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DEPARTMENT OF PHYSICS

NAME OF THE SUBJECT : PHYSICS FOR ELECTRONICS ENGINEERING

SUBJECT CODE : PH8253

REGULATION : 2017

UNIT – I :ELECTRICAL PROPERTIES OF MATERIALS

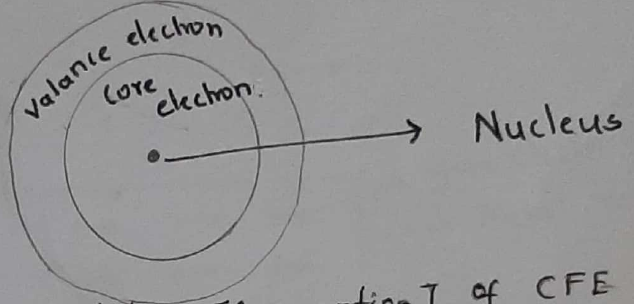
8 Mark

CLASSICAL FREE ELECTRON THEORY: [CFE]

Free electron theory of metals was proposed by Drude. P. in 1900.

PRINCIPLE:

This theory is based on the principle that a metal consists of a very large number of free electrons which can move freely throughout the metal. These free electrons are fully responsible for the electrical conduction in metal



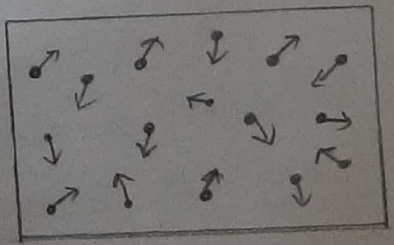
EXPLANATION: (postulates [Assumption] of CFE Theory)

1) An atom consists of a central nucleus with positive charge surrounded by electrons of negative charges.

2) The electrons in the closed shell are called core electron and those in the outermost shell is called valence electro

3) In metal the valence electrons get detached and they move freely throughout the metal. Hence they are called free electrons or valance electrons.

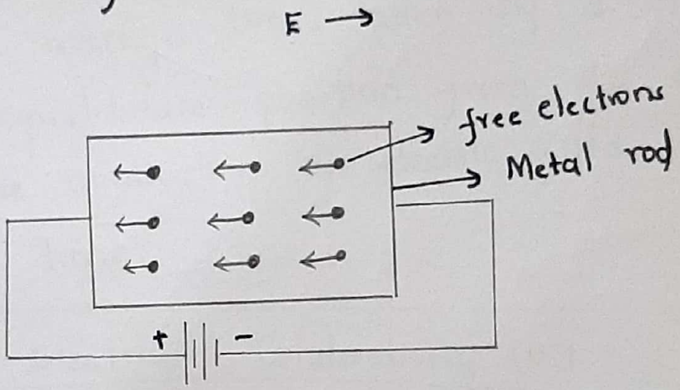
4) The electrons in a metal are free to move in all possible directions.



Free electrons move in random directio without electrical field.

5) In the absence of electric flield, the free electrons move in random manner. They collide with other free electrons, walls of the container and positive ion core. This collision is called <u>elastic collision</u>.

6) When the electric field is applied, the electrons get Some amount of energy from the applied electric field and they begin towards the positive potential. As a result these electrons acquire constant Velocity called as drift velocity.



Free electrons with external applied electric field

7) Since the electrons are assumed to be a perfect gas, they obey classical kinetic theory of gases.

Drift Velocity: (V_d)

It is defined as the average Velocity acquired by the free electrons of a metal in a particular direction by the application of electric field.

Mean free path (λ):

The average distance travelled by a free electron between two succesive collisions in the presence of an applied electric field is known as mean free path.

It is the product of drift velocity (V_d) and collision time (τ_c)

$$\boxed{\lambda = V_d \times \tau_c}$$

- **Collision time : (τ_c)**

The average time taken by a free electron between any two successive collisions is known as collision time. $\tau_c = \frac{\lambda}{V_d}$ where λ - mean free path

V_d - drift velocity.

- **Relaxation time:**

The average time taken by a free electron to reach its equilibrium position from its disturbed position by the application of electric field is known as relaxation time.

★. Derivation of Electrical Conductivity (σ)

8 mark

2 mark → **Definition:** The amount of electrical charge (Q) flowing per unit time (t) across unit area (A) in the metal for unit applied electric field (E) is called electrical conductivity. (σ)

$$\sigma = \frac{Q}{tAE} = \frac{J}{E}$$

$\sigma = Q$ (where $t = 1\,s$; $A = 1\,m^2$; $E = 1\,A$)

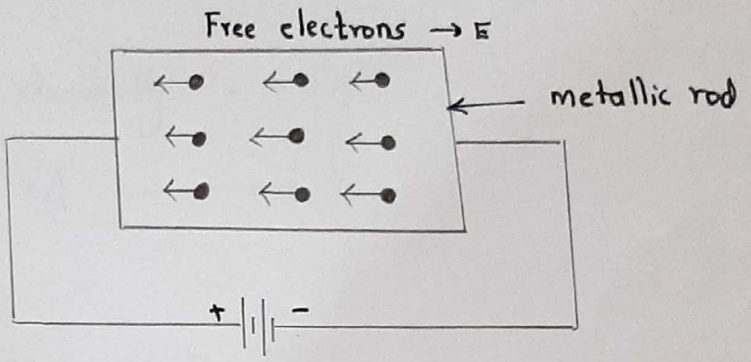
Current density $J = \frac{Q}{tA}$ Also $J = \sigma E$ (ohm's law)

Derivation of Electrical Conductivity:

(Based on Drude and Lorentz classical free electron theory)

When an electrical field (E) is applied to an electron of charge 'e' of a metallic rod, the electron moves in opposite direction to the applied field with a Velocity V_d (as in fig)

This velocity is known as drift Velocity.



Movement of electrons in a metallic rod.

