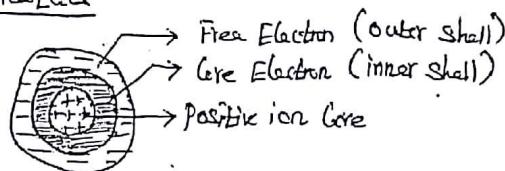


Free Electron theory of metals

In isolated atom



Free Electron - determines its electrical property

Free Electron theory explains electrical conductivity of metals & other properties. Applicable to both metals & non-metals

Developed in three main stages

- 1) Classical Free Electron theory - Proposed by Drude & Lorentz in 1900. According to this theory "Free Electron in metals obeys classical mechanics"
- 2) Quantum Free Electron theory - Proposed by Sommerfeld in 1928. According to this theory "Free Electron in metals obeys quantum laws"
- 3) Zone (or) Band theory - Proposed by Bloch in 1928. According to this theory "Free Electrons move in a periodic field provided by the lattice"

D) Classical Free Electron theory

Based on following Postulates

- 1) In an atom electrons revolve around nucleus and metal is composed of such atoms
- 2) Valence electrons of atom are free to move about the whole volume of metal like molecules of gas in container
- 3) Free Electron move in random direction & collide with Positive ions fixed to lattice (or) other free electrons - All these collision are elastic (No gain/loss of energy)
- 4) When Electric field is applied to metal, free electrons are accelerated in the direction opposite to direction of applied electric field.
- 5) Electron distribution is based on Maxwell - Boltzmann distribution law

Assuming free electrons as gas molecules & applying kinetic theory of gases - drift velocity, mean free path & relaxation time of electrons were explained

Drift velocity - Additional velocity + random velocity of electron in presence of electric field

Mean free path - Average distance travelled by electron between two successive collisions in presence of Electric field

Relaxation time - Time taken by electron to move from disturbed position to rest position when Electric field is switched off.

Success of free Electron theory

- 1) Verifies Ohms law
- 2) Explains Electrical & thermal conductivity of metals
- 3) Finds relation between Electrical & thermal conductivity of metals

Drawbacks of free Electron theory

- D) Photoelectric effect, Compton effect & Black body radiation couldn't explained
- 2) The specific heat of metal is find to be $4.5R$ but experimental value is $3R$
- B) Electrical conductivity of semiconductor / Insulator couldn't explain
- A) Ferromagnetism couldn't explained. Also theoretical value of paramagnetic susceptibility is greater than experimental value

Quantum free Electron theory

This theory obeys quantum mechanical laws

Sommerfeld applied Schrödinger's wave equation & de-Broglie wave concept to find expression for electron energies

Fermi-Dirac statistics were considered for particle distribution instead of Maxwell-Boltzmann statistics

According to quantum mechanics — Moving particle has some sort of wave motion

Then wavelength $(\lambda) = \frac{h}{P}$ (de-Broglie wavelength)

To characterize moving particle having wave motion $\rightarrow (\psi)$ — wavefunction is introduced [Tells us probability of finding e^- in a atom]

By connecting (ψ) & de-Broglie wavelength, Schrödinger gave wave equation for moving particle having wave motion in one dimension as

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

Based on Schrödinger's wave equation, Energy of particle is calculated as $(E) = \frac{n^2 h^2}{8mL^2}$ & wavefunction of particle $\psi(x) = A \sin \frac{n\pi x}{L}$

Postulates Made

- 1) potential of electron is uniform (or) constant within the crystal
- 2) Electron possess wave nature
- 3) Allowed energy levels of electrons are quantized
- 4) Electrons move freely within crystal & not allowed to leave the crystal due to large potential barrier at the surface
- 5) Distribution of electrons obey Fermi-Dirac Statistics

Merits

- 1) Electrons are having wave motion
- 2) Explains Electrical conductivity / thermal conductivity
- 3) Specific heat of metal
- 4) Photoelectric effect & Compton effect were explained

Demerits

- 1) Fails to give difference of metals / semi-conductors / Insulator
- 2) Fails to explain the charge transport properties of metals

Density of Energy states

Defined as number of available electron states per unit volume in the energy interval E & $E+dE$ and is denoted by $Z(E)$

To find $Z(E)$ Expression

In a given material, number of electrons per unit volume in a given range of interest is given by

$$N_e = \int_E^\infty Z(E) F(E) dE$$

where $Z(E)$ in the range E & $E+dE$ is given by.

