

Quantum Physics :- It is the study of matter and energy at the most fundamental level.

Example :- laser, electron microscope, magnetic resonance imaging (MRI) devices.

Dual Nature of Light :- It describes that light has dual nature. It behaves as both particle i.e., corpuscular nature (energy particle of plank) and wave nature (i.e., electromagnetic waves)

Photons :- Light is composed of discrete packets of energy called quanta or photons. Each photon carry an energy $E = h\nu$ and momentum $p = \frac{h}{\lambda}$ which depends on the frequency of incident radiation not on the intensity.

De-Broglie Hypothesis :- Since radiation have dual nature & the universe compose of radiation & matter. \therefore De-Broglie concluded that moving particle must possess dual nature.

Acc to him moving particle must act as wave and sometimes as particle.

Wave associated with moving particle is De-Broglie wave, whose wavelength is

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

$$E^2 = p^2 c^2 + m_0^2 c^4$$

\therefore Rest mass, $m_0 = 0$

$$E^2 = p^2 c^2$$

$$E = pc \Rightarrow p = \frac{E}{c} = \frac{h\nu}{c} = \frac{hc}{c\lambda} = \frac{h}{\lambda}$$

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

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

where, $p = mc$ = momentum of photon

Acc. to De Broglie, above equation must also be true for material like electrons, photons, neutrons etc. Hence, a particle of mass m moving with ' v ' velocity must associate with wave of wavelength

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

Compton Effect:- It is defined as the effect that is observed when x-rays or gamma rays are scattered on a material with increase in wavelength.

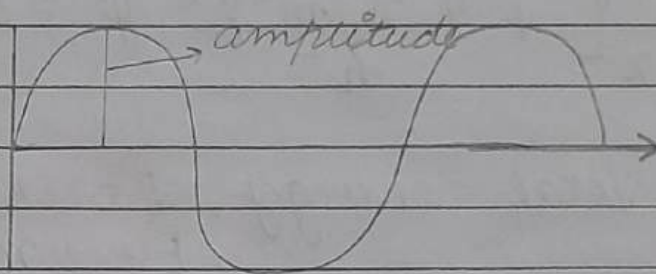
During study Compton discovered that wavelength is not dependent on intensity of incident radiation.

Schrodinger wave equation:-

It is the linear partial differential equation that governs the wave function of a quantum mechanical process system. It is a key result in quantum mechanism and its discovery was a significant landmark in the development of the subject.

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{8\pi^2 m (E - V)}{h^2} \Psi = 0$$

- $m =$ mass of e^-
- $E =$ Total energy
- $V =$ Potential energy
- $\Psi =$ wave function



For a particle whose energy doesn't vary with time Schrodinger wave equation can be written as

$$\hat{H} \Psi = E \Psi \quad \text{--- (1)}$$

$$\hat{H} = \hat{T} + \hat{V}$$

put in eq- (1)

$$(\hat{T} + \hat{V}) \Psi = E \Psi$$

Let us consider wave eq in X axis

$$\Psi = A \sin 2\pi \frac{x}{\lambda} \quad \text{--- (2)}$$

differentiate w.r.t x

$$\frac{\partial \Psi}{\partial x} = A \left(\frac{2\pi}{\lambda} \right) \cos \frac{2\pi x}{\lambda}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -A \left(\frac{2\pi}{\lambda} \right)^2 \sin \frac{2\pi x}{\lambda} \quad \text{--- (3)}$$

put value of Ψ from (2)

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{4\pi^2}{\lambda^2} \psi \quad \text{--- (4)}$$

From, De-Broglie equation,
 $\lambda = \frac{h}{mv}$

put the value of λ in eq (4)

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{-4\pi^2}{\left(\frac{h}{mv}\right)^2} \psi = \frac{-4\pi^2 m^2 v^2}{h^2} \psi$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2 m^2 v^2}{h^2} \psi = 0 \quad \text{--- (5)}$$

As Total energy, $E = KE + PE$
 $E = \frac{1}{2} mv^2 + V$

$$2 \left(\frac{E - V}{m} \right) = v^2$$

$$v^2 = \frac{2(E - V)}{m}$$

put in eq - (5)

