

I N D E X

NAME: Surbhi Shekhare ROLL NO.: 20BCSI14
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[illegible]

Energy band Structure of a Solid & classification of Solids on the basis of energy diagram.

In a crystal (solid) there are a no. of atoms arranged in a regular periodic structure. The extent of energy level splitting depends on the nearness of atoms in it. Let N identical atoms form the crystal. An isolated atom has discrete energy levels. as shown in fig, fig(b) shows an atom sitting at origin of coordinate system and let us assume that other atoms approaches this along the z axial direction and half at the equilibrium distance a called lattice constant of crystal. As atom approach a continuously rising electrostatic interaction occurs b/w them & each energy level splits up into many distinct levels and form energy band as shown in fig. (a) depicts the effect of slicing of fig(b) at a_0 & represents the energy band structure of crystal. It is seen that corresponding to equal allowed energy level of an isolated atom, there form an allowed energy level band & also separated forbidden bands of energy N empty levels.

Degree of splitting depends upon their depth in atom. The e^- s in atom shells screen the core e^- s belonging to inner shells due to which the energy levels of inner shell e^- s splits to a lesser degree. They form narrow core bands. They are always completely filled & do not participate in conduction. In contrast the energy levels of valance e^- s are split more & form wider bands.

In general N interacting atoms cause an energy level to split into $(2l+1)N$ levels. Thus s level ($l=0$) splits into N levels whereas p -level consists of p_x, p_y, p_z splits up into $3N$ levels.

Consequently maximum e^- capacity of an s -band is $2Ne^-$ s whereas the capacity of a p -band is $6Ne^-$ s.

While occupying an energy band, e^- s start from the lowest energy level in the band fill in level after the other in the ascending order of energy. When $2Ne^-$ s occupy N -levels available in the band, the band is said to be completely filled. In the case of non-availability of $2Ne^-$ s the energy band gets partially filled. When there are no energy e^- s to occupy the levels the energy band remain vacant.

The width of an allowed or forbidden energy band is generally of the order of a few eV. As N is very

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large, the energy separation b/w successive energy levels in an allowed band is very large, the energy separation 'small' is of $\sim 10^{-27} \text{ eV}$. At room temp. K.E of $e^-s \sim KT (\approx 0.026 \text{ eV})$ which is very large as compared to the energy level separation in an allowed band. So e^-s can easily move into higher vacant levels within allowed energy band either due to thermal energy or due to a small externally applied field. On other hand e^-s can not jump across a forbidden band under normal thermal energy possessed by them or due to an applied electric field. High temperature required to cause inter-band e^- transition.

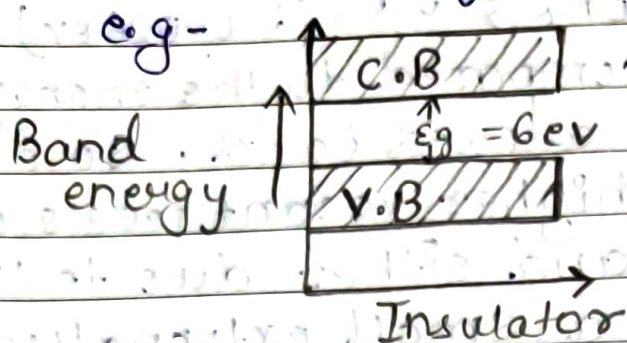
Classification of Bands in Solids:

- Valance band
- Conduction band
- forbidden energy gap.

Valance Band:- e^-s in outermost orbits are called valance e^-s . The range of energies possessed by the valance e^-s is known as valance band,

Conduction Band:- In some solids valance e^-s are loosely band (attracted) to nucleus. At room temp. these e^-s move. The range of energies possessed by conduction e^-s known as conduction band. For insulators this band is completely empty & for conductors this band is partially filled. ~~forbidden energy gap~~

forbidden Energy gap :- Separation both C.B & V.B on energy level diagram called forbidden energy gap.

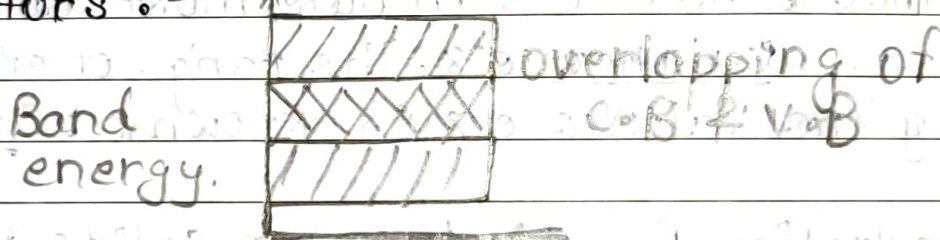


➤ Classification :-

- **Insulator :-** At room temp. valance e^- s of solids not have sufficient energy to cross over to the C.B.