$$Z(E)dE = \frac{\pi}{2} n^2 dn \rightarrow (1)$$

$$\text{Also, Energy of particle } E = \frac{h^2 n^2}{8mL^2} \rightarrow (2)$$

$$n^2 = \frac{E 8mL^2}{h^2} \rightarrow (3)$$

$$n = \left[\frac{8mL^2}{h^2} E \right]^{1/2} \rightarrow (4)$$

Diff of (3) on both sides

$$2ndn = \frac{8mL^2}{h^2} dE$$

$$dn = \left[\frac{8mL^2}{h^2} \right] \left[\frac{1}{2n} \right] dE$$

$$= \left[\frac{8mL^2}{h^2} \right] \frac{1}{2} \left[\frac{1}{\frac{8mL^2}{h^2} E} \right]^{1/2} dE$$

$$dn = \frac{1}{2} \left[\frac{8mL^2}{h^2} \right]^{1/2} \frac{dE}{(E)^{1/2}} \rightarrow (5)$$

Substituting of (5) & (2) in (1) we get

$$\begin{aligned} Z(E) dE &= \frac{\pi}{2} \left[\frac{8mL^2}{h^2} \right] \cdot \frac{E}{E^{1/2}} \cdot \left[\frac{8mL^2}{h^2} \right]^{1/2} dE \\ &= \frac{\pi}{4} \left[\frac{8mL^2}{h^2} \right]^{3/2} (E)^{1/2} dE \end{aligned}$$

According to Pauli's exclusion principle, two electrons of opposite spin can occupy each states & hence number of energy states available is

$$2(E) dE = 2 \times \frac{4\pi}{A} \left[\frac{8mL^2}{h^2} \right]^{3/2} (E)^{1/2} dE$$

$$\therefore 2(E) dE = 2 \times \frac{4\pi}{A h^3} (2m)^{3/2} (8) \cdot (L)^3 (E)^{1/2} dE$$

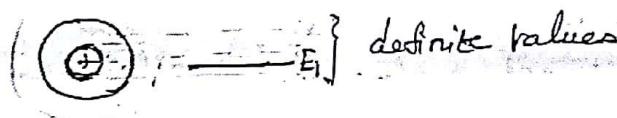
$$2(E) dE = \boxed{\frac{4\pi}{h^3} (2m)^{3/2} (L)^3 (E)^{1/2} dE}$$

$$\begin{aligned} \text{Here } (8m)^{3/2} &= 8m \cdot 8m \\ &= (4 \times 2)m [(4 \times 2)m]^{1/2}, \\ &= (4 \times 2) L^3 m^{3/2} [2^2 \times 2] \\ &= A \times 2 (2m)^{3/2}, \\ &\boxed{= (8) (2m)^{3/2}} \end{aligned}$$

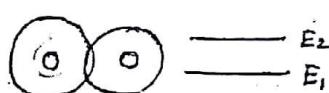
Energy bands in solid

According to quantum mechanical law, the energies of electrons in a free atom can not have arbitrary values but only some definite values

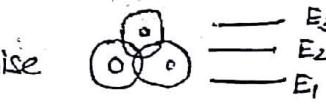
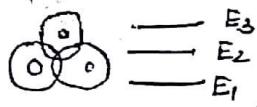
In Isolated atom



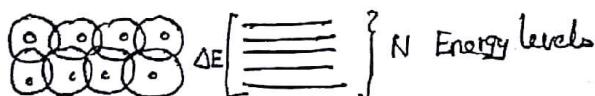
When two identical atoms are brought closer, the outermost orbit of atom overlap and interact



Likewise



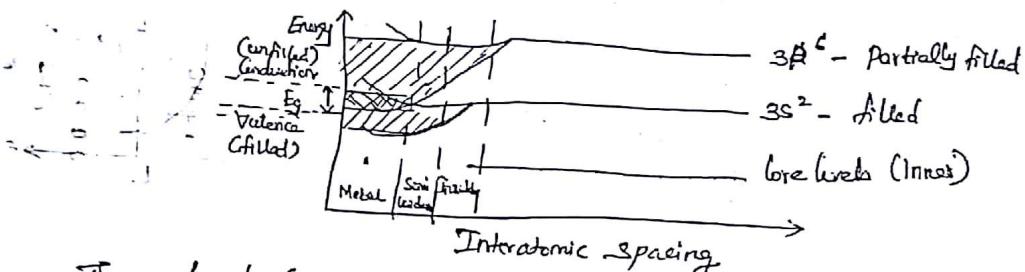
For N atoms to form solid



Thus when N atoms are considered to form solid, energy levels of atom split into N levels & becomes closer that they form continuous band. The width of this band depends on degree of overlap of electrons of adjacent atoms and is largest for outer most atomic electrons.

If Si is considered, electronic configuration is $1s^2, 2s^2, 2p^6, \frac{3s^2}{\text{filled}}, \frac{3p^2}{\text{unfilled}}$

If no. of Si atoms are brought closer (a) interatomic spacing is reduced than



This band corresponds to outer most orbit in "conduction band" and inner (α) next lower orbit band is "valence band". The gap available between these two allowed energy bands is called forbidden energy gap (E_g)

According to width of this forbidden energy gap, solids are broadly classified as metals, semiconductors & Insulators

In the above diagram

The completely filled $3s^2$ overlaps with partially filled $3p^6$ at lower atomic spacing - metals

As atomic spacing increases - small gap occurs between filled $3s^2$ & $3p^6$ - semiconductors

As atomic spacing is large - forbidden gap between filled $3s^2$ & $3p^6$ increases - Insulator

Kronig - Penney model

It is assumed in quantum free electron theory of metals that free electrons in metal express a zero potential (or) constant potential and is free to move in the metal. Based on this many phenomena were explained for solids but could not explain why some are conductors/semiconductors/insulators.