Lorentz force acting on the electron F = eE ——— ①

This force is known as the driving force of the electron.

Due to this force, the electron gains acceleration 'a',

$$\text{Acceleration } (a) = \frac{\text{Drift velocity } (V_d)}{\text{Relaxation time } (\tau)}$$

$$\boxed{a = \frac{V_d}{\tau}} \quad \text{——— ②}$$

From Newtons' second law of motion, the force

F = Mass of the electron (m) × acceleration (a)

$F = ma$ ——— ③

Sub ② in ③

$$F = \frac{mV_d}{\tau} \quad \text{——— ④}$$

Equating ① and ④

$$\frac{m V_d}{\tau} = eE$$

$$V_d = \left(\frac{e\tau}{m}\right) E \quad \text{———} ⑤$$

From Ohm's law

$J = \sigma E$ (or) $\sigma = \frac{J}{E}$; where σ – electrical conductivity of the electron.

But Current density

$$J = ne V_d \quad \text{———} ⑥$$

Sub ⑤ in ⑥

$$J = \frac{ne\, e\tau E}{m} = \frac{ne^2\tau E}{m}$$

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

$J = \sigma E$ where $\boxed{\sigma = \frac{ne^2\tau}{m}}$

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

Thermal Conductivity (k):

Thermal conductivity is defined as the amount of heat flowing per unit time through the material having unit area of crosssection per unit temperature gradient

$$\therefore K = \frac{Q}{\left(\frac{dT}{dx}\right)}$$

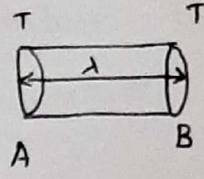
k – Thermal conductivity of the material.

Q – Amount of heat flowing per unit time through unit area.

$\frac{dT}{dx}$ – Temperature gradient.

Thermal Conductivity of a metal: (Derivation)

Consider two cross sections A at high temperature (T) and B at low temperature (T-dT) in a uniform metallic rod AB. These two cross sections are seperated by a distance λ. The heat conduction takes place from A to B through the electrons.



Let the density of conduction electrons be n and Velocity of electrons be V.

During the collision, electrons near A lose their kinetic energy while electrons near B gains the energy.

At A average kinetic energy of an electron $= \frac{3}{2} KT$.

where k - Boltzmann Constant.

T - Temperature at A.

At B average kinetic energy of an electron $= \frac{3}{2} k(T-dT)$

Excess kinetic energy of an electron from A to B $\Big\} = \frac{3}{2} KT - \frac{3}{2} k(T-dT)$

$$= \frac{3}{2} \cancel{KT} - \cancel{\frac{3}{2}} KT + \frac{3}{2} k dT$$

$$= \frac{3}{2} k dT$$

Number of electrons crossing unit area per unit time from A to B $\Big\} = \frac{1}{6} nv$

The excess of energy carried upwards (A to B) in unit area in unit time $\Big\} = \frac{1}{6} nv \times \frac{3}{2} k dT$

$$= \frac{1}{4} nv\, k dT$$

|||arly the deficient of energy carried downward (B to A) in unit area in unit time $= -\frac{1}{4} nvk\,d$

Net amount of energy transfered from A to B per unit area per unit time $\Big\}$ $Q =$

$$= \frac{1}{4} nvk\,dT - \left(-\frac{1}{4} nvk\,dT\right)$$

$$= \frac{1}{4} nvk\,dT + \frac{1}{4} nvk\,dT$$

$$= \frac{1}{2} nvk\,dT.$$

Thermal conductivity $Q = K\frac{dT}{dx} = K\frac{dT}{\lambda}$

$$\frac{1}{2} nvk\,dT = \frac{K\,dT}{\lambda}$$

$$\boxed{K = \frac{1}{2} nvk\lambda}$$

Mean free path $\lambda = \tau v$

$$K = \frac{1}{2} nvk(\tau v)$$

$$\boxed{K = \frac{1}{2} nv^2 k\tau}$$

This is the expression for thermal conductivity of a metal.

State and prove Weidmann Franz law:

Wiedemann - Franz law:

Statement:

It states that for the metals, the ratio of the thermal conductivity to the electrical conductivity is directly proportional to the absolute temperature. This ratio is constant for all metals at a given temperature.

$$\frac{K}{\sigma} \propto T$$

$$\frac{K}{\sigma} = LT$$

K - Thermal conductivity.

σ - Electrical conductivity.

L - Lorentz number - value = $2.44 \times 10^{-8}\ W\Omega K^{-2}$ at T = 293 K.

Derivation:

Wiedemann Franz law is derived from electrical & thermal conductivity of a metal.

Electrical conductivity of a metal $\sigma = \frac{ne^2\tau}{m}$ —— ①

Thermal conductivity of a metal $K = \frac{1}{2} nv^2 k\tau$ —— ②

$$\frac{\text{Thermal conductivity (K)}}{\text{Electrical conductivity }(\sigma)} = \frac{\frac{1}{2} nv^2 k\tau}{\frac{ne^2\tau}{m}} = \frac{1}{2}\frac{mv^2 k}{e^2}$$

$$\frac{K}{\sigma} = \frac{1}{2}\frac{mv^2 k}{e^2} \quad \text{—— ③}$$

kinetic energy of electron $\frac{1}{2}mv^2 = \frac{3}{2}kT$

Sub ④ in ③

$$\frac{K}{\sigma} = \frac{3}{2}\frac{kTk}{e^2} = \frac{3k^2T}{2e^2}$$

$$\frac{K}{\sigma} = \frac{3}{2}\left(\frac{k}{e}\right)^2 T$$

$$\frac{K}{\sigma} = LT$$

Where $L = \frac{3}{2}\left(\frac{k}{e}\right)^2$ is a constant & is called as Lorentz number

$$\frac{K}{\sigma} \propto T$$

Thus it is proved that the ratio of thermal conductivity to electrical conductivity of a metal is directly proportional to the absolute temperature.