When temp. is $\uparrow$ ed there e^- s gain energy enough & cross the energy gap. Hence the resistance of insulator $\downarrow$ ed with increase in temp. Hence it has -ve temp. coeff. -

- **Conductors :-**

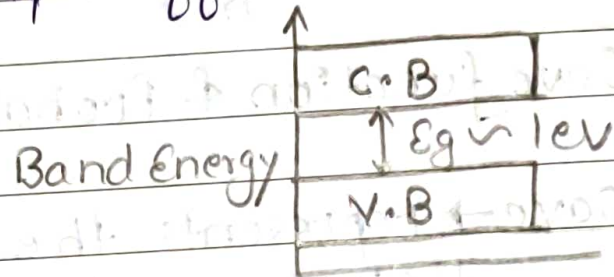


current can easily flow :- of free e^- s. metals good conductor due to the flow that valence e^- s metals being essentially free. on the band theory this is depicted as an overlap of V.B and C.B. so that at least a fraction of valence e^- s can move through material Cu, Al, Au (gold).

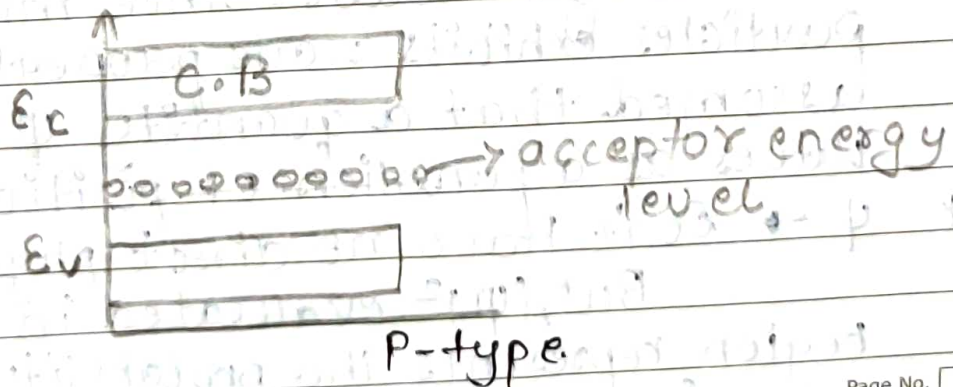
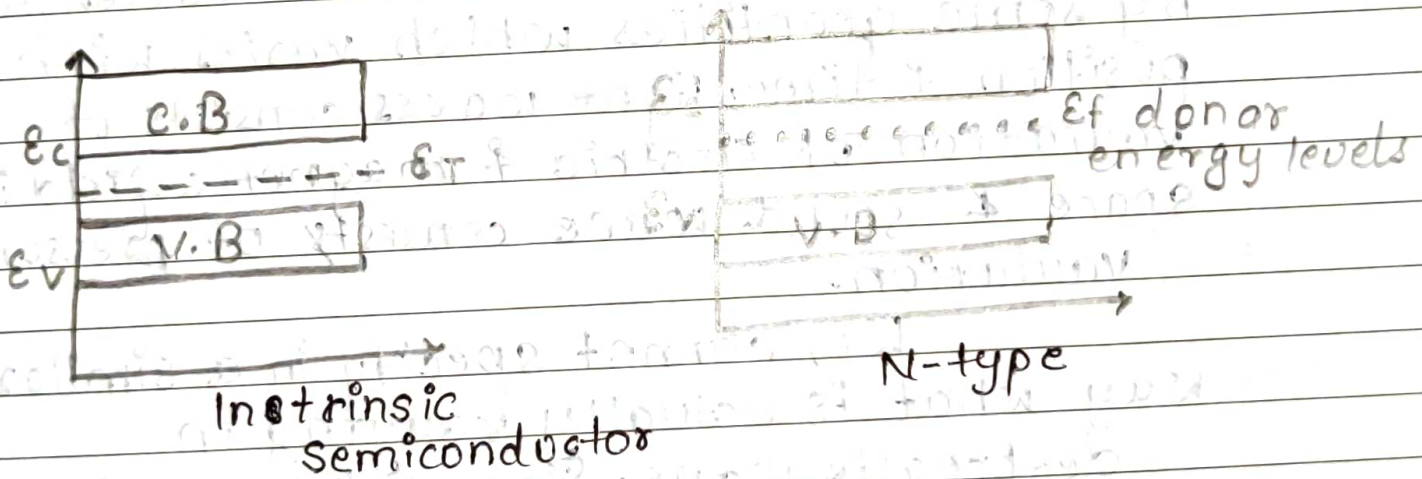
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- Semiconductors - Electrical conductivity both insulator and conductor can be varied under external electrical field. In semiconductor v.B is almost filled & c.B is also empty $E_g \sim 0.5$ to 1 eV .