Hence the failure was overcome in band / zone theory which states that electron move in a periodic potential produced by the ~~ions~~ cores. The potential of electron varies periodically with periodicity of ion core

(i) V is maximum when e^- is lying between adjacent nuclei
 (ii) V is zero near the ion core (or) nucleus V

Apply Schrodinger's time independent wave eq. for the two regions

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

for $0a$ in diagram $V=0$ then

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

for $-b0$ in diagram $V=V_0$ then

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

$$\text{Put } \alpha^2 = \frac{2m}{\hbar^2} (E) \psi \text{ & } \beta^2 = \frac{2m}{\hbar^2} (V_0 - E) \psi \text{ then } (\because V_0 > E)$$

$$\frac{d^2\psi}{dx^2} + \alpha^2 \psi = 0 \rightarrow (3) \quad \& \quad \frac{d^2\psi}{dx^2} - \beta^2 \psi = 0 \rightarrow (4)$$

According to zone theory we know $\psi = u_k(x) e^{ikx} \rightarrow (7)$

Diffr. eq. (5) w.r.t. x

$$\frac{d\psi}{dx} = \frac{\partial}{\partial x} [u_k(x) e^{ikx}] \quad \left[\frac{\partial}{\partial x} \cdot \text{uv} \right]$$

$$\frac{d\psi}{dx} = u_k \frac{\partial u_k}{\partial x} e^{ikx} + u_k i k e^{ikx}$$

Again diffr. w.r.t. x

$$\frac{d^2\psi}{dx^2} = \left[e^{ikx} \frac{\partial^2 u_k}{\partial x^2} + \frac{\partial u_k}{\partial x} (i k e^{ikx}) \right] + i k \left[u_k i k e^{ikx} + e^{ikx} \frac{\partial u_k}{\partial x} \right]$$

$$\frac{d^2\psi}{dx^2} = e^{ikx} \frac{\partial^2 u_k}{\partial x^2} + i k e^{ikx} \frac{\partial u_k}{\partial x} - k^2 u_k e^{ikx} + i k e^{ikx} \frac{\partial u_k}{\partial x} \rightarrow (8)$$

Substituting (8) in (5)

$$e^{ikx} \frac{\partial^2 u_k}{\partial x^2} + i k e^{ikx} \frac{\partial u_k}{\partial x} - k^2 u_k e^{ikx} + i k e^{ikx} \frac{\partial u_k}{\partial x} + \alpha^2 e^{ikx} u_k = 0$$

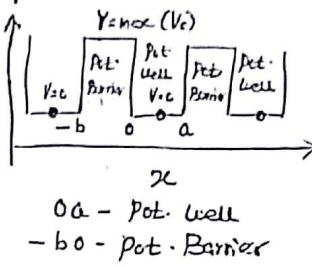
\therefore by e^{ikx}

$$\frac{\partial^2 u_k}{\partial x^2} + i k \frac{\partial u_k}{\partial x} - k^2 u_k + i k \frac{\partial u_k}{\partial x} + \alpha^2 u_k = 0$$

$$\frac{\partial^2 u_k}{\partial x^2} + 2 i k \frac{\partial u_k}{\partial x} + (\alpha^2 - k^2) u_k = 0 \rightarrow (9)$$

similarly for (8) in (6)

$$\frac{\partial^2 u_k}{\partial x^2} + 2 i k \frac{\partial u_k}{\partial x} + (\beta^2 + k^2) u_k = 0 \rightarrow (10)$$



Solutions for eq (7) & (8) is

$$U_1 = A e^{i(\alpha-k)x} + B e^{-i(\alpha+k)x} \rightarrow (11)$$

$$U_2 = C e^{(B-ik)x} + D e^{-(B+ik)x} \rightarrow (12)$$

Apply boundary conditions to above equation such that

$$U_1(x=0) = U_2(x=0) = 0$$

$$U_1(x=a) = U_2(x=b) = -b$$

$$\frac{\partial U_1}{\partial x} \Big|_{x=0} = \frac{\partial U_2}{\partial x} \Big|_{x=0} = 0$$

$$\frac{\partial U_1}{\partial x} \Big|_{x=a} = \frac{\partial U_2}{\partial x} \Big|_{x=b} = -b$$

$$\text{Then we get, } A + B = C + D \rightarrow (13)$$

$$A i(\alpha-k) - B e^{i(\alpha+k)} = C(B-ik) - D(B+ik) \rightarrow (14)$$

$$A e^{i(\alpha-k)a} + B e^{-i(\alpha+k)a} = C e^{-(B-ik)b} + D e^{(B+ik)b} \rightarrow (15)$$

$$A i(\alpha-k) e^{i(\alpha+k)a} - B e^{i(\alpha+k)} e^{i(\alpha+k)a} = C(B-ik) e^{-(B-ik)b} - D(B+ik) e^{(B+ik)b} \rightarrow (16)$$

