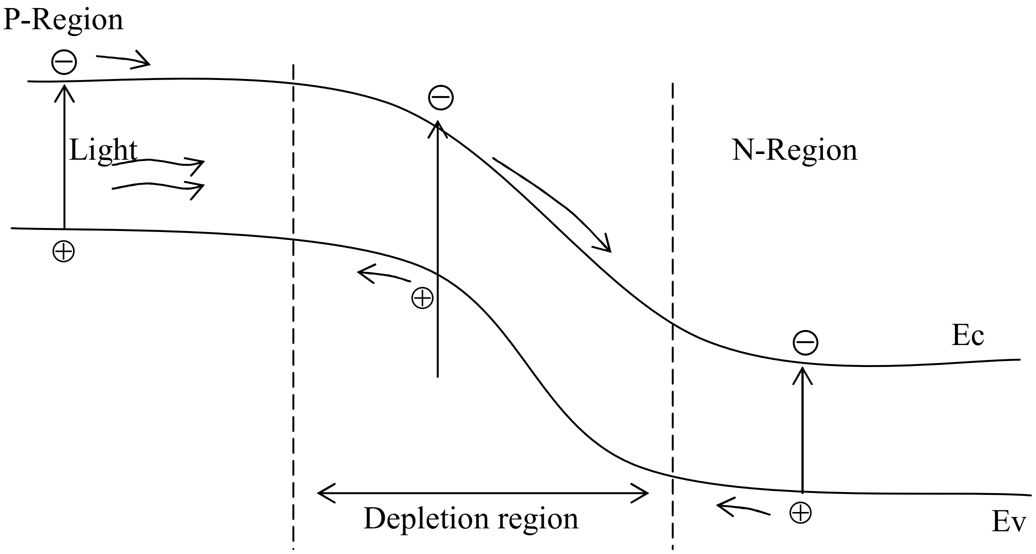


Figure (2) Energy band diagram of a photodiode

When reverse bias is applied, the depletion layer is widened, the junction capacitance reduced. Here in this situation the junction will not conduct current. However the reverse biased junction can conduct current when free carriers are generated in the junction by radiation of sufficient energy.

The magnitude of the photo current depends on the number of charge carriers generated and also on the illumination and the diode.

The photocurrent also depends upon the frequency of light falling on the photodiode.

The magnitude of the current with large reverse bias is given by

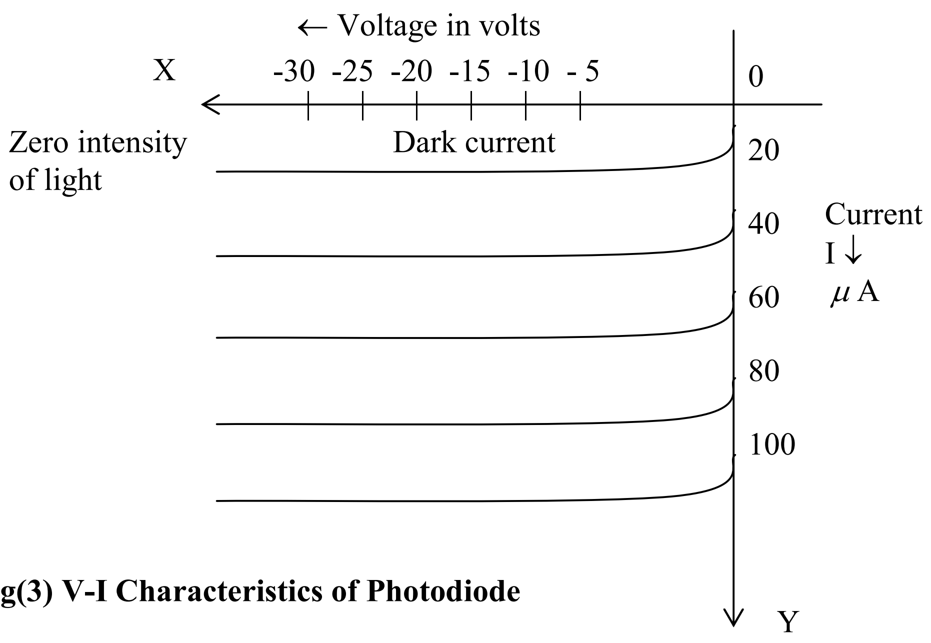
$$I = I_S + I_0\left(1 - e^{\frac{v}{\eta VT}}\right)$$