Conclusion:

1) Wiedemann Franz law clearly shows that if a metal has high thermal conductivity, it will also have high electrical conductivity.

2) Among the metals, the best electrical conductors (silver, copper, Aluminium) are also best conductors of heat.

Kinetic energy of electron $\frac{1}{2}mv^2 = \frac{3}{2}kT$ — ④

Sub ④ in ③

$$\frac{K}{\sigma} = \frac{\frac{3}{2}kTk}{e^2} = \frac{3k^2T}{2e^2}$$

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2) Among the metals, the best electrical conductors (silver, copper, Aluminium) are also best conductors of heat.

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2 mark

Lorentz Number:

The ratio of thermal conductivity (k) of a met
to the product of electrical conductivity of a metal (σ) of the metal and absolute temperature (σ) of the metal is constant.
It is known as Lorentz number

$$L = \frac{k}{\sigma T} \quad \text{where} \quad L = \frac{3}{2}\left(\frac{k}{e}\right)^2$$

$$k = 1.38 \times 10^{-23} \ JK^{-1}$$

$$e = 1.602 \times 10^{-19} \ \text{Colomb}$$

$$\text{So} \quad L = \frac{3}{2}\left(\frac{1.38 \times 10^{-23}}{1.602 \times 10^{-19}}\right)^2$$

$$\boxed{L = 1.12 \times 10^{8} \ W\Omega K^{-2}}$$

★.
2 mark

Merits of classical free electron theory:

It is used to

i) Verify Ohm's law.
ii) explain the electrical and thermal conductivity of metals.
iii) derive Wiedemann - Franz law.
iv) explain the optical properties of metals.

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Drawbacks of classical free electron theory: (or) Demerits:

1) Contradiction in the absorption of supplied energy:

By classical theory all the free electrons absorb energy. But by quantum theory only a few electrons absorb energy.

2) Fails to explain the concept of non metals:

Classical theory fails to explain the electrical conductivity of semiconductors and insulators. For solids Band theory explain these concepts Successfully

Fails to explain the concept of photoelectric effect, Compton effect and Black body radiation:

Classical theory fails to explain photo electric effect, compton effect and black body radiation, because this phenomena is based on quantum theory.

4) Specific heat of solids:

Molar electronic specific heat calculated by this theory does not agree with the experimental results.

5) Temperature dependence of electrical conductivity.

It is experimentally observed that for metals, the electrical conductivity (σ_{exp}) is inversely proportional to temperature.

$$\sigma_{exp} \propto \frac{1}{T} \quad \text{——} \quad ①$$

But main assumption of CFE theory

$$\sigma \propto \frac{1}{\sqrt{T}} \quad \text{——} \quad ②$$

From ① & ② it is clear that the prediction of classical free electron theory is not agreeing with the experimental results.

6) Paramagnetism of metals:

Experimentally, the paramagnetism of metals is nearly independent of temperature. This is not at all explained by this theory.

7) Wiedemann - Franz law:

By electron theory the value of $\frac{k}{\sigma T}$ is found agree with theoretical value at ordinary temperature, but deviation occur at low temperature.

Quantum Free electron theory

It is a microscopic theory proposed by Sommerfeld in the year 1928. This theory obeys the law of quantum mechanics.

Basic assumptions of quantum free electron theory

i) According to quantum theory, the electrons are treated as matter waves.

ii) The electrons possess kinetic energy only.

iii) The free electrons obey Fermi Dirac statistics and Pauli's exclusion principle.

iv) At 0K, the electrons are distributed from the ground state to the Fermi level.

v) Only electrons nearer to the Fermi level are contributing for thermal conduction and electronic specific heat capacity.

Merits of quantum free electron theory:

i) This theory treats the electron quantum mechanically.

ii) This theory explains the electrical conductivity, thermal conductivity, specific heat capacity of metals, photoelectric effect, compton effect etc.

nits of quantum free electron theory:

1) It fails to explain the difference between metals, Semiconductors and insulators.

2) It also fails to explain the positive value of Hall coefficient.

FERMI DISTRIBUTION FUNCTION

Fermi - Dirac statistics deals with the particles having half integral spin. The particles like electrons are the examples of half integral spin and hence they are known as Fermi particles or Fermions.

★ 2 mark

Definition: The expression which gives the distributions of electrons among the various energy levels as a function of temperature is known as Fermi distribution function.

It is the probability function F(E) of an electron occupying a given energy level at absolute temperature.

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

where
F(E) – Fermi function.
E – Energy of the level whose occupancy being considered.
E_f – Fermi energy.
k – Boltzmann constant.
T – Absolute temperature.

The probability value F(E) lies between 0 and

If F(E) = 1 the energy level is occupied by electro

If F(E) = 0 the energy level is vacant.

If F(E) = 0.5 (or) $\frac{1}{2}$, there is 50% chance of finding the electron in the energy level.

V.V.★ 10 Mark

Effect of temperature on Fermi function:

(or)

Variation of Fermi distribution function.

The dependance of fermi distribution function and temperature and its effect on the occupancy of energy level is shown in fig (a) & (b)

case (i) probability of occupation for $E < E_f$ at $T=0$:

$$F(E) = \frac{1}{1+e^{\frac{(E-E_f)}{KT}}}$$

$$\left[e^{-\infty} = 0\right]$$

$$\left[e^{\infty} = \infty\right]$$

When $T = 0k$ & $E < E_f$, we have

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

$$\boxed{F(E) = 1}$$

At T = 0k, there is 100% chance for the electrons to occupy the energy levels below the fermi energy level ie: below the fermi energy level, all the energy levels are occupied with the electrons.