For eq (13), (14), (15) & (16) a non zero solution exist only if the determinant of the coefficient A, B, C, D vanishes

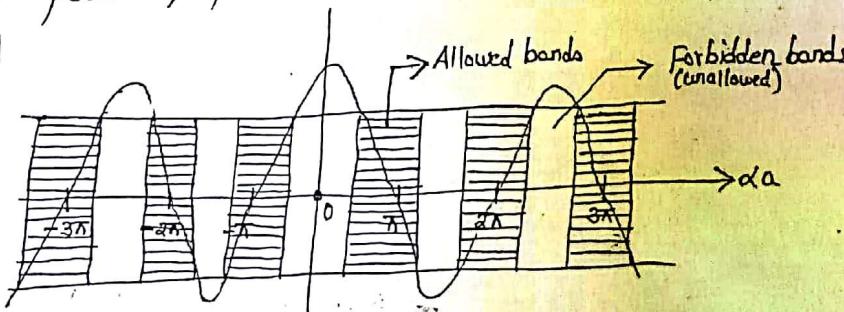
$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ i(\alpha-k) & -i(\alpha+k) & (B-ik) & -(B+ik) \\ e^{i(\alpha+k)a} & -e^{i(\alpha+k)a} & e^{-(B-ik)b} & e^{(B+ik)b} \\ i(\alpha-k)e^{i(\alpha+k)a} & -i(\alpha+k)e^{i(\alpha+k)a} & (B-ik)e^{-(B-ik)b} & -(B+ik)e^{(B+ik)b} \end{bmatrix} = 0$$

By solving the determinant we get

$$\frac{\beta^2 + \alpha^2}{\alpha \beta} \sin \beta b \sinh \alpha a + \cosh \beta b \cosh \alpha a = \cos k(a+b) \rightarrow (17)$$

$$\text{Again solving the above eq, } \frac{P}{\alpha a} \sin \alpha a + \cos \alpha a = \cos ka \rightarrow (18)$$

Here P - power of potential well & coska takes value between +1 and -1



To find Energy of particles

Consider $p = \alpha$ then eq (18) becomes

$\sin \alpha = 0$ and we know $\sin n\pi = 0$

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

From eq (3) $\alpha^2 = \frac{2mE}{\hbar^2}$

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

$$\frac{n^2\pi^2 \hbar^2}{a^2 2m} = E \Rightarrow \frac{\hbar^2 \pi^2 h^2}{a^2 2m 4\pi^2} = E \quad [\because \hbar = h/2\pi]$$

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

Discrete Energy of particle - states Insulating nature of solid

Consider $p=0$ then eq (18) becomes

$$\cos \alpha = \cos ka \Rightarrow \alpha = k \Rightarrow \alpha^2 = k^2$$

we know $k = \frac{2\pi}{\lambda} \Rightarrow k^2 = \frac{4\pi^2}{\lambda^2}$

Also $\alpha^2 = \frac{h^2}{m^2 v^2}$ (According to de-Broglie wave equation)

then $k^2 = \frac{4\pi^2 m^2 v^2}{h^2}$ and $\alpha^2 = \frac{2mE}{\hbar^2}$ (from eq 3)

Then $\frac{2mE}{\hbar^2} = \frac{4\pi^2 m^2 v^2}{h^2}$

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

$$E = \frac{4\pi^2 m^2 v^2 \hbar^2}{4\pi^2 2m h^2} \quad [\because \hbar = h/2\pi]$$

$$E = \frac{1}{2} mv^2$$

Above indicates kinetic energy of particle states conducting nature of solid. (ie) particle is completely free and no energy levels exist.

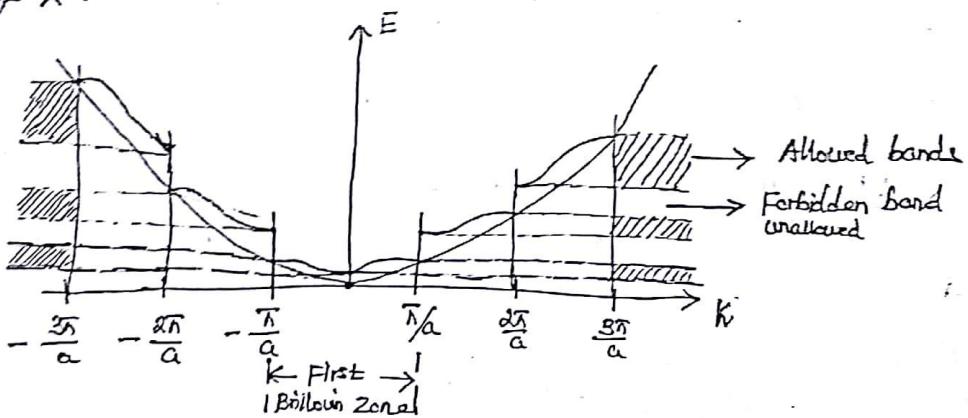
Brillouin Zone is representation of permissible values of k of the electrons in one, two or three dimension system. This is the energy spectrum of electrons moving in a periodic potential field is divided into allowed zones and forbidden zones.