Where I_0 = Reverse saturation current
I_s = Short circuit current which is proportional to the intensity of light.
V = Voltage across the diode.
V_T = volt equivalent of temperature.
η = A constant
For Ge, η=1
Si, η=2

The volt ampere characteristics of a photodiode are shown in the figure (3).

The reverse current increases with increase in illumination. Even if there is no light is falling on the photodiode, there is a minimum leakage current called dark current, flowing through the device.

Germanium has a higher dark current than silicon, but it also has a higher level of reverse current.



Fig(3) V-I Characteristics of Photodiode

Applications of photodiode

1. Photodiodes are used as light detectors, demodulators and encoders.
2. They are used in optical Communication systems.
3. They are used in high speed counting circuits.
4. They are used in high speed switching circuits.
5. They are used in high operated switches.
6. They are used in computer card punching and tapes.
7. They are used in electronic control circuits.
8. They are used in retrieving of sound from sound track film.

Liquid Crystal Display (LCD)

Liquid crystal displays came under passive types of display since no light generation is required.

There are two types of LCD’s namely.

- i) Reflective type, requiring illumination on the front side.
- ii) Transmittive type requires illumination on the rear side.

The liquid crystal state is a phase of matter exhibited by a large number of organic molecules of organic material over a restricted temperature range.

The material becomes a crystalline solid at the lower temperature range while it changes into a liquid at the upper temperature range.

In the liquid state, molecules will have the shape of rod. In any small volume of liquid crystal state the orientation of the molecules is described in terms of a unit vector called Directors**.**

They are basically two liquid crystal materials commonly used as LCD’s.

They are Nematic and Cholestric

The arrangement of molecules is shown in the figure (1) and figure (2) for Nematic and Cholesteric type of LCD’s.

The properly used liquid crystal structure (NLC). In Nematic type the molecules are aligned parallel to each other as shown in figure (1). But these molecules are free to move relative to each other. Hence they represent a liquid phase. Here the molecules will have complete translational motion.