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

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

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

Relationship b/w group & phase velocity.

wave packets \rightarrow group of waves
(group velocity, phase velocity)

Phase Velocity :-

As, $E = h\nu$ $\nu = \frac{E}{h}$

$$E = mc^2$$

$$\nu = \frac{mc^2}{h}$$

$$V_p = \nu \lambda = \frac{mc^2}{h} \times \frac{h}{mv}$$

$V_p = \frac{c^2}{v}$

phase velocity

As, we know that

$E = h\nu$ $E = mc^2$ $\nu = \frac{E}{h}$

$$\nu = \frac{mc^2}{h}$$

$$V_p = \nu \lambda = \frac{mc^2}{h} \times \frac{h}{mv}$$

$V_p = \frac{c^2}{V_g}$

$\therefore V_p \times V_g = c^2$

Free Electron Theory

The classical free electron theory was proposed by Drude and Lorentz. Acc. to this theory the e^- are moving freely and randomly moving in entire volume of metal like gas atoms in the gas container. When an electric field is applied the free e^- gets accelerated.

Classical free electron theory :-

- (a) The valence electrons are considered to be free e^- in metal. These electrons are not bound to any atoms and move freely through volume of metal.
- (b) The valence e^- of atoms are responsible for the conduction of electricity by metal and for this reason these e^- are called conduction electrons.
- (c) The conduction e^- move about inside the metal without any collision or thermal agitation much like molecules of ideal gas. The assembly of e^- in metal is called electron gas.
- (d) The forces b/w conduction e^- and other 'core' e^- are neglected just like the molecules of perfect gas.

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(e) The free e^- move randomly in all possible direction with different velocity. The distribution of velocities is in accordance with Maxwell-Boltzmann distribution for a gas.

(f) The average kinetic energy of e^- is $\frac{3}{2}kT$ where k is Boltzmann constant and T is absolute temperature.

(g) The absence of external electric field there is no net motion of e^- thus net current density is zero.

(h) The average distance travelled by a free e^- b/w 2 successive collision with positive ion is known as mean free path and represented by λ .

However, free e^- gas in metal differ from ordinary gas in some respect;

(i) The free e^- gas is charged while the ordinary gas molecules are mostly neutral.

(ii) The concentration of e^- in metal is large than ordinary gas.

Success:—

- * Electrical conductivity
- * Ohm's law
- * Thermal Conductivity
- * Wiedemann-Franz law

* Complete opacity of metal and their high luster.

Drawback :-

- * It fails to explain electric specific heat and the specific heat capacity of metal.
- * It fails to explain superconducting properties of metal.
- * It fails to explain new phenomena like photo-electric effect, Compton effect, Black body radiation etc.

Quantum free e^- theory :-

Acc. to this theory, the free e^- occupy different energy level, up to Fermi level at 0K, So, they possess different energies and hence they possess different velocities.

Density of states :- The density of state gives the no. of allowed e^- for whole state per unit volume at a given energy.

$$D E = \frac{2 \cdot dn}{dE_n}$$

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

diff. both sides

$$dE_n = \frac{h^2}{2m} \left(\frac{\pi}{L} \right)^2 2n \cdot dn$$

$$D(E) = 2 \frac{dn}{dE_n} = 2 \frac{2m}{h^2} \left(\frac{L}{\pi}\right)^2 \frac{1}{2n}$$

Energy Band Diagram

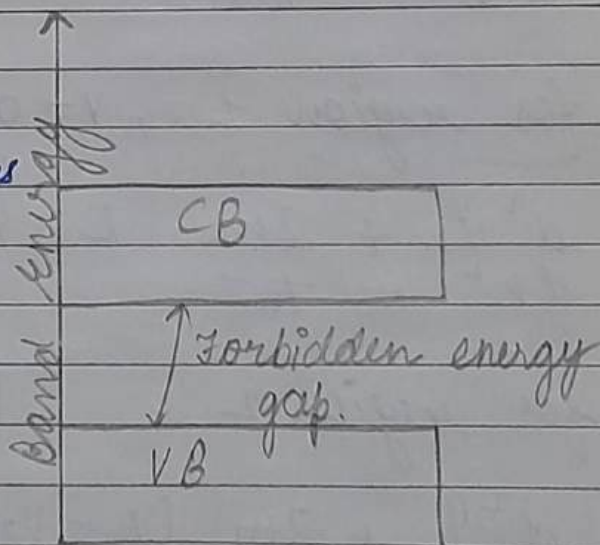
Range of energies possessed by an e^- in a solid