At low temp. semiconductor behaves as insulator but at room temp. some e^- cross over the c.B. As temp. $\uparrow$ and more valence e^- cross over to c.B so conductivity $\uparrow$ hence, resistivity $\downarrow$. So, it has -ve temp. coefficient of temp.



> fermi energy - highest occupied energy level of a material at absolute zero temperature.



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* Density of States -

In 1924 de-broglie extended the wave particle dualism of light to the material particle. Nature exhibit symmetry.

light can
 sometimes
 act as
 → wave
 → particle

moving particle is associated with wavelength
 $\lambda = \frac{h}{mv}$

Wave function & Probability of Interpretation:

Wave → represents the propagation of a disturbance in medium. We are familiar with light, water & sound wave.

These waves are characterised by some quantities which varies with position & time. light waves consists of variation of electric & magnetic field in space & sound wave consists of pressure variation.

We, cannot specify in a similar way what is actually varying in de-broglie wave. Since microscopic particles exhibits wave properties, "it is assumed that a quantity ψ describes the waves as a function of position & time".

→ ψ → Don't have no direct physical signature
 But, $(\psi)^2$ evaluated in a particular region represents the probability of finding in that region.

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* Properties of ψ

- ① It must be finite everywhere and single valued at all points & must be continuous.

In 1926, Erwin Schrodinger measured that the de-broglie waves associated with e^- would resemble the classical waves of light and developed a differential eqⁿ that describes the behaviours of matter waves.

mass(m), Energy (E) & momentum (P)

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

$$E = K.E + P.E \\ = \frac{1}{2}mv^2 + V \\ = \frac{P^2}{2m} + V$$

$$\psi = Ae^{\frac{i}{\hbar}(Et - Px)} \\ \eta = \frac{h}{2\pi}$$

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar} \psi \\ \frac{\partial \psi}{\partial x} = \frac{iP}{\hbar} \psi$$

Multiplying both side by ψ
 $\psi \cdot \left(\frac{P^2}{2m} + V \right) \psi$

- ① $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$ (Single directional time independent)

- ② $\nabla^2 \psi + \frac{2m}{\hbar^2} \psi (E - V) = 0$ (3-D time independent eqⁿ)

∇ → Del or variable operator

$$\nabla = \hat{i} \frac{d}{dx} + \hat{j} \frac{d}{dy} + \hat{k} \frac{d}{dz}$$

∇^2 is called laplacian operator.

$$\nabla^2 = \hat{i}^2 \frac{d^2}{dx^2} + \hat{j}^2 \frac{d^2}{dy^2} + \hat{k}^2 \frac{d^2}{dz^2} \rightarrow \text{To be continued on XYZ.}$$

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(3) $\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V\right) \psi = i\hbar \frac{d\psi}{dt}$ (single directional time dependent eqn)

(4) $-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = i\hbar \frac{d\psi}{dt}$ (3-D eqn) (time independent)

ψ is the function at x (position) & t (time) so writing ψ is equivalent to writing $\psi(x, t)$ in all above eqn.

Using these eqn we can explain energy spectrum of particle in 1-D box.

$\psi=0$ $V=0$ $\psi=0$ $V=0, 0 < x < a$
 $\psi \neq 0$ $\psi \neq 0$ $= V_0, x \leq 0 \text{ \& } x \geq a$

In the box pot. of particle is always zero so we can use this information with previous eqn to create a differential eqn.