When a parabola representing the energy of free electron is compared with electron energy in periodic field, discontinuities in parabola occurs at values of k given by

$$k = \frac{n\pi}{a} \quad \text{where } n = \pm 1, \pm 2, \pm 3 \dots$$

We know $k = \frac{2\pi}{\lambda} \Rightarrow \frac{2n}{\lambda} = \frac{n\pi}{a} \Rightarrow [2a = n\lambda]$ is in the form of Bragg's diffraction law $d \sin\theta = n\lambda$, ($\sin 90^\circ = 1$)

Thus we find electrons travelling through the periodic array of atom in crystal get diffracted when they satisfy Bragg's law. Thus two electron positions of different P.E are possible for same value of k .



For the region $k = +\frac{\pi}{a}$ to $-\frac{\pi}{a}$, electrons has allowed Energies.

This Zone is called First Brillouin Zone

Then $k = \frac{\pi}{a}$ to $\frac{2\pi}{a}$ & $-\frac{\pi}{a}$ to $-\frac{2\pi}{a}$, electron has next allowed Energy. This Zone is called Second Brillouin Zone

A discontinuity in energy of electron between first & second zone is called Forbidden band

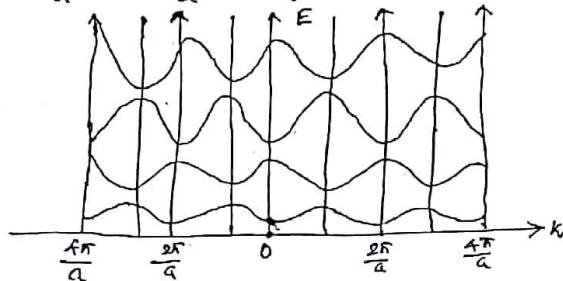
E-k diagram

The dependence of energy of electron on the wave number 'k' is given by E-k diagram.

There are three types of E-k diagrams:

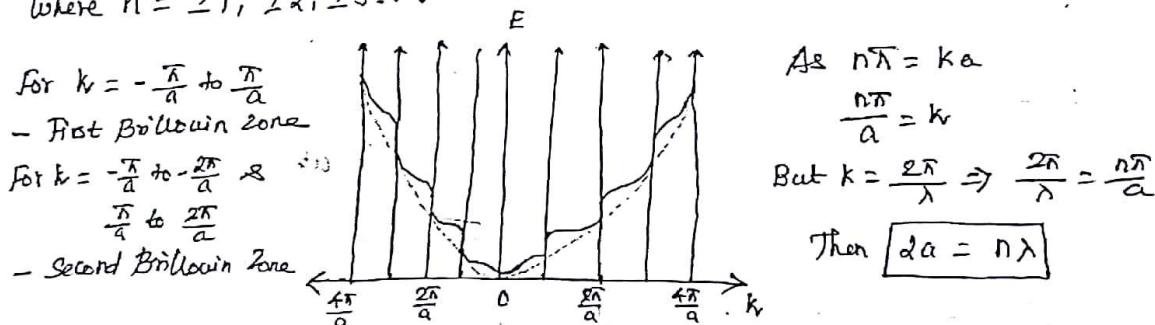
1) Periodic Zone Scheme - (E-k) diagram

Here periodic repetition of allowed energy values corresponding to each allowed band can be represented as being obtained by the periodic repetition of the region $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$ through whole of k-space.



2) Extended Zone Scheme - (E-k) diagram

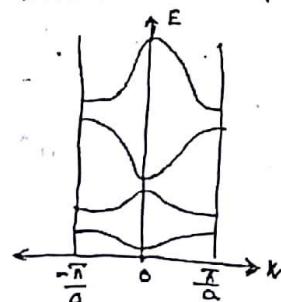
In this scheme, different bands are drawn in different zones in k-space. Hence a discontinuity is observed at $k = \pm \frac{n\pi}{a}$ where $n = \pm 1, \pm 2, \pm 3, \dots$



The discontinuity in the curve is due to Bragg law & reflections at edges of allowed bands (i.e.) $k = \pm n\pi/a$

3) Reduced zone scheme - (E-k) diagram

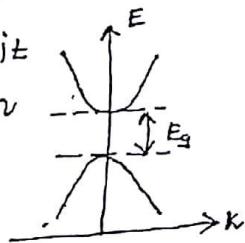
In this scheme, from right or left through distance $\frac{2\pi}{a}$ which are integral multiples of $\frac{2\pi}{a}$ so that they all fit within the interval $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$ the first Brillouin zone.