* Valance Band :- The e^- in outermost orbit of an atom are known as valance ~~band~~ e^- . These e^- have highest energy. In case of solid valance e^- are confined in a band or energy range. The range of energy possessed by valance e^- is called valance band.

* Conduction :- In certain material the valance e^- are loosely attached to nucleus are called conduction electron and the range of energy possessed by conduction e^- is called a conduction band.

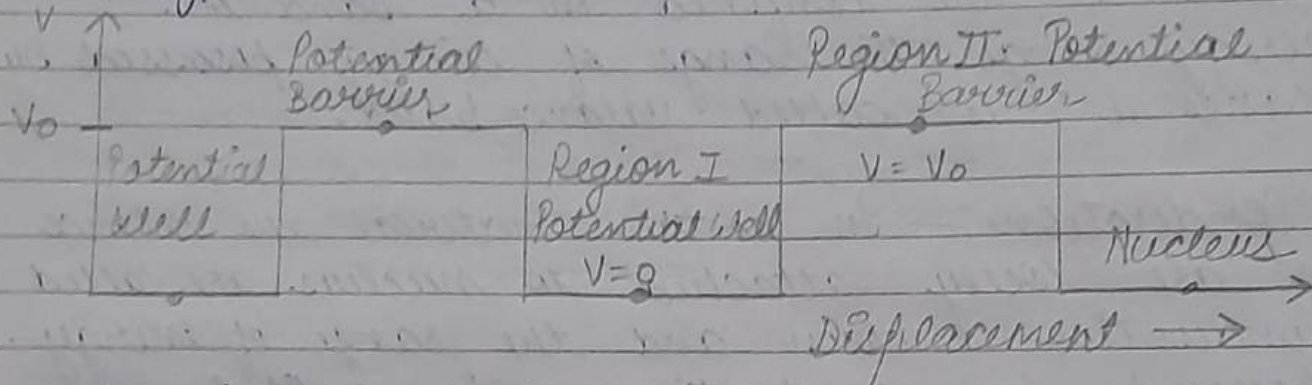
* Forbidden energy gap :- The separation b/w conduction band and valance band on the energy level diagram.

The greater energy gap more tightly the valance electrons are bound to the nucleus



The Kronig-Penny Model

Acc to this theory, the potential of e^- varies periodically with periodicity of ion core i.e., nucleus, and potential energy of e^- is zero near nucleus and maximum when it is lying b/w the adjacent nuclei which are separated by inter atomic spacing i.e., 'a'.



Apply Schrodinger time independent eqⁿ:-
for region 1 and 2

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

for region 1, $V = 0$

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

for region 2, $V = V_0$

$$\frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \psi = 0 \quad \text{--- (2)}$$

$$\text{put } \frac{2m}{\hbar^2} E = \alpha^2 \quad \& \quad \frac{-2m}{\hbar^2} (E - V_0) = \beta^2 \quad \text{--- (3)}$$

Now eq (1) & (2) becomes :-

$$\frac{d^2 \psi}{dx^2} + \alpha^2 \psi = 0 \quad \text{--- (4)}$$

$$\frac{d^2 \psi}{dx^2} - \beta^2 \psi = 0 \quad \text{--- (5)}$$

Now, solution of eqⁿ (4) & (5) is

$$\psi = e^{ikx} \cdot U_k(x) \quad \text{--- (6)} \quad [U = \text{periodicity}]$$

Now, double differentiate eq (6) wrt x

$$= \frac{d^2 \psi}{dx^2} = e^{ikx} \frac{d^2 U_k(x)}{dx^2} + ike^{ikx} \frac{dU_k(x)}{dx} - k^2 \cdot U_k e^{ikx} + ike^{ikx} \frac{dU_k(x)}{dx} \quad \text{--- (7)}$$