(1) $\Rightarrow \frac{d^2\psi}{dx^2} + \psi \frac{2mE}{\hbar^2} = 0$ (using)

let $k = \frac{\sqrt{2mE}}{\hbar}$

$\frac{d^2\psi}{dx^2} + k^2\psi = 0$

soln of this eqn

$\psi = A \sin(kx) + B \cos(kx)$

Initial condition, $x=0, \psi=0$

$0 = A \cdot 0 + B \cdot 1$

$[B=0]$

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$\psi=0$ & $x=a$

$0 = A \sin(ka) + 0$

$ka = n\pi$ $n \in \mathbb{Z}^+$

$[k = \frac{n\pi}{a}]$

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

$\psi = \sin(\frac{n\pi x}{a})$

$[E_n = \frac{n^2\hbar^2}{8ma^2}] \rightarrow E_1 = \frac{\hbar^2}{8ma^2}$

$[E_n = n^2 E_1]$

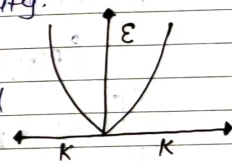
* for free particle in space (No restriction)

k vector describes wave property.

$[E = \frac{\hbar^2 k^2}{2m}]$ $E \propto k^2$

Energy is not quantised

$[\psi_n = A \sin \frac{n\pi x}{a}]$



{ continuous energy spectrum

for each value of n there is corresponding quantum state ψ_n whose energy can be given by

$[E = \frac{\hbar^2}{8ma^2} n^2]$

(1) The lowest energy of particle called zero point energy.

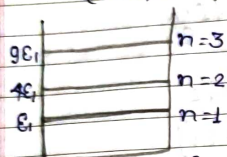
$E_1 = \frac{\hbar^2}{8ma^2}$ (lowest energy or zero point energy)

$[E_n = n^2 E_1]$

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- (2) Bonded e^- can have only discrete energy value corresponding to $n=1,2,3$ & not any arbitrary value.
- (3) Spacing b/w 2 consecutive levels $\uparrow$ as $(n+1)^2 \epsilon_1 - n^2 \epsilon_1 = (2n+1) \epsilon_1$



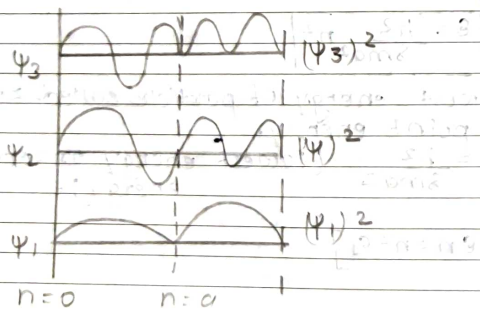
The value of A could be determined by normalizing ψ a/q to which the total probability that the particle is somewhere in the box must be unity.

$$\int P(x) dx = \int (\psi_n)^2 dx = 1$$

$$\int_0^a A^2 \sin^2 n\pi x/a dx = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$$

On integration

Normalised wave function $\psi_n = \sqrt{\frac{2}{a}} \sin n\pi x/a$



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for e^- moving in 3-dimensional box of side a .

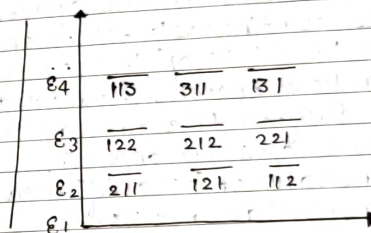
$$k_x = \frac{n_x \pi}{a}, k_y = \frac{n_y \pi}{a}, k_z = \frac{n_z \pi}{a}$$

$$\psi = A \sin(k_x x) \sin(k_y y) \sin(k_z z)$$

$$\left[\epsilon_0 = \frac{h^2}{8ma^2} (n_x^2 + n_y^2 + n_z^2) \right] = \left[\frac{h^2}{8ma^2} n^2 \right]$$

$\downarrow \quad \quad \quad \downarrow$
 $3=0 \quad \quad \quad 1=0$

(38)



- classically a particle in a box could have any i.e. energy but quantum theory shows that the particles are restricted to take only certain discrete value. These allowed values called quantum no. and it a/sec can sequence of boundary conditions imposed.

$n=0$ is not allowed, ψ & $(\psi)^2 \rightarrow 0$ will become zero at every point inside the box.

lower energy state is $E_1 \rightarrow (1,1,1)$ for next higher energy states having there are 3 diff. possibilities

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(112, 121, 211).

These energy states same energy but diff. value of n .

$$E_{112} = E_{121} = E_{211} = \frac{6n^2}{8ma^2}$$

for some example value of n energy is inversely proportional to mass and square of the length of box.