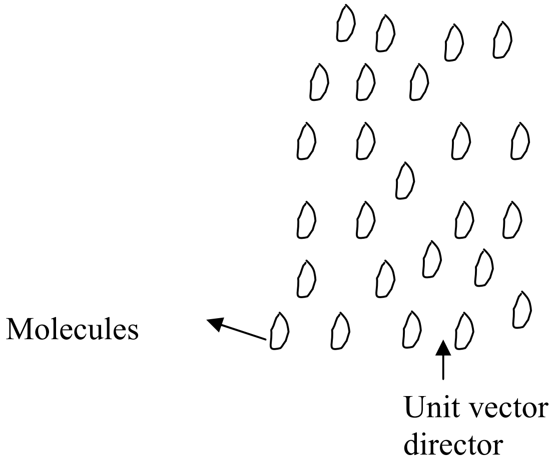


Figure (1) : Arrangement of Molecules in a Nematic liquid crystal

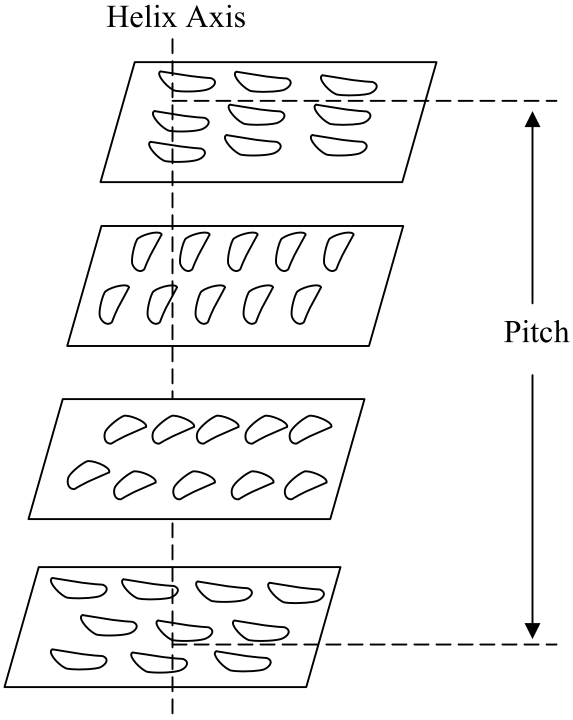


Figure (2) Arrangement of molecules in a cholesteric liquid crystal

The liquid is completely transparent. When the liquid is subjected to a strong electric field, the well ordered liquid crystal structure is disturbed.

This makes the liquid to polarize and turns opaque. When the electric field is removed, the liquid crystal regains its original structure and form.

Here the material becomes transparent.

In the cholesteric phrase the molecules are arranged in a large number of planes.

In each plane all the molecules are arranged in the direction of director as shown in figure (2).

The director directions thus display a helical twist through the material.

The distance between planes having the same director's direction is called the Pitch P.

Depending on the construction LCDs are classified into two types.

Dynamic scattering type

The dynamic scattering type liquid crystal cell is shown in the figure (3).

This consists of two thin glass plates, each coated with tin oxide on the inner side. This is transparent and act as electrodes.

These two glass plates are separated by a liquid crystal layer of 5-50 μm thick.

The front glass sheet is etched to produce a single or multi segment pattern of characters.

When a week electric field is applied to a liquid crystal, the molecules align in the direction of the field.

When the voltage exceeds a certain threshold value, the liquid crystal structure entirely distributed and the appearance changes.

As the voltage further increases, the flow becomes turbulent and the material turns optically inhomogeneous.

In this disordered state, the liquid crystal scatters light.

Thus when there is not external electric field applied, the liquid crystal is transparent.

When electric field is applied, the disturbance causes scattering of incident light in all directions. Here the cell appears bright.

Field effect type

The field effect type of liquid crystal is similar to Dynamic type. This is also known as twisted nematic field effect display.

Its construction is same as dynamic type. But it is sand witched between two pieces of polarized.

The polarized directions of the two polaroids are perpendicular to each other.

1st polarized is called polarizes and the 2nd one is called Analyses.

The 1st polarizes is infront of the LCD cell and the 2nd one is at its back. Both of these are arranged perpendicular to each other. Beyond Polaroid 2 a reflector is placed in reflective mode.

When a beam of polarized light passes through the polarizes, plane polarized light rotates though 90^0 as transverses the cell.

When no electric field is applied, it passes through the analyses and then reflects back at the mirrors and light retraces the path.

Thus when no field is applied the device reflects light and appears bright.

When a field is applied, the direction of polarization of light traversing the cell is not rotated. Hence it is stopped by the second polarizes (Analyses).

No, light is reflected from the device and hence it appears dark. This means that in the absence of the field he incident light is reflected while it is blocked when the field is applied.

Advantages

1. Liquid crystals consume small amount of energy.
2. Hence the voltages required are loss.
3. Because low power consumption, a Seven segment display requires about 140w (20w per segment), whereas LEDs require 40mw per numerical.
4. They are economical and cheap.
5. In a seven segment display, the current drawn in 25µA for dynamic scattering cells and 300µA for field effect type cells.
6. LCDs require AC voltage supply.
7. They are economical and cheap.
8. They are used as temperature, measuring sensor.
9. Since thin layers are used, they are must suitable for display devices.

Disadvantages

1. Angle of viewing is limited.
2. External light must be used.

3. LCDs are slow devices. The ON and OFF times are quite large. ON time is a few ms. and off time is 10 ms.
4. When used with DC, there life time is less. Hence they are used with AC supply only.