Now put eq (7) in eq (4) and (5) and also divide throughout with e^{ikx}

\therefore we get,

$$\frac{d^2 U_k(x)}{dx^2} + 2ik \cdot \frac{dU_k(x)}{dx} + [\alpha^2 - k^2] U_k(x) = 0 \quad \text{--- (8)}$$

$$\frac{d^2 U_k(x)}{dx^2} + 2ik \cdot \frac{dU_k(x)}{dx} - [\beta^2 - k^2] U_k(x) = 0 \quad \text{--- (9)}$$

Now, the general solution for eqⁿ (8) & (9) is:-

$$U_1 = A e^{i(\alpha - k)x} + B e^{-i(\alpha - k)x} = 0 \quad \text{--- (10)}$$

$$U_2 = C e^{(\beta - ik)x} + D e^{-(\beta - ik)x} = 0 \quad \text{--- (11)}$$

Now, solving eq (10) & (11)

$$\frac{P}{\alpha a} \sin \alpha a + \cos \alpha a = \cos ka \quad \text{--- (12)}$$

This equation is Kronig-penny model.

$P = \text{power}$

$a = \text{interatomic distance}$

Case I, when $P \rightarrow \infty$

Divide eq (12) by P

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

$$\sin \alpha a = 0$$

$$\alpha a = n\pi$$

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

a

$$\alpha^2 = \frac{n^2 \pi^2}{a^2} \quad \text{--- (a)}$$

general solution

from eq- (3)

$$\alpha^2 = \frac{2m}{\hbar^2} E \quad \text{--- (b)}$$

Equate (a) and (b)

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

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

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

$n =$ integer
 $m =$ mass of e^-
 $h =$ plank's const.

This $P = \infty$ represents the nature of insulator.

Case-2, $P = 0$

$$\cos \alpha a = \cos Ka$$

$$\therefore \alpha = K$$

$$\alpha^2 = K^2 \quad \text{--- (c)}$$

put in eq (3)

$$\alpha^2 = \frac{2m}{h^2} E \quad \text{--- (d)}$$

$$K^2 = \frac{2m}{h^2} E$$

$$\frac{4K^2}{\lambda} = \frac{2m E}{h^2}$$

$$\left[K = \frac{2m}{\lambda} \right]$$

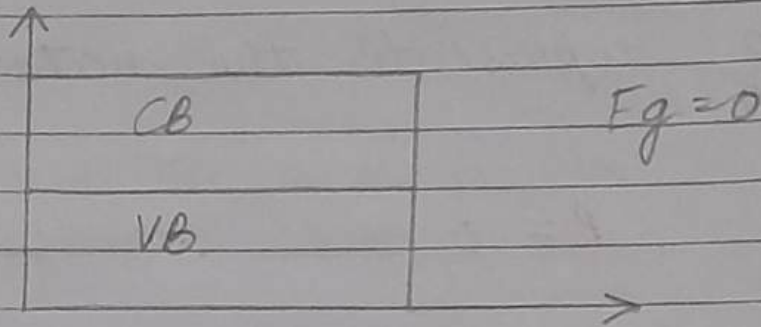
$$E = \frac{h^2}{2m \lambda^2} = \frac{h^2 / \lambda^2}{2m}$$

$$E = \frac{P^2}{2m} \quad \left[\lambda = \frac{h}{P}, \quad P = \frac{h}{\lambda} \right]$$

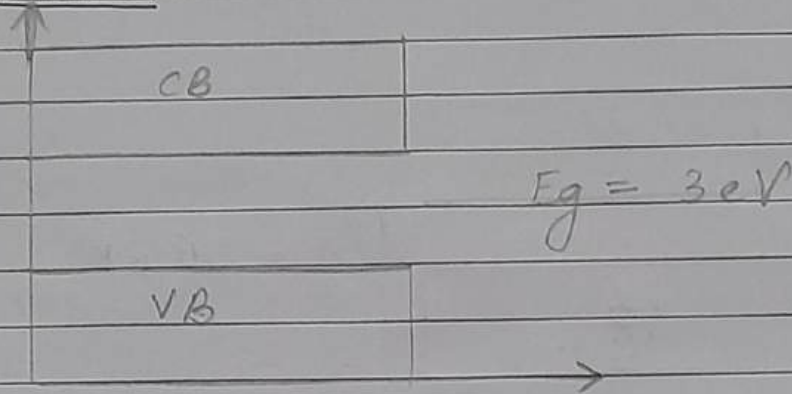
This $P = 0$ represents the nature of conductor.