The energy is quantised in the space, so it can't varies continuously. It is only possible when " ma^2 " is of the order of h^2 . As the particle become heavier & box become larger the energy levels becomes more closely spaced.

i.e. permitted energies of e^- confined in a box of 0.1 nm wide are 38 eV.

$$E_1 = 38 \text{ eV}$$

$$E_2 = 152 \text{ eV}$$

$$E_3 = 342 \text{ eV}$$

for a box of microscopic size say 1 cm wide $En = 3.8 \times 10^{-16} n^2 \text{ eV}$. In such cases energy levels becomes so closely spaced that they seem to continuous

The quantum mechanical formula, therefore gives classical for system with dimension $ma^2 \gg h^2$. This is illustration of Bohr's correspondence principle which states the quantum mechanics must yield identical result with those of classical physics in the limit of large quantum n .

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The degeneracy breaks when a small modification is introduced in system by changing length of the box or applying external field.

This aspect is relevant in explaining the fact such as splitting of spectral lines in magnetic & electric field under action of field the degenerated level breaks into separate levels.

Q) Determine the degeneracy of energy level $38h^2$ of a particle in a cubical $8ma^2$ box of side a .

$$\text{Here, } nx^2 + ny^2 + nz^2 = 38$$

$$(nx, ny, nz) \text{ can be } (116, 161, 611)$$

$$\rightarrow (532, 352, 325, 253, 523, 235)$$

$\rightarrow$ 6 fold degeneracy

* Electron Distribution in Solids (fermi dirac statistics)

two types -

Quantum Statistics

- (1) fermi dirac statistics (main focus in course)
- (2) Bose statistics

Fermi Dirac

Particle called fermions

Follows poly exclusion!

Half integral spin

Bose-Stat

particle called Boson

Integral spin & doesn't follow poly exclusion

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Note:- Quantum mechanical character will be lost if energy is given.

Fermi-Dirac Statistics

Assumption of classical Mechanics

[Any no. of particles may have identical energy]

Classical mechanics fails to explain electron contribution to specific heat & magnetic susceptibility.

The electron in solid behaves as fermi particles & follow fermi-dirac stats. In solid we consider

A/q to pauli exclusion principle not more than 2 e-s will go into ground state, two 2 e-s in next higher energy & so on, until all e-s are allocated state of lowest possible energy. Since no. of e- are very large, it is thus understood that even at absolute zero of temp, some electrons have K.E of several e.v for a piece of metal of macroscopic dimension say cm^3 , the energy of ground state (III) is of the order of $5.7 \times 10^{-15} \text{ eV}$ and hence may be taken zero for practical purpose. Also the max. spacing b/w consecutive level less than 10^{-6} eV so that distribution of energy may be regarded as almost continuous or some times quasi-continuous since we are talking

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about an almost continuous range of energies we can represent the probability of occupying a given state by a continuous distribution function. The energy distribution of e-s at any temp. T or the probability ($F(E)$) of an e- occupying a given energy level is expressed by F.D distribution function.

$$F(E) = \frac{1}{1 + \exp. \left(\frac{E - E_F}{kT} \right)}$$

The probability that an electron occupies an energy level E at thermal equilibrium is given by.

where,

$E_F \rightarrow$ fermi level

$F(E) \rightarrow$ fermi factor

- Note - (1) In general E_F may or may not correspond to an energy level but a reference with which other energies can be compared.
(2) The energy probability of the electron to occupy the energy level E rises with temp.

Case-01 ($T=0K$)

At absolute zero, electrons occupy energy levels in pairs starting from bottom of the band up to an upper level designated as E_F leaving the uppermost level vacant.

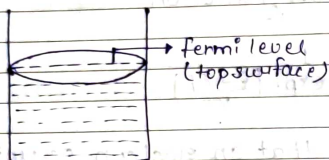
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Fermi level can be defined as the uppermost filled energy level in a conductor at 0K.

Fermi Energy is defined as the max^m energy that a free electron can have in a conductor at 0K.



(Analogy) water at rest

① for $E < E_f$, $E - E_f = -ve$

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

Note: $f(E) = 1$, indicates that all the energy level lying below the level E_f , are occupied.