Direct and Indirect band gap in Semiconductors

1) Direct bandgap in Semiconductors

As we know $P = \hbar k$, then $P \propto k$, if the condition is observed in E-K diagram in particular [reduced zone (E-K) diagram] then it is called Direct bandgap Semiconductor. Here the minimum energy level of Valence band aligns with the minimum energy level of Conduction band. A direct recombination occurs with release of energy equal to energy difference (forbidden gap) between two levels. The probability of radiative recombination is high and hence direct bandgap Semiconductors are preferred for making optical sources [LED, Display, Laser].

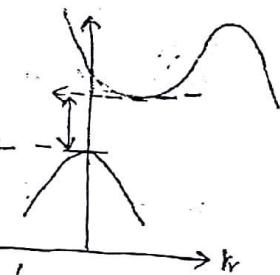


Also the k values of bottom of Conduction band and top of Valence band are same. Photon assisted transition occurs and so low change in momentum can cause recombination process to proceed.

Eg for Direct bandgap Semiconductors : GaAs, ZnS.

2) Indirect bandgap in Semiconductors

Here $P \neq k$, if the condition is observed in E-K diagram in particular [reduced zone (E-K) diagram] then it is called indirect bandgap Semiconductor. Here the maximum energy level of Valence band and minimum energy level of Conduction band are misaligned with respect to momentum. Due to relative difference in momentum, first the momentum is concerted by release of energy and only after both the momenta align themselves. The probability of radiative recombination is comparatively less.



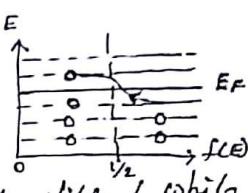
Also k values of bottom of Conduction band and top of Valence band are different. Here phonon assisted transition occurs which is horizontal in nature & the momentum of phonons are high. Therefore band to band transition with emission of photons must be accompanied by the emission/absorption of a phonons.

At $T=0K$, all the levels below E_F are filled & all levels above E_F are completely empty for given system

When $T > 0K$ then $E = E_F$

$$f(E) = \frac{1}{1 + e^{\frac{E-E_F}{kT}}} = \frac{1}{1+1} = \frac{1}{2}$$

When $T > 0K$, some levels above E_F are partially filled while some levels below E_F are partially empty



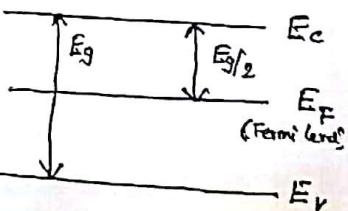
Influence of donor and acceptor in Semiconductors

In pure Semiconductor like Si, Ge, all the valence electrons are intact and no free electrons are available for current conduction. In order to conduct, the electron from top of the full valence band have to move into the conduction band by crossing the forbidden energy gap.

The electric field that needs to be applied to do this work is extremely large. The other possibility by which this transition can be brought is by thermal excitation.

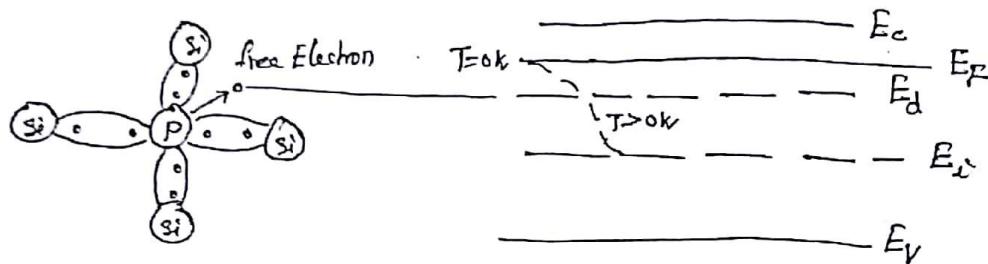
At room temperature, thermal energy available can excite limited number account for conduction. In Intrinsic Semiconductor the conduction is due to the intrinsic processes characteristic of the crystal in question.

If Si & Ge are considered, the electrons that are excited from top of valence band to bottom of conduction band by thermal energy are responsible for conduction. (E_F) in such cases lies middle of forbidden energy gap (E_g). Then, electrons require large energy to cross this Energy band gap. So Electrical Conductivity always decreases. In order to increase electrical conductivity, we have to add impurities to pure Semiconductor which will increase concentration of charge carriers and shift the Fermi level.