Types of electronic material

(A) Conductors :-

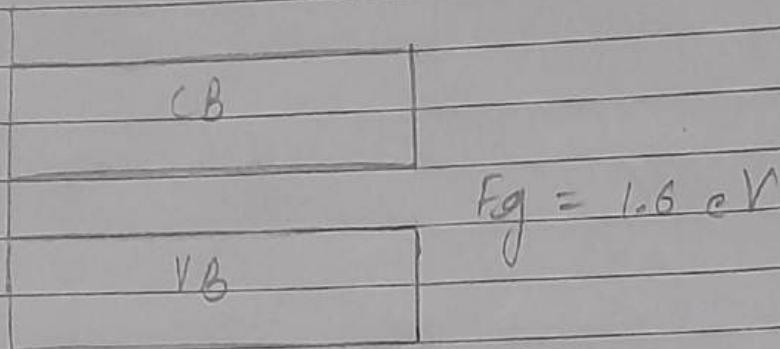


- * In conductors, it has incompletely filled valance band then there are enough no. of e^- available for conduction i.e they can behave as free e^- and some as charge carrier.
- * Example:- alkali earth metals such as Na, K, Li and noble metal such as Cu, Ag, Au.
- * There is no forbidden energy gap and valance band and conduction band, overlaps each other.
- * They possess very low resistivity (10^{-12} to 10^{-8} ohm meter) and very high conductivity (10^2 to 10^8 $S m^{-1}$)

(B) Insulators :-

- * For solids which have a certain no. of energy bands are completely filled and other bands being completely empty are known as insulators.
- * There is no effective free e^- all the bands upto valance band are full and the topmost band has almost zero, when the crystal is at lowest energy.
- * The forbidden energy gap is very wide, due to this fact e^- can't jump from valance band to conduction band.
- * The resistivity is very high more than $10^8 \Omega \text{ cm}$, conductivity is zero.
- * Example \rightarrow wood, plastic.

(C) Semiconductors :-



- * Semiconductor are those solids whose valance band is completely filled but is separated from empty conduction band by small energy gap at absolute zero.
- * Its conductivity lies between metal and insulator and increase with temperature.
- * Due to narrow energy gap, they have no. of electronic properties which make it useful in manufacturing electronic equipments.
- * At absolute zero, pure semiconductor have no broken bonds and electrical properties as an insulator.
- * Conductivity of semiconductor is mainly due breaking of covalent bond and the substance is called intrinsic semiconductor.
- * When a certain impurity atom are added into crystal with produce energy state

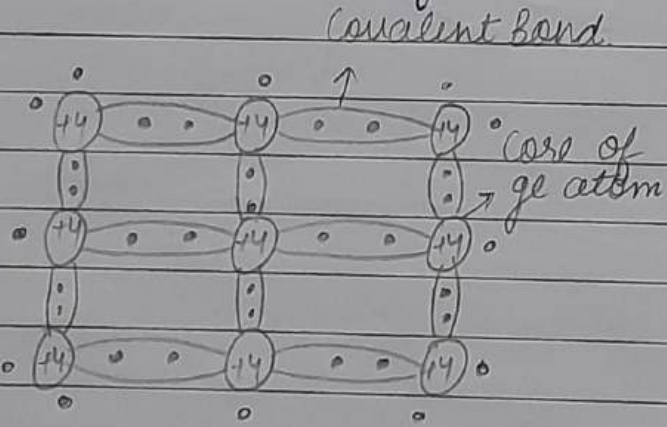
lying in a forbidden energy state lying in forbidden energy gap and results in forbidden electronic conductivity and they are called extrinsic semiconductor. The added element are called dopant and process is called doping.