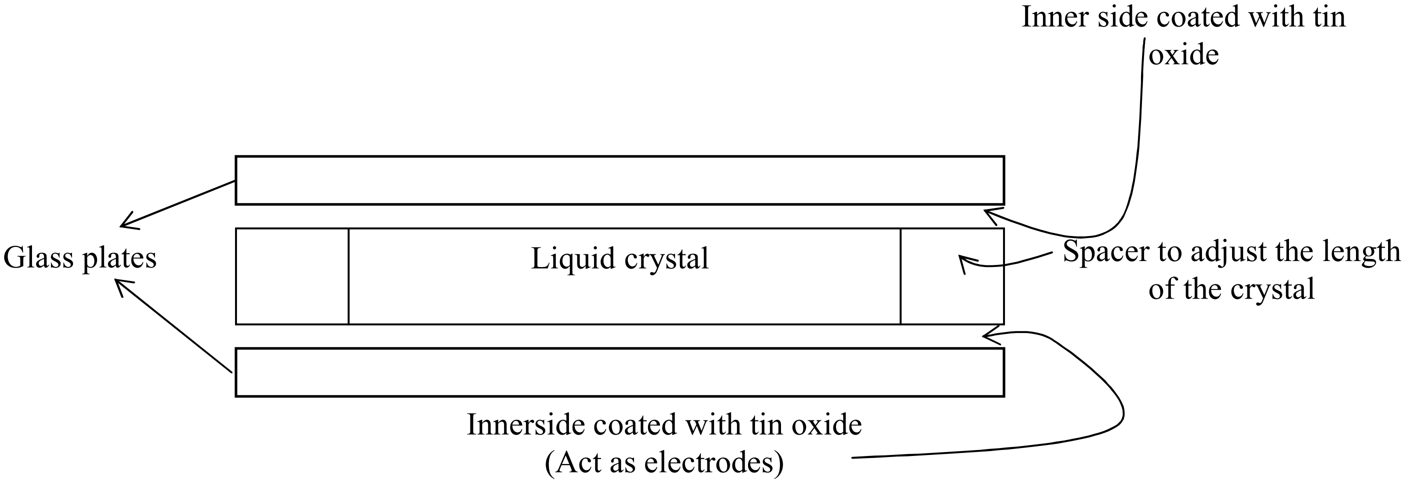


Figure (3) Construction of dynamic scattering LCD.

Drift current:

In a perfect crystal the periodic electric field enables electrons and holes to move freely as if in vacuum.

When there is no electric field, there is no net current. This is because charge movement in any direction is balanced by charge movement in the other direction. In the presence of the electric field field, the carriers experience directed movement. This is called drift.

Definition Of drift: **Forcible movement of Charge carriers under the influence of an Electric field is called drift**.

With the field carriers drift and this results in current flow through the semiconductor.

Movement of charge carries under the influence of an applied electric field is called drift.

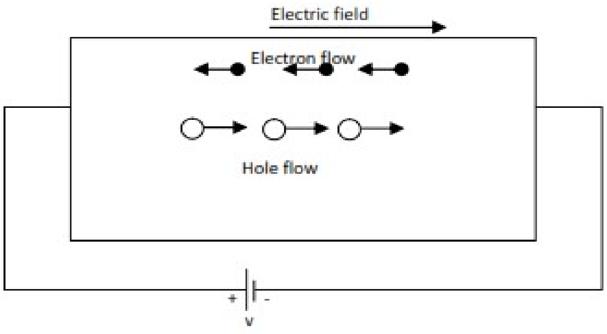


Fig. 1. Drift in semiconductor

The current density is given by

$J = neV_d$ --------------- (1)

Here $V_d =$ drift velocity.

Also $V_d \alpha E \Rightarrow V_d = \mu E$ ------------- (2)

Where μ is called the mobility of the carriers. E= Electric field.

From equations (1) and (2),

Now current density $J = nev_d$ ----------- (3)

$J = ne\mu E$ ---------------(4)

In semi conductors, the current flow is due to electrons and holes.

Electron current density is given by

$J_n\left(drift\right) = ne\mu_n E$ ------------- (5)

Hole current density is given by

$J_p\left(drift\right) = pe\mu_p E$ ----------- (6)

The two charge carriers move in the opposite direction.