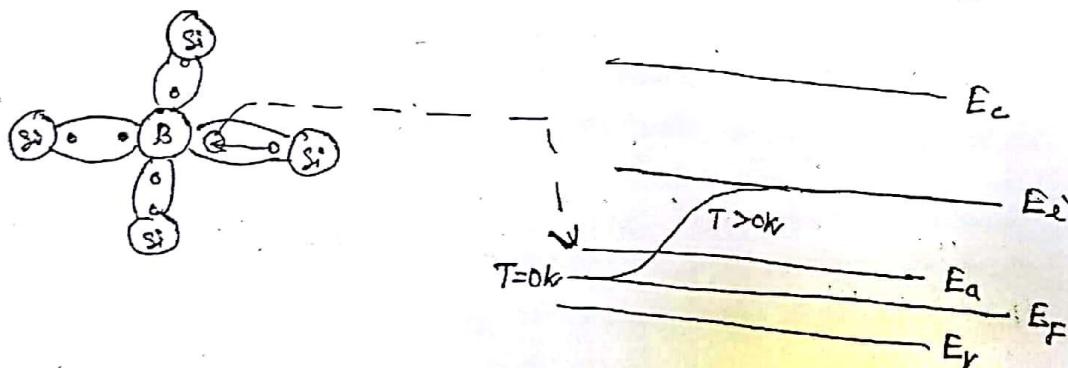
1) Influence of Donor

Consider pure Semiconductor is added with pentavalent impurity. The addition of pentavalent impurity gives free electrons to present near the conduction band and shift fermi level (E_F) between conduction band and free electron level called donor level (E_d)



2) Influence of acceptor

Consider pure Semiconductor is added with trivalent impurity. The addition of trivalent impurity gives holes to present near the top of valence band and shift fermi level (E_F) between valence band (E_v) and hole level called acceptor level (E_a)



Concept of phonons

Particles derived from the vibrations of atoms in a solid called phonons. Also called quasiparticles.

Characteristics of phonons

- 1) Phonons carry momenta, Energy
- 2) Phonons do not carry any part in altering the internal structure of any host body
- 3) According to current studies, Phonons do not have a rest mass so that overall mass change in the particle or in collisions is negligible.
- 4) It can travel from one object to another.
- 5) They are responsible for electrical and thermal properties of Condensed matter
- 6) It has rest mass (or) Average mass.
- 7) Longitudinal waves

$$\text{The Energy of Phonons} = \frac{\hbar\omega}{= \hbar(2\pi)^2}$$

Hence in Lattice structure, vibrations are created by atoms, the quantised lowest state energy of vibration is called Phonon

Non-equilibrium carrier densities - (Properties of carriers)

Up until now, we have only considered the thermal equilibrium carrier densities, n_0 and p_0 . However most devices of interest are not in thermal equilibrium.

The constant temperature is not a sufficient condition for thermal equilibrium. In fact, applying a non-zero voltage to a device (or) illuminating it with light will cause a non-equilibrium condition, even if the temperature is constant.

To describe a system that is not in thermal equilibrium, we assume that each of the carrier distributions is still in equilibrium with itself. Such assumption is justified on the basis that electrons weakly interact with each other and interact with holes only on much larger time scale.

As a result, the electron density can still be calculated using the Fermi-Dirac distribution function, but with a different value of Fermi Energy. The total carrier density for a non-degenerate Semiconductor is then described by

$$n = n_0 + \delta n = n_i \exp \left[\frac{E_n - E_F}{kT} \right]$$

Where δn - excess electron density

E_n - quasi-Fermi Energy for electrons

Similarly

$$p = p_0 + \delta p = n_i \exp \left[\frac{E_p - E_F}{kT} \right]$$

Where δp - excess hole density

E_p - quasi-Fermi energy for holes

Effective mass of electron and hole (m^*)

When an electron in a periodic potential of lattice is accelerated by an electric field or magnetic field, then the mass of electron is called effective mass (m^*).

$$\text{Force acting on electron } (F) = m^* \times a \Rightarrow a = F/m^* \rightarrow (1)$$

According to Quantum theory, electron moving with velocity (v) can be treated as wave packet moving with group velocity.

$$V_g = \frac{d\omega}{dk} = \frac{d}{dk}(2\pi\nu) \quad [\because \omega = 2\pi\nu]$$

$$V_g = \frac{\partial P}{\partial k} \cdot 2\pi \Rightarrow \frac{\partial}{\partial k} \left[\frac{E}{h} \right] 2\pi \quad [\because P = E/h]$$

$$V_g = \frac{2\pi}{h} \left[\frac{\partial E}{\partial k} \right] \Rightarrow \frac{1}{\hbar} \left[\frac{\partial^2 E}{\partial k^2} \right] \rightarrow (2) \quad [\because h = 2\pi\hbar]$$

$$\text{Since, acceleration } (a) = \frac{dV_g}{dt} = \frac{\partial}{\partial t} \left[\frac{1}{\hbar} \left(\frac{\partial^2 E}{\partial k^2} \right) \right] \rightarrow (3)$$