(ii) <u>probability of occupation for $E > E_f$ at $T=0$:</u>

when $T = 0k$ & $E > E_f$

$$F(E) = \frac{1}{1+e^{\frac{+ve}{0}}} = \frac{1}{1+e^{\infty}} = \frac{1}{1+\infty} = \frac{1}{\infty} = 0.$$

$$F(E) = 0$$

There is 0% chance for the electrons to occupy the energy level above Fermi energy level. (ie) all the energy levels above the fermi energy level not occupied.

fig (a)

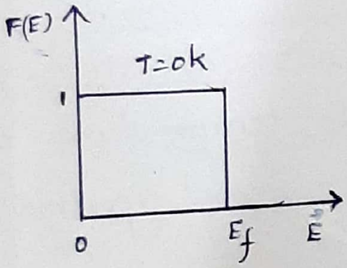
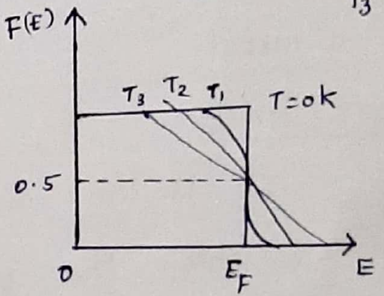


fig : b

$T_3 > T_2 > T_1 > 0k$



Variation of Fermi distribution function with E at different temperatures.

<u>Case iii :</u>

<u>Probability of occupation at ordinary temperature :</u>

At ordinary temperature, the value of probability starts, reducing from 1 for values of E close to but lesser than E_f

when temperature $T > 0$ & $E = E_f$

$$F(E) = \frac{1}{1+e^{0}} = \frac{1}{1+1} = \frac{1}{2} = 0.5.$$

There is 50% chance for the electron to occupy the Fermi energy level. ie: the value of $F(E) = \frac{1}{2}$ at $E = E_f$.

case : iv At high temperature:

when $KT >> E_F$ or $T \to \infty$ the electrons lose their quantum mechanical character and Fermi distribution function reduces to classical Boltzmann distribution.

uses of Fermi distribution function:

1) It gives the probability of electron occupying the energy level at a given temperature.

2) It is used in the calculation of number of free electrons per unit volume at a given temperature.

3) It is useful in the calculation for the fermi energy of a metal.

Fermi level:

It is the energy level at finite temperature above 0K in which the probability of electron occupation is $\frac{1}{2}$ and it is also the level of maximum energy of the filled states at 0K.

(or) [The highest energy level occupied by the electrons at absolute zero is called Fermi energy level.
- The probability of occupation of electron at Fermi level is 50%]

Fermi Energy:

It is the energy of the state at which the probability of electron occupation is $\frac{1}{2}$ at any temperature above 0K. It is also the maximum energy of filled states at 0K.

(or)

Fermi energy is the energy of the highest energy level occupied by the electron at absolute zero.

nsity of energy states:

question:

[• Derive an expression for the density of states and based on that calculate the carrier concentration in metals (or)

- With a neat diagram, derive an expression for density of states. (or)
- Define density of states in metals. Derive an expression for the Fermi energy of a system of free electron.
- Define Fermi energy. obtain a general expression for the Fermi energy of electrons in solid at 0K. Show that at same temperature the average energy of the electron is $\frac{3}{5}$th of the Fermi energy.]

Definition: Density of state is defined as the number of available electron states per unit volume in an energy interval E & E + dE

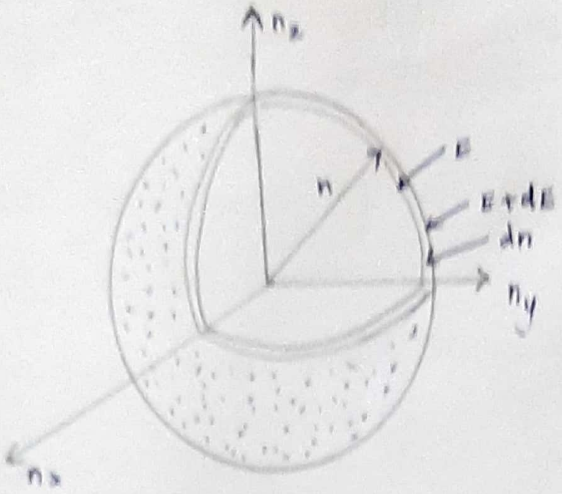
$$\underset{\text{(Density of states)}}{Z(E)\,dE} = \frac{\text{Number of energy states in energy interval } E \,\&\, E+dE \text{ in a metal piece } N(E)\,dE}{\text{Volume of the metal piece } (V)}$$

Consider a cubical metal piece of side 'a'. Construct a sphere of radius 'n' in space such that

$$n^2 = n_x^2 + n_y^2 + n_z^2$$

n_x, n_y and n_z are the quantum numbers along the three directions.

Calculation of Density of States\



Let the sphere is divided into many shells and each shell is represented by a particular combination of quantum numbers (n_x, n_y and n_z).

All the three quantum numbers n_x, n_y and n_z must be positive, it is satisfied only by one octant of the sphere. [$\frac{1}{8}$ of the sphere]

Every integer represents one energy state and therefore unit volume of the sphere contains one energy state.

Volume of the sphere $= \frac{4}{3}\pi n^3$.