* Example :- Si^{14} and Ge^{32}

Types of Semiconductor

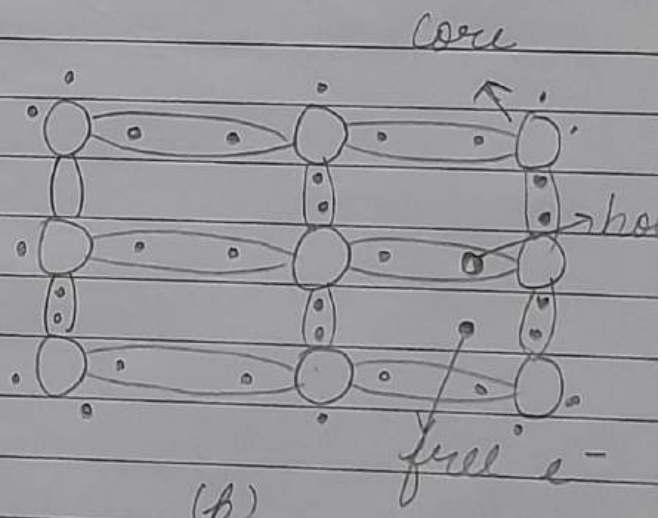
(A) Intrinsic Semiconductor.

- * Pure Ge and Si are known as intrinsic semiconductor.
- * Pure Ge atom has 32 e^- out of which 28 are tightly bound to the nucleus and remaining 4 revolve in the outermost level, these are called as valance electrons.
- * Nucleus with 28 tightly bound e^- forms a +ve core of the atom.



(a)

Ge Structure with covalent bond.



(b)

Ge crystal with e^- hole pair

Density of state :-

It is defined as no. of electronic state (or orbital) per unit area energy range. It is denoted by $D(E)$.

Mathematically it can be written as,

$$D(E) = 2 \frac{dn}{dE}$$

where 2 is due to spin degeneracy.

As we know,

$$E_n = \frac{h^2}{2m} \left(\frac{n\pi}{L} \right)^2 \quad \text{--- (1)}$$

Differentiate w.r.t. n

$$\frac{dE_n}{dn} = \frac{h^2}{2m} \left(\frac{\pi}{L} \right)^2 2n$$

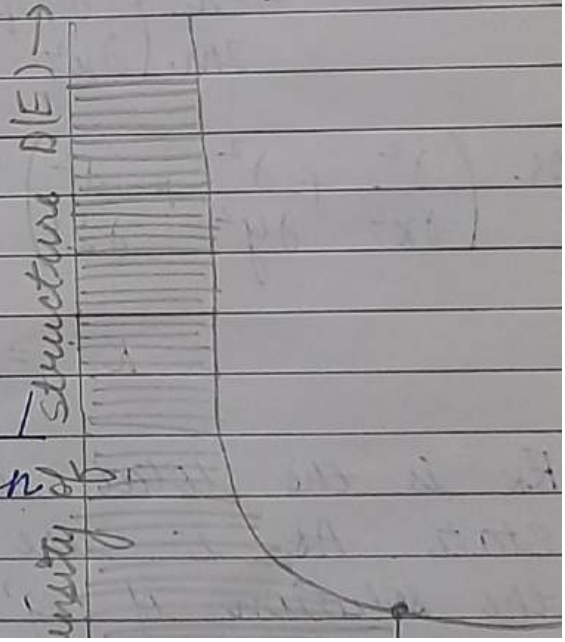
$$dE_n = \frac{h^2}{2m} \left(\frac{\pi}{L} \right)^2 2n \, dn$$

Now dn/dE_n denotes energy level as per unit energy.

Thus the density of states for a free electron is given by

$$D(E) = \frac{2 \, dn}{dE_n} = \frac{2 \cdot 2m(L)^2}{h^2 (\pi)^2 2n}$$

$$D(E) = \frac{4L}{m} \left(\frac{1}{\pi} \right)^2$$



This graph indicates the energy range in which all levels are filled. The filled level extent from 0 to E_f . At absolute zero the level which divides the filled and the empty level is known as fermi level and energy corresponding to ~~fer~~ fermi level is called fermi energy.