$$= \frac{1}{\hbar} \frac{\partial^2 E}{\partial k \cdot \partial t} = \frac{1}{\hbar} \frac{\partial^2 E}{\partial k^2} \cdot \frac{dk}{dt} \rightarrow (3)$$

$$\text{we know } P = \hbar k \quad (\text{i.e. } k = \frac{2\pi}{\lambda} \Rightarrow \frac{2\pi P}{\hbar})$$

$$k = P/\hbar \Rightarrow \frac{1}{\hbar} k = P \rightarrow (4)$$

$$\text{Diff. eq. (4) w.r.t. } (t) \text{ then } \frac{dp}{dt} = \frac{1}{\hbar} \frac{dk}{dt}$$

$$F = \frac{1}{\hbar} \frac{dk}{dt} \quad [\because \frac{dp}{dt} = F]$$

$$\frac{F}{\hbar} = \frac{dk}{dt} \rightarrow (5)$$

$$\text{Sub (5) in (3) then } a = \frac{1}{\hbar} \frac{\partial^2 E}{\partial k^2} \left(\frac{F}{\hbar} \right)$$

$$a = \frac{F}{\hbar^2} \left(\frac{\partial^2 E}{\partial k^2} \right) \rightarrow (6)$$

Comparing eq. (6) and eq. (1), then

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \left(\frac{\partial^2 E}{\partial k^2} \right)$$

$$m^* = \hbar^2 \left(\frac{\partial k^2}{\partial E} \right) \text{ (or)} \quad \boxed{m^* = \hbar^2 / \left(\frac{\partial^2 E}{\partial k^2} \right)}$$

The above eq shows effective mass is determined by $\left(\frac{\partial^2 E}{\partial k^2} \right)$

which is curvature \rightarrow If large - m^* is low

If small - m^* is high

Fermi Level is important in theory of solids which decides electrical conductivity and in particular for Semiconductors

The concept actually comes from Fermi Dirac statistics

$$(i.e) \text{ For a given system } n_i = \frac{g_i}{e^{(E_i + \beta E_i)/kT} + 1} \quad (or) \quad \frac{g_i}{e^{(E_i - E_F)/kT} + 1}$$

n_i - number of particles in energy range (dE)

E_F - Fermi Energy

E_i - Energy of allowed levels

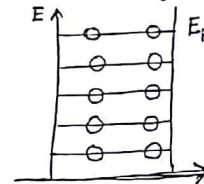
g_i - Allowed Energy states in the energy range (dE)

Fermi Level is determined by Fermi Energy

Energy of highest occupied level at $T=0K$ for the given system

when $T=0K$

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



when $T > 0K$

$$E_F = E_{F_0} \left(1 - \frac{\pi^2}{12} \left(\frac{kT}{E_{F_0}} \right)^2 \right) \quad \text{where } E_{F_0} \text{ Fermi Energy at } T=0K$$

when Temperature increases, E_F slightly decreases

Probability of occupation - determined by using Fermi Dirac distribution function.

If $f(E)$ is Fermi Dirac distribution function then $f(E) = \frac{N(E)}{M(E)}$

$M(E)$ - Allowed Energy States in energy range (dE)

$N(E)$ - Number of Particles in the same range

$$f(E) = \frac{N(E)}{M(E)} = \frac{1}{e^{(E_i - E_F)/kT} + 1}$$

$f(E)$ has values between (0) and (1)

The probability of particle occupation for given system at

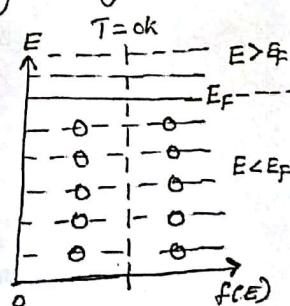
$T=0K$

(i) When $E < E_F \Rightarrow E - E_F = -ve$ quantity

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

(ii) When $E > E_F \Rightarrow E - E_F = +ve$ quantity

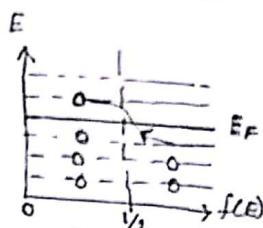
$$f(E) = \frac{1}{1 + e^{\infty}} = \frac{1}{1 + \infty} = 0$$



At $T=0K$, all the levels below E_F are filled & all levels above E_F are completely empty for given system.

When $T > 0K$ then $E = E_F$

$$f(E) = \frac{1}{1+e^{\frac{E-E_F}{kT}}} = \frac{1}{1+1} = \frac{1}{2}$$



When $T > 0K$, some levels above E_F are partially filled while some levels below E_F are partially empty

Influence of donor and acceptor in Semiconductor

In pure Semiconductor like Si, Ge, all the valence electrons are intact and no free electrons are available for current conduction. In order to conduct, the electron from top of the full valence band have to move into the conduction band by crossing the forbidden energy gap.

The electric field that needs to be applied to do this work is extremely large. The other possibility by which this transition can be brought is by thermal excitation.