$\therefore$ The number of energy states in the sphere $= \frac{4}{3}\pi n^3$. —①

$\therefore$ Number of energy states in $\frac{1}{8}$th of the sphere $= \frac{1}{8} \times \frac{4}{3}\pi n^3$. —②

Simillarly the number of energy states within one octant of the sphere of radius $(n+dn)$ with energy $(E+dE)$ $= \frac{1}{8}\left[4\pi(n+dn)^3\right]$

The number of energy states between the shell of radius n & n+dn N(E)dE $= \frac{1}{8}\left[\frac{4}{3}\pi(n+dn)^3\right] - \frac{1}{8}\left[\frac{4}{3}\pi n^3\right]$

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

$$= \frac{1}{8}\frac{4\pi}{3}\left[\cancel{n^3} + dn^3 + 3n^2dn + 3ndn^2 - \cancel{n^3}\right]$$

$$\because (a+b)^3 = a^3 + b^3 + 3a^2b + 3ab^2$$

glecting higher order terms

$$N(E)\,dE = \frac{1}{8}\,\frac{4\pi}{3} \times 3n^2 dn$$

$$= \frac{\pi}{2} n^2 dn = \frac{\pi}{2} n(ndn) \quad \text{—— ④}$$

Energy of the electron $E = \frac{n^2h^2}{8ma^2}$

$$n^2 = \frac{8ma^2E}{h^2} \quad \text{—— ⑤}$$

$$n = \left(\frac{8ma^2E}{h^2}\right)^{1/2} \quad \text{—— ⑥}$$

Differentiating eqn ⑤

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

$$ndn = \frac{8ma^2}{2h^2} dE \quad \text{—— ⑦}$$

from ⑥ & ⑦

Eqn ④ ⇒ $N(E)\,dE = \frac{\pi}{2} n(ndn)$

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

$$= \frac{\pi}{4}\left(\frac{8ma^2}{h^2}\right)^{1/2}\left(\frac{8ma^2}{h^2}\right)E^{1/2}dE$$

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

Pauli's exclusion principle states that two electrons of opposite spins can occupy each state

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

$$= \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{3/2} a^3 \sqrt{E}\, dE$$

$$= \frac{\pi}{2} \frac{(8m)^{3/2}}{h^3} a^3 \sqrt{E}\, dE$$

$$\Big[(8m)^{3/2} = (8m)\,(8m)^{1/2} = (4\times 2m)\;(4\times 2m)^{1/2}$$

$$= 4 \times 2m \;\; 2^{\cancel{2}\times 1/\cancel{2}} \times (2m)^{1/2}$$

$$= 8 \times (2m)^{3/2} \Big]$$

$$N(E)\, dE = \frac{\pi}{2} \frac{8\,(2m)^{3/2}}{h^3} a^3 \sqrt{E}\, dE$$

$$= \frac{4\pi}{h^3} (2m)^{3/2} a^3 \sqrt{E}\, dE$$

Density of states is given by

$$Z(E)\, dE = \frac{N(E)\, dE}{V}$$

$$= \frac{\frac{4\pi}{h^3} (2m)^{3/2} \cancel{a^3} \sqrt{E}\, dE}{\cancel{a^3}}$$

$$= \frac{4\pi}{h^3} (2m)^{3/2} E^{1/2}\, dE$$

This is the expression for density of charge carriers.

rier concentration in metals

(or)

Density of electrons and Fermi energy at absolute zero

At absolute zero, the topmost filled energy level is the Fermi level and its energy is E_F

$$dN = N(E)\, dE\, F(E)$$

Below E_F, $F(E) = 1$

$$\therefore dN = N(E)\, dE$$

$$N = \int dN = \int_0^{E_F} \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{3/2} E^{1/2}\, dE$$

$$N = \frac{\pi}{\cancel{2}} \left(\frac{8m}{h^2}\right)^{3/2} \frac{E_f^{3/2}}{3/\cancel{2}}$$

$$= \frac{\pi}{3} \left(\frac{8m}{h^2}\right)^{3/2} E_f^{3/2} \quad \text{——} ①$$

N is the number of electrons per unit volume called concentration of electrons, from ①

$$E_F^{3/2} = \frac{3N}{\pi} \left(\frac{h^2}{8m}\right)^{3/2}$$

$$E_F = \left(\frac{h^2}{8m}\right) \left(\frac{3N}{\pi}\right)^{2/3} \quad \text{——} ②$$

eqn ② represents the Fermi energy of electrons at absolute zero.

Average Energy of an electron at absolute

$$E_{av} = \frac{E_t}{N}$$

$$E_t = \int dN\, E$$

$$= \int_0^{E_F} E\, \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{3/2} E^{1/2}\, dE$$

$$= \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{3/2} \int_0^{E_F} E^{3/2}\, dE$$

$$= \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{3/2} \frac{E_f^{5/2}}{5/2}$$

$$= \frac{\pi}{5} \left(\frac{8m}{h^2}\right)^{3/2} E_f^{5/2}$$

$$E_{av} = \frac{E_t}{N} = \frac{\frac{\pi}{5}\left(\frac{8m}{h^2}\right)^{3/2}}{\pi/3 \left(\frac{8m}{h^2}\right)^{3/2}} \frac{E_f^{5/2}}{E_f^{3/2}}$$

$$= \frac{3}{5} E_f$$

hon in periodic potential.

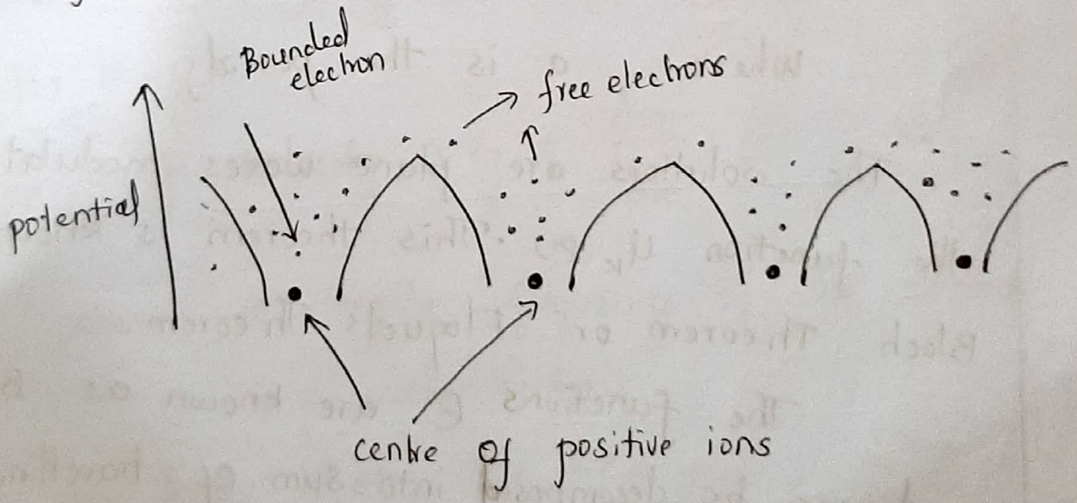
Band theory of solids (Zone theory)

The free electron theory fails to explain why some solids are conductors, some are insulators and others are semiconductors.