② for $E > E_f$, $E - E_f = +ve$

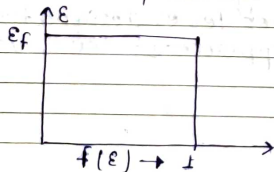
$$f(E) = \frac{1}{1 + e^{(E - E_f)/0}} = \frac{1}{1 + e^{+\infty}} = \frac{1}{\infty} = 0$$

Note: $f(E) = 0$, implies that all the levels above E_f are vacant.

③ for $E = E_f$, $E - E_f = 0$,

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

This implies $0 < \text{occupancy} < 1$ of e^- s.



Case-02

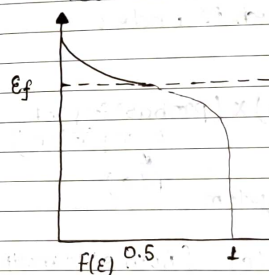
On heating e^- get excited to higher energy levels.

In general $E_f \gg kT$

Therefore, e^- s lying deep under conduction band energy not sufficient for transition to upper unoccupied energy level.

→ At normal temp. e^- s near Fermi level can be excited. These levels make up a narrow band of width kT directly adjacent to Fermi level.

→ Due to Result of thermal excitation the E_f probability of finding e^- s just below Fermi level $\downarrow$ es.



→ Fermi level can also be defined as the energy level with occupancy 0.5 at $T > 0K$.

② Fermi energy is the avg. energy possessed by electrons participating in conduction in metal.

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Density of States

→ The fermi function doesn't by itself give the no. of e^- which have a certain energy, it gives us only the probability of occupation of energy by a single e^- .

Since even at the highest energy, the diff. b/w neighbouring energy levels is as small as 10^{-6} eV, we can say that in a macroscopically small energy interval small but discrete energy levels are present.

To know the actual no. of e^- s with a given energy one should know the no. of states in system which is under consideration.

$$\text{Actual No. of } e^- = (\text{No. of states}) \times (\text{probability of occupation})$$

$N(E)$

$Z(E)$

$F(E)$

$E \rightarrow$ Energy of system

$$N(E) = Z(E) \times F(E)$$

$$N(E)dE = Z(E)dE F(E) \quad (\text{Both side multiply by } dE)$$

Calculation of density of state of e^- s in any energy range (E to $E+dE$).

Consider a cube of side l and we are assuming e^- s travel absolutely freely within volume of specimen, their wave properties limit the energy values that they may take.

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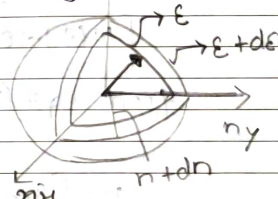
$$E = \frac{h^2}{8m l^2} (n_x^2 + n_y^2 + n_z^2) \quad \text{--- (1) } \quad \text{(Sw. e) } \quad \text{one-3}$$

$$n^2 = n_x^2 + n_y^2 + n_z^2 \Rightarrow E = \frac{h^2}{8m l^2} n^2 \quad \text{--- (2) } \quad \text{--- (3)}$$

Sphere radii n & $n+dn$ (n_x, n_y, n_z) integer value represents an energy state at that point.

Thus, all point on the surface of sphere of radius n will have same energy.

All points within sphere represents quantum states with energies smaller than E .



$\therefore$ no. of energy states within sphere of radius $n \propto$ Vol. of sphere $= \frac{4}{3} \pi n^3$ --- (4)

Re. $n_x, n_y, n_z \rightarrow$ +ve integers.

no. of states of energy $\propto E$ will be given by the octant of sphere i.e. the n value can only be defined in the octant of sphere.

Total no. of quantum states with energy less than equal to $E \propto$ Vol. of 1st octant of sphere

No. of state within one octant of sphere of radius $n = \frac{1}{8} \times \frac{4}{3} \pi n^3$ --- (5)

Similarly the no of states within one octant of a sphere of radius $(n+dn)$ corresponding to energy $E+dE$ is $= \frac{1}{8} \times \left[\frac{4}{3} \pi (n+dn)^3 \right] - \frac{1}{8} \times \left[\frac{4}{3} \pi n^3 \right]$ --- (6)

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∴ No. of energy states having energy values b/w ϵ & $\epsilon + d\epsilon$ given by -

$$N(\epsilon) \cdot d\epsilon = \frac{1}{8} \times \frac{4}{3} \pi (cn + dn)^3 - n^3$$

$$\approx \frac{\pi}{6} (3n^2 dn)$$

terms corresponding to higher power of dn are negligible (such as $(dn^2) \approx 0$).