Density of states in 3D :-

Consider that the metal may be described by a free e^- gas which is confined to a cube of edge L .



The potential inside the crystal is 0 while outside the crystal the potential being large. The free particle schrodinger equation in 3D is.

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi_k(\mathbf{r}) = E_k \psi_k(\mathbf{r})$$

$$\text{or } \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi_k(\mathbf{r}) + k^2 \psi_k(\mathbf{r}) = 0 \quad \text{--- (1)}$$

$$k^2 = \frac{2m E_k}{\hbar^2}$$

E_k is the total energy of the electrons in k state. As e^- are confined to a cube of edge L the solution of eqⁿ (1) is the ~~analog~~ analog to one dimensional wave function and can be written as.

$$\psi_k(\mathbf{r}) = A \sin(k_x x) \sin(k_y y) \sin(k_z z)$$

where,

$$k_x = \frac{n_x \pi}{L}, \quad k_y = \frac{n_y \pi}{L}, \quad k_z = \frac{n_z \pi}{L}$$

with $k^2 = k_x^2 + k_y^2 + k_z^2$ and n_x, n_y, n_z are +ve integers which satisfies periodic boundary conditions. The required wave functions are to be periodic in x, y, z with period L . Thus appropriate boundary conditions are

$$\Psi(x+L, y, z) = \Psi(x, y+L, z) = \Psi(x, y, z+L) = \Psi(x, y, z) \quad (2)$$

$$\Psi_{k(r)} = A e^{i(k_x x + k_y y + k_z z)}$$

Provided that component of the wave vector $k(k_x, k_y, k_z)$ satisfy

$$k_n = 0, \pm \frac{2\pi}{L}, \pm \frac{4\pi}{L}, \dots$$

We know,

$$E_k = \frac{\hbar^2 k^2}{2m}$$

The energy E_k of orbital with wave vector k . The magnitude of wave vector is ~~separated~~ related to wavelength λ by

$$k = \frac{2\pi}{\lambda}$$

using normalising equation

$$\int \Psi^*(r) \Psi(r) d\tau = 1$$

$$\int_0^L \int_0^L \int_0^L A^2 e^{-i\mathbf{k}\cdot\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} dx dy dz = 1$$

$$A = \left(\frac{1}{L^3}\right)^{1/3} = \left(\frac{1}{V}\right)^{1/2}$$

Hence, Normalized wave function

$$\psi_{\mathbf{k}}(\mathbf{r}) = \left(\frac{1}{V}\right)^{1/2} e^{i\mathbf{k}\cdot\mathbf{r}}$$

and density of state in 3D

$$D(E) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$$

EK diagram :-

It is a graph that represent the same property of semiconductor such as type of band gap energy of matter and its momentum. In this two curve are drawn. One curve represents the conduction and other curve represents the valance band.

As we discuss in Kronig - penny model

Case I $\rightarrow p = \infty \Rightarrow E = \frac{\hbar^2 k^2}{8ma^2}$ [p = momentum]

Case II $\rightarrow p = 0 \Rightarrow E = \frac{p^2}{2m}$

But we will use energy of \mathbf{k}

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

Since E_k diagram relate to momentum

$$E = \frac{P^2}{2m}, \text{ where } P = mv \text{ acc. to classical mechanics}$$

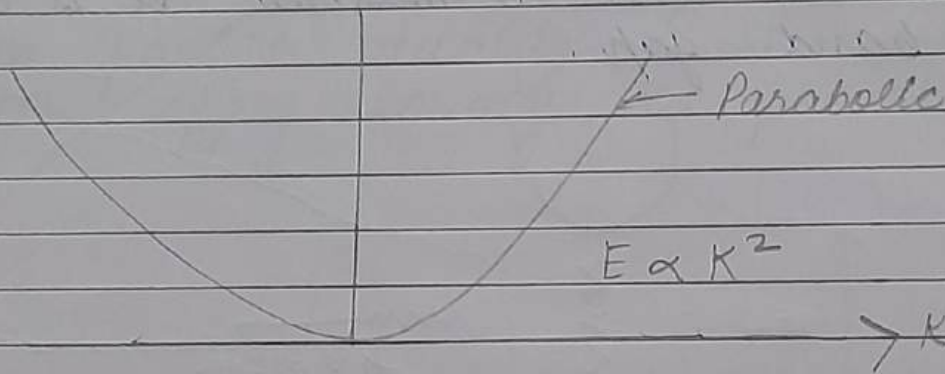
But acc. to quantum mechanics momentum of e^-