A solution to this problem was given by band theory of solids and is called zone theory.

Postulates:

Potential energy of electron within the crystal is periodic ie free electrons move inside periodic lattice field.



Therefore the potential energy of the electron near by the centre of positive ion is maximum and will not be able to move freely, but the electrons which are above these potentials peaks are free to move inside the metal and hence they are termed as free electrons.

Bloch Theorem:

Bloch theorem is a mathematical statement of an electron wave function moving in a perfectly periodic potential. These functions are called bloch functions.

Let us consider an electron moving in a periodic potential. The schrodinger equation is

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

There exist solutions of the form

$$\psi(x) = e^{\pm ikx}\, u_k(x) \quad \text{———} \quad ②$$

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

Where a is the period,

The solutions are plane waves modulated by the function $u_k(x)$. This theorem is known as the Bloch Theorem or Floquet's Theorem.

The functions ② are known as Bloch functions and can be decomposed into sum of travelling waves.

Effective mass of Electron and Hole

Effective mass of electron:

The mass acquired by an electron when it is accelerated in a periodic potential is called effective mass of an electron. It is denoted by m^*.

Explanation:

When an electron is accelerated the mass of the electron is not a constant, but it varies. This varying mass is called effective mass (m^*).

Derivation of effective mass of electron:

When electric field is applied to, crystal the electron gains velocity described by wave vector k.

$$\therefore \text{Group velocity } v_g = \frac{d\omega}{dk} \quad \text{——} \quad ①$$

where ω - angular frequency of the electron.

k - wave vector

We know that $E = h\nu$

$$\because \omega = 2\pi\nu$$

$$\nu = \frac{\omega}{2\pi}$$

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

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

$$= \hbar\omega$$

$$\omega = \frac{E}{\hbar} \quad \text{——} \quad ②$$

Substituting ② in ①

$$V_g = \frac{d}{dk}\left(\frac{E}{\hbar}\right)$$

$$V_g = \frac{1}{\hbar}\frac{dE}{dk} \quad \text{———} ③$$

The acceleration 'a' is

$$a = \frac{d(V_g)}{dt}$$

$$= \frac{d}{dt}\left[\frac{1}{\hbar}\left(\frac{dE}{dk}\right)\right] \quad (\times \,\&\, \div \text{ by } dk)$$

$$= \frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{dk}{dt} \quad \text{———} ④$$

Momentum (p) of an electron

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

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

$$= \hbar k \quad \text{———} ⑤$$

Differentiating ⑤ w.r.t 't'

$$\frac{dp}{dt} = \hbar\frac{dk}{dt} \qquad \left[\because \text{Force on the } \bar{e} \quad F = \frac{dp}{dt}\right]$$

(or)

$$F = \hbar\frac{dk}{dt}$$

$$\frac{dk}{dt} = \frac{F}{\hbar} \quad \text{———} ⑥$$

Substituting ⑥ in ④

$$a = \frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{F}{\hbar}$$

$$= \frac{1}{\hbar^2}\frac{d^2E}{dk^2}F$$

$$F = \left[\frac{\hbar^2}{\left(\frac{d^2E}{dk^2}\right)}\right]a \quad \text{———} \quad ⑦$$

When an electrical field is applied, acceleration is

$$a = \frac{eE}{m^*} = \frac{F}{m^*} \qquad [\because F = eE]$$

$$F = m^* a \quad \text{———} \quad ⑧$$

Comparing ⑦ & ⑧

$$m^* a = \left[\frac{\hbar^2}{\left(\frac{d^2E}{dk^2}\right)}\right]a$$

$$\boxed{m^* = \frac{\hbar^2}{\left(\frac{d^2E}{dk^2}\right)}} \quad \text{———} \quad ⑨$$

from ⑨ effective mass is not constant but depends on $\frac{d^2E}{dk^2}$

Special cases:

case : i

If $\frac{d^2E}{dk^2}$ is positive then m^* is also positive

case : ii

If $\frac{d^2E}{dk^2}$ is negative then m^* is also negative.

case : iii

If $\frac{d^2E}{dk^2}$ is more then electrons behave as light particle.

case : iv

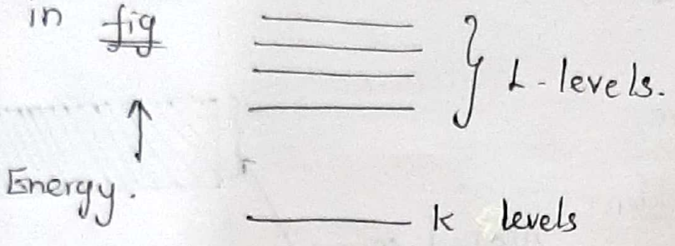
If $\frac{d^2E}{dk^2}$ is very small, then the electrons behave as heavy particle.

Energy bands in Solids:

A solid contains an enormous number of atoms packed closely together. Each atom has a discrete set of electron energy levels 1s, 2s, 2p, - - - - -

The energies of electrons within any one isolated atom obey the conditions.