Now the total drift current density is given by

$J(drift) = J_n(drift) + J_p(drift)$

$J(drift) = ne\mu_n E + pe\mu_p E$

$J(drift) = E(ne\mu_n + pe\mu_p)$ -------- (7)

For intrinsic semiconductors $n = p = n_i$

$J(drift) = En_i(e\mu_n + e\mu_p)$

$J(drift) = n_i Ee(\mu_n + \mu_p)$ ------------- (8)

Equation(8) gives current density equation.

Diffusion current :

Usually directed movement of charge carriers will give rise to electric current.

The movement of charge carriers may be due to either drift or diffusion.

Usually non-uniform concentration of carriers gives rise to diffusion.

Definition: **Movement of charge carriers from high concentration region to low Concentration region in a semiconductor is known as diffusion.**

Let us suppose that the concentration of electrons varies with distance x in the semi conductors. Here the concentration gradient is given by $\frac{\partial n}{\partial x}$.

Ficks law states that the rate at which carriers diffuse is proportional to the density gradient and the movement is in the direction of negative gradient.

Mathematically, the rate of flow of electrons can be written as

$f_n \alpha -\frac{\partial n}{\partial x}$ ------------(1) Here f_n = rate of flow of electrons across unit area.

The rate of flow of electrons is given by

$f_n = -D_n \frac{\partial n}{\partial x}$ ----------- (2)

Here D_n = Diffusion coefficient for electrons.

Partial derivatives are used because n is a function of temperature and distance.

This flow of electrons constitutes an electron diffusion current density. Since conventional current is the rate of negative charge, we have

$J_n\left(diffusion\right) = -\left(e\right)\left(\text{Rate of flow of electrons across unit area}\right)$

$J_n\left(diffusion\right) = \left(-e\right)(-D_n \frac{\partial n}{\partial x})$

$J_n\left(diffusion\right) = eD_n \frac{\partial n}{\partial x}$ ----------- (3)

If an excess hole concentration is created in the same region, hole diffusion takes place in the same direction at a rate per unit area.

The rate of flow of holes per unit area is given by

$f_p = -D_p \frac{\partial p}{\partial x}$ ------------- (4)

This results in a hole diffusion current density .

Now $J_p\left(diffusion\right) = +e\left(\text{rate of flow of holes across unit area}\right)$

$J_p\left(diffusion\right) = -e\,D_p \frac{\partial p}{\partial x} ------ (5)$

Here $D_p =$ Hole diffusion coefficient for holes.

Einstein Relations *or* **Einstein Equations**

At equilibrium with no field, the free electron distribution is uniform and there is no net current flow. Any tendency to disturb the state of equilibrium which would lead to diffusion current creates an internal electric field.

This internal electric field creates a drift current balancing the diffusion current component.

Under equilibrium conditions, we have therefore the drift and diffusion currents.

These currents are due to an excess density of electrons.

Now $J_n\left(\text{drift}\right) = n\mu eE$ ----------------------- (1)

$J_n\left(\text{diff}\right) = eD_n \frac{\partial n}{\partial x}$ --------------- (2)

Under equilibrium conditions, $J_n(drift) = J_n(diff)$

$$\therefore n\mu_n eE = eD_n \frac{\partial n}{\partial x} ------(3)$$

The force F on excess carriers restoring equilibrium is given by the product of excess charge and Electric field.

$$F = (ne)E \qquad \text{--------------- (4)}$$

$$(3) \Rightarrow n = \frac{D_n \frac{\partial n}{\partial x}}{\mu_n E} \qquad \text{----------- (5)}$$

Now from (4) and (5),we get

$$\therefore F = e\frac{D_n}{\mu_n}\frac{E}{E}\frac{\partial n}{\partial x}$$

$$F = \frac{e\,D_n}{\mu_n}\frac{\partial n}{\partial x} \qquad \text{------------- (6)}$$

This force F depends on the thermal energy of the excess carriers.