$$P = \hbar K \quad \text{--- (2)}$$

put (2) in (1) , $E = \frac{\hbar^2 K^2}{2m}$

let $\frac{\hbar^2}{2m} = A$ (constant)

$$E = AK^2 \quad \therefore E \propto K^2$$



This expression tells us the R/n b/w momentum and energy of electron.

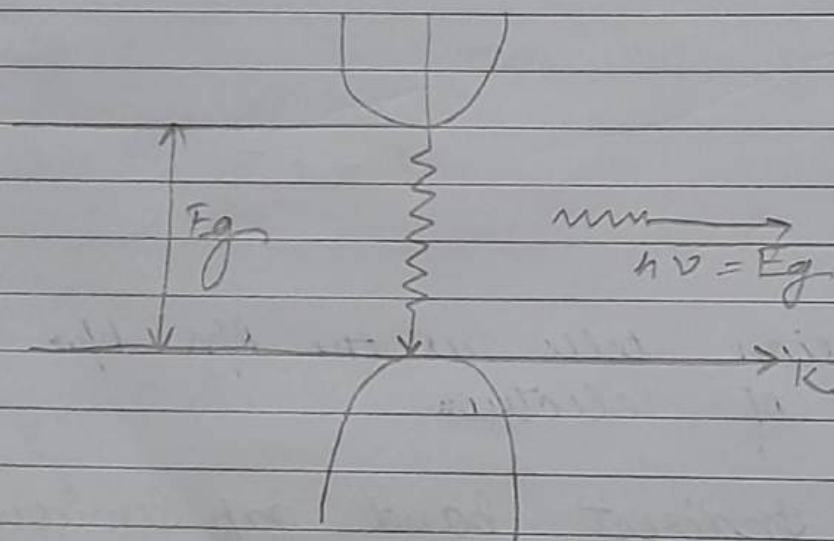
Direct and Indirect Band gap Semiconductor:-

There are 2 types of semiconductor.

- * Direct band gap
- * Indirect band gap

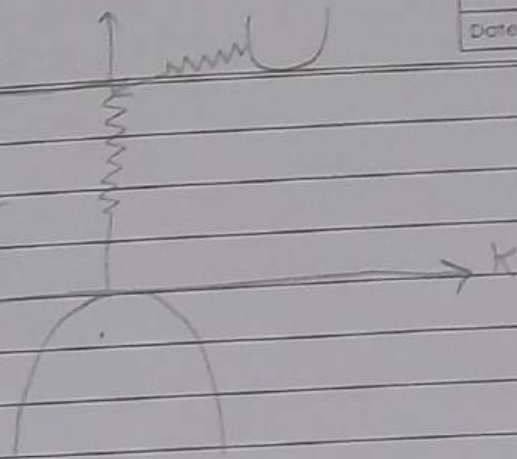
Direct Band gap semiconductor :-

The band represent the minimum energy difference b/w the top of Valance Band and bottom of conduction band. However the top of the valance band (VB maxima) and the bottom of conduction band (CB minima) are not generally at the same value of e^- momentum. Minimum energy state in the conduction band (CB minima) and max-energy state in valance band (VB maxima) are characterised by certain crystal momentum and k vector (propagation constant) in Brillouin zone. If the k -vector are same for CB minima and VB maxima. It is called direct band gap.



Indirect Band gap Semiconductor :-

If the k vector is diff. for the CB minima and VB maxima is known as 'indirect band gap semiconductor'.



Phonons.

The energy in lattice vibration or elastic wave is quantized. The quantum of energy in an elastic wave is called phonon in analogy with the quantum of electromagnetic wave, the photon, almost all of the concepts such as the wave particle duality, which apply to photon apply equally to phonons.

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