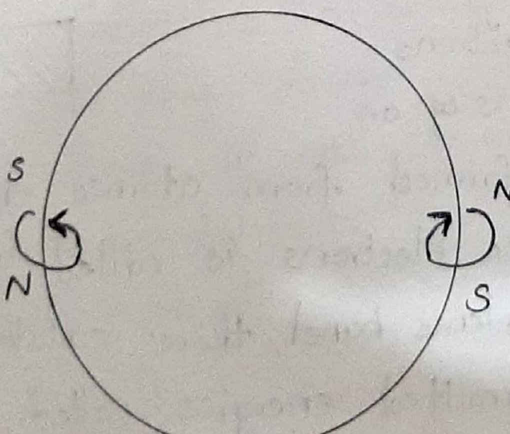
i) There are specific electronic energy levels in each atoms as in fig



Electrons cannot occupy space between these levels.

ii) Electrons fill the lowest energy levels first. A specific quantity of energy, called a quantum of energy must be supplied to move an electron to the next higher level.

iii) Pauli's exclusion principle states that, not more than two electrons can occupy any one energy level. Two electrons of opposite spins occupy the same energy level.

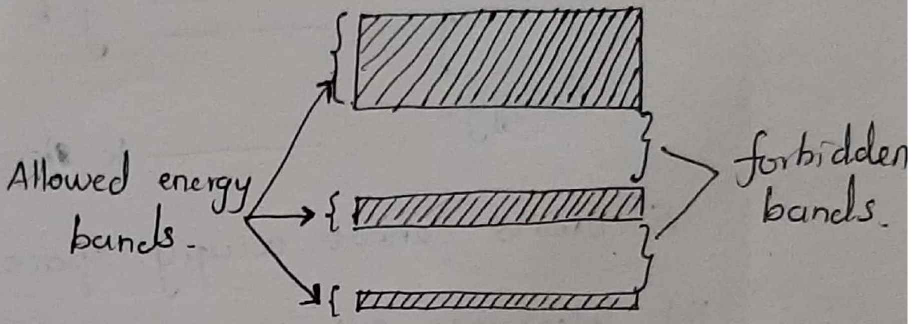


Valence electrons of adjacent atoms interact constitu a single system of electrons, and their outermost electronic orbits overlap.

Each atomic energy level is split up into a large number of closely spaced energy levels.

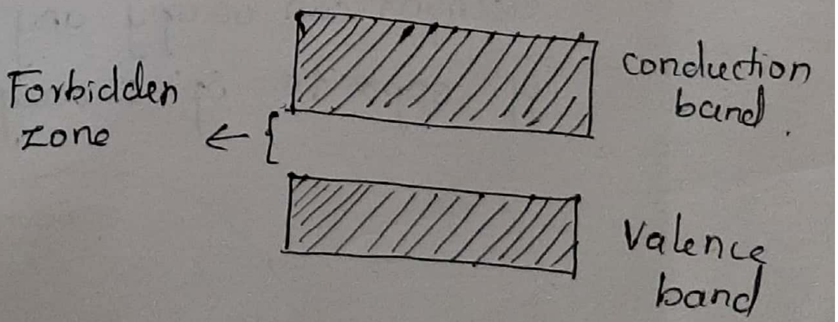
A set of such closely spaced energy levels is called an energy band.

These regions are known as forbidden bands or energy gaps



Each quantum state is occupied by a maximum of two electrons with opposite spins. Thus each energy band can be occupied by 2N electrons.

The valence band consists of a group of states containing the outermost electrons or valence electrons of an atom. The band formed from atomic energy levels containing valence electrons is called Valence band.



Above the valence band, there exists the band of next higher permitted energies called conduction band. It is seperated from the valence band by a gap.

The conduction band corresponds to the first excited states and it is normally the lowest unfilled energy band. In conduction band the electrons can move freely and they are generally called conduction electrons.

According to free electron theory, the potential energy of the electron inside the crystal through which an electron moves is supposed to be constant (zero) and so it is completely free to move.