By making an analogy between the excess carriers in a semiconductors and gas molecules in a low pressure gas, the force F corresponds to pressure gradient.

Pressure gradient = $K_B T \frac{\partial n}{\partial x}$

$$\therefore K_B T\frac{\partial n}{\partial x} = \frac{eD_n}{\mu_n}\frac{\partial n}{\partial x} \Rightarrow K_B T = \frac{e D_n}{\mu_n}$$

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

$$D_n = \frac{K_B T}{e}\mu_n \qquad \text{--------------- (7)}$$

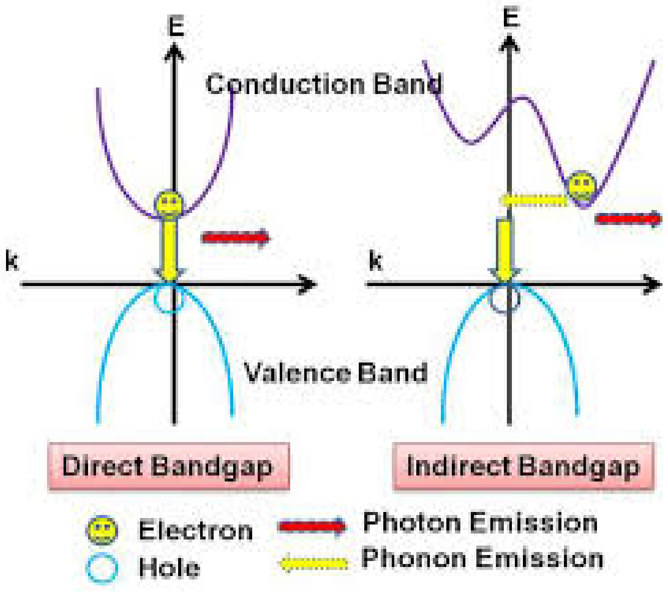
Similarly for holes $D_p = \frac{K_B T}{e}\mu_p$ ---------------- (8)

$$\frac{7}{8} \Rightarrow \frac{D_n}{D_p} = \frac{\mu_n}{\mu_p} \qquad \text{------------ (9)}$$

Equations (7), (8) and (9) are called Einstein’s Relations.

Direct Bad Gap and Indirect Band Gap Semiconductor.

Direct Band Gap Semiconductors	**IndirectBandGapSemiconductors**
1.Emperical formula $GaAs_{1-x}P_x$ Where x is molar concentration. If $x \le 0.45$, then semiconductor is called **Direct Band Gap Semiconductor.** **2.** Transition of electrons from conduction band to valence band takes place directly. 3. Intra band Transition occurs with high probability. 4. Radiative recombination mechanism is dominant. 5. Momentum of Charge carries is conserved. 6. Life time of emitted photons is large. 7. Life time Charge carriers is less. 8. Natural or Artificially occurring. materials. Like InP, Ga, GaAs, CdS. 9. Used in LEDs and Semiconductor Laser diodes.	**1.Emperical formula** $GaAs_{1-x}P_x$ Where x is molar concentration.. If $x > 0.45$,then semiconductor is called **Indirect Band Gap Semiconductor.** **2.** Transition of electrons from conduction band to valence band takes place indirectly. 3. Intra band Transition occurs with low probability. 4. Recombination centers are present in the form of impurities to enhance radiative process. 5. Momentum of Charge carries is not conserved. 6. Life time of emitted photons is less. 7. Life time Charge carriers is large. 8. Artificially or naturally occurring materials. Like Gap, PbS, PbTe, Si, Ge. 9.Used in LEDs



Zener Diode:

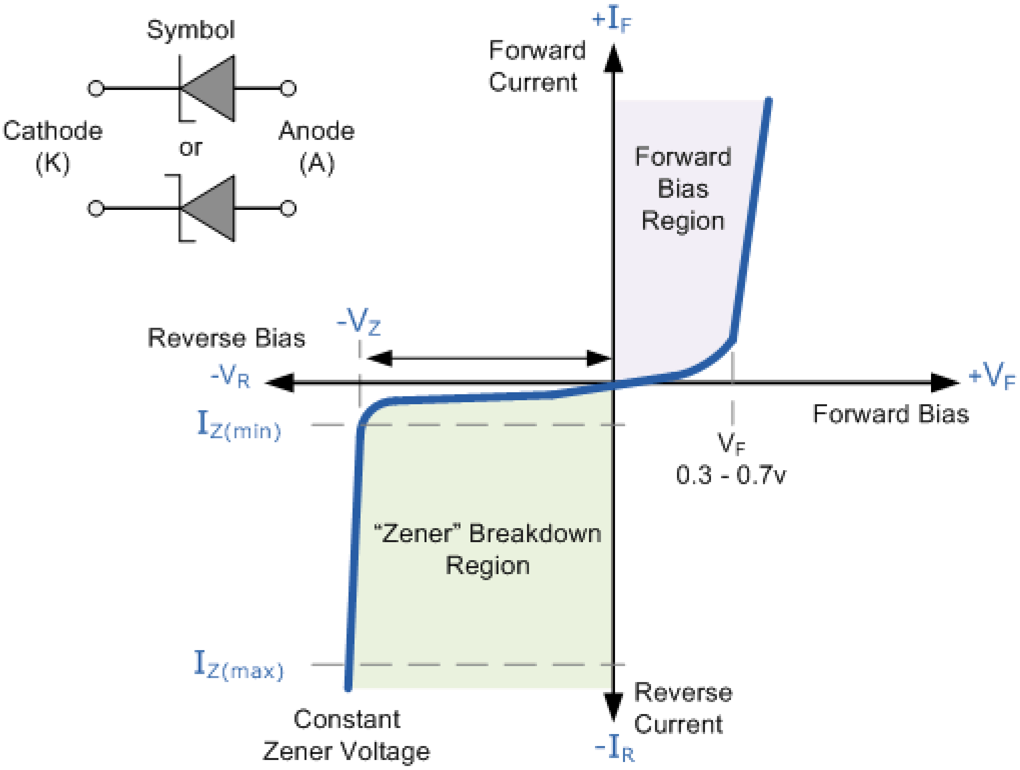


Fig (1) Zener Diode symbol and V-I Characteristics

Zener diode is similar to ordinary PN junction Diode.

The PN junction is moderately doped.

Zener diode is having a sharp breakdown voltage.

A Zener diode must be always connected in reverse bias.

Zener Diode Symbol and V-I Characteristics are shown in figure (1).

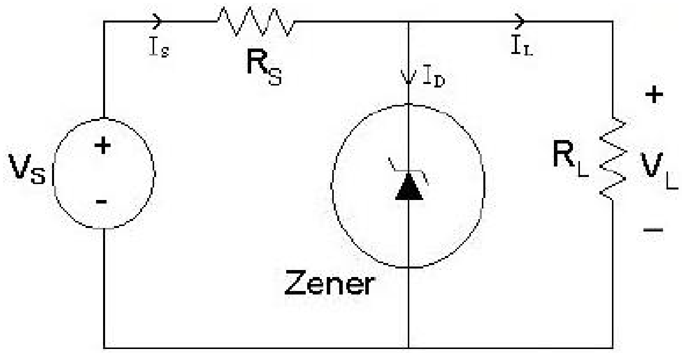
In forward bias, current increases slowly. At voltage called forward voltage (V_f) or Knee voltage (V_{knee}) current increase sharply.

In reverse bias originally current is very less. But with increase in reverse voltage , at a voltage called zener breakage voltage (V_Z) current increases abnormally.This breakdown voltage is negative.

Zener Diode Voltage Regulator:

A voltage regulator circuit with Zener diode is shown in figure(2).

Figure (2) Zener diode -voltage Regulator.



In fig (2), V_S= Variable voltage source.
I_S =Source current.
R_S = source Resistance.
R_L= Load resistance.
V_L =Load voltage.

With increase in source voltage, at a voltage called Zener breakdown voltage, voltage across the Zener diode remains constant.

This constant voltage appears across the diode and hence the same appears across the load.