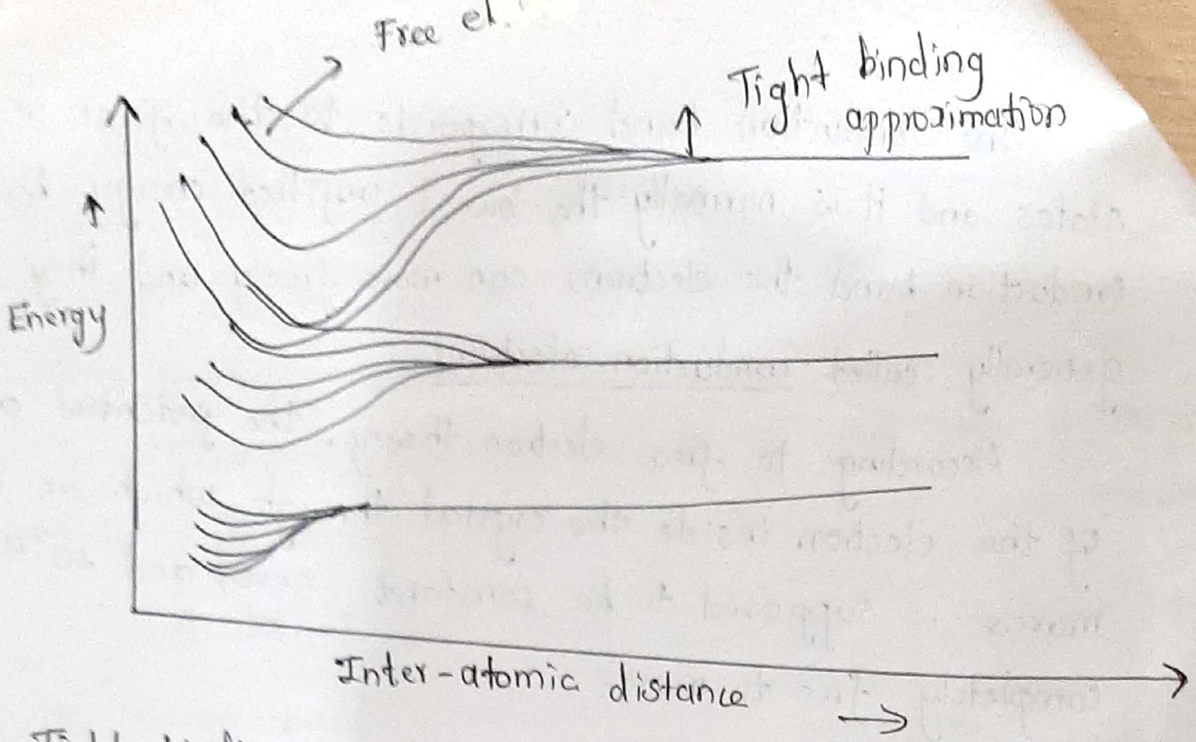
Tight Binding approximation

In solids, there exist the Ionic core which are tightly bounded to the lattice location, while the electrons are free to move here and there. This is called free-electron approximation.

In free electron approximation

In free electron approximation is assumed to be

1. The potential energy of the electron is lesser than its total energy.
2. The width of the forbidden bands (E_g) are smaller than the allowed bands as in the fig.
3. Therefore, the interaction between the neighbouring atoms will be very strong.
4. As the atoms are closer to each other, the inter atomic distance decreases and hence the wave functions overlap with each other.



Tight binding approximation:

Tight binding approximation is opposite to free electron approximation.

All the electrons are bounded to the atoms. The atoms are free, while the electrons are tightly bounded. Hence, this is called tight binding approximation.

In tight binding approximation,

1. The potential energy of the electrons is nearly equal to the total energy.
2. The width of the forbidden bands (Eg) are larger than the allowed bands as in the fig
3. Therefore, the interactions between the neighbouring atoms will be weak.
4. As the atoms are not closer, the interatomic distance increases and the wave functions will not overlap.

concept of hole (or) Effective or Negative mass of electron

The effective mass m^* is negative near the zone edges of filled valence bands. The electrons in these regions are accelerated in a direction opposite to the direction of the applied field. This is called the negative mass behaviour of the electrons.

The electrons with the negative effective mass is considered as the same positive mass of that of an electron, but with positive charge. This new entity is given the name "hole"

The holes are not real particles like electrons or positrons, but it is a way of looking at the negative mass behaviour of the electrons near the zone edge.

The positive hole conduction and effective negative electron mass conduction are in equilibrium. The calculations made on the hole appear to be more convenient and hence the hole concept is retained.

Several phenomena like Hall effect, Thomson effect etc find explanation on the basis of the hole concept.

Electrons in metals - Particle in a Three dime

The Solution of one dimensional potential well extended for a three-dimensional potential box.

In a three - dimensional potential box, the particle can move in any direction. So we use three quantum numbers, n_x, n_y and n_z to the three co-ordinate axes namely x, y and z respectively.

If a, b, c are the lengths of the box along x, y & z axes then,

$$\text{ie, } E_{n_x n_y n_z} = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8mb^2} + \frac{n_z^2 h}{8mc^2}$$

If $a=b=c$ as for a cubical box then

$$E_{n_x, n_y, n_z} = \frac{h^2}{8ma^2}\left[n_x^2 + n_y^2 + n_z^2\right] \quad \text{—— ①}$$

The corresponding normalised wave function is

$$\psi_{n_x, n_y, n_z} = \sqrt{\frac{2}{a} \times \frac{2}{a} \times \frac{2}{a}} \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{a} \sin \frac{n_z \pi z}{a}$$

$$= \sqrt{\frac{8}{a^3}} \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{a} \sin \frac{n_z \pi z}{a} \quad \text{—— ②}$$

From the equations ① & ② we understand that several combinations of the three quantum number (n_x, n_y & n_z) lead to different energy eigen values and eigen functions.

Example:

Suppose a state has quantum numbers, then

$n_x = 1$, $n_y = 1$, $n_z = 2$

Then $n_x^2 + n_y^2 + n_z^2 = 6$

Similarly for a combination $n_x = 1$, $n_y = 2$, $n_z = 1$ and for a combination $n_x = 2$, $n_y = 1$, $n_z = 1$

We have $n_x^2 + n_y^2 + n_z^2 = 6$

$$\therefore E_{112} = E_{121} = E_{211} = \frac{6h^2}{8ma^2} \quad \text{———} ③$$

The corresponding wave functions are written as

$$\left.\begin{aligned} \psi_{112} &= \sqrt{\frac{8}{a^3}} \sin\frac{\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{\pi z}{a} \\ \psi_{121} &= \sqrt{\frac{8}{a^3}} \sin\frac{\pi x}{a} \sin\frac{2\pi y}{a} \sin\frac{\pi z}{a} \\ \psi_{211} &= \sqrt{\frac{8}{a^3}} \sin\frac{2\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{\pi z}{a} \end{aligned}\right\} \text{———} ④$$

Degenerate States:

From ③ & ④ for several combinations of quantum numbers, we have the same energy eigen value but different eigen functions. Such a state of energy levels is called degenerate state.

The three combinations of quantum numbers (112), (121), and (211) which give the same eigen value but different eigen functions are called 3-fold degenarate state.

Non-degenerate state:

when only one wave function corresponds to the energy eigen value, such a state is called non-degenerate state.

Suppose $n_x = 2$, $n_y = 2$, $n_z = 2$

Then $E_{222} = \frac{12h^2}{8ma^2}$

and $\psi_{222} = \sqrt{\frac{8}{a^3}} \sin\frac{2\pi x}{a} \sin\frac{2\pi y}{b} \sin\frac{2\pi z}{a}$

21/12/17

Unit 1 & 2