$$[N(\epsilon) d\epsilon = \frac{\pi}{2} n^2 dn] \quad \text{--- (7)}$$

from eqn (3)

$$n^2 = \frac{8m^2 \epsilon}{h^2} \quad \text{--- (8)}$$

$$n = \left[\frac{8m^2 \epsilon}{h^2} \right]^{1/2} \epsilon^{1/2} \quad \text{--- (9)}$$

(8) differentiating both side -

$$2n dn = \frac{8m^2}{h^2} d\epsilon$$

$$n dn = \frac{4m^2}{h^2} d\epsilon$$

$$N(\epsilon) d\epsilon = \frac{\pi}{2} n (n dn)$$

$$N(\epsilon) d\epsilon = \frac{\pi}{2} \left[\frac{8m^2}{h^2} \right]^{1/2} \epsilon^{1/2} \cdot \frac{4m^2}{h^2} d\epsilon$$

$$\therefore N(\epsilon) d\epsilon = \frac{\pi}{4} \left[\frac{8m^2}{h^2} \right]^{3/2} \epsilon^{1/2} d\epsilon \quad \text{--- (10)}$$

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There are 2 spin states for e^- ($+\frac{1}{2}$, $-\frac{1}{2}$) $2e^-$ of opp. spine can occupy in same state (A/q to Pauli Exclusion pri.)

∴ No. of energy states available for e^- occupancy is double the above value & equal to

$$N(\epsilon) d\epsilon = \frac{\pi}{2} \left[\frac{8m^2}{h^2} \right]^{3/2} \epsilon^{1/2} d\epsilon$$

$$N(\epsilon) d\epsilon = \frac{4\pi}{n^3} (2m)^{3/2} \epsilon^{1/2} d\epsilon \quad \text{--- (11)}$$

Now, density of energy state is given by No. of available e^- states per unit vol. per unit energy range at a certain energy level ϵ .

$$Z(\epsilon) d\epsilon = \frac{N(\epsilon) d\epsilon}{V} = \frac{4\pi}{n^3} (2m)^{3/2} \epsilon^{1/2} \quad \text{--- (12)}$$

$Z(\epsilon)$ called density of state function.

$Z(\epsilon)$ is independent of dimensions (l) of the box & hence applicable for any case.

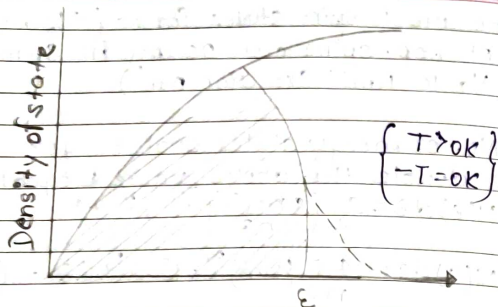
[$Z(\epsilon)$ defined as the NO. of available energy states per unit energy interval centered around ϵ .]

Energy distribution of e^- s

Density of states in the energy interval ϵ to $\epsilon + d\epsilon$ given by eqn (12).

Note that the no. of available energy levels at the lower end of the parabola is considerably less than at higher higher energies.

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The plot $\chi(E)$ vs E at $T=0K$ abruptly to zero at $E=E_F$. This distribution of e^- s is understandable. The electrons cannot crowd in lower levels since they obey Pauli excl. principle (start filling with lowest level till all of them are accommodated) highest level is E_F . Area under curve at $T=0K$ & $T>0K$ must be equal. On heating the conduction e^- s are excited to higher levels giving new distribution of e^- s.

Actually the e^- energy vary from 0 to E_F & also the no. of e^- s increases with the increase of energy which becomes max^m at E_F since at absolute zero $F(E) = 1$, hence the total no. of e^- s is

$$N = \int_0^{E_F} N(E) dE = \frac{4\pi}{h^3} (2m)^{3/2} \int_0^{E_F} E^{1/2} dE$$

$$N = \frac{2}{3} \times \frac{4\pi}{h^3} (2m)^{3/2} E_F^{3/2} \quad \text{--- (1)}$$

The no. of e^- s per unit vol. (density of e^- s) is $n = \frac{N}{V} = \frac{8\pi}{3h^3} (2m)^{3/2} E_F^{3/2}$

$\therefore$ The fermi energy at absolute zero is $E_F \rightarrow E_F = \frac{h^2}{2m} \left(\frac{3n}{8\pi} \right)^{2/3} = 3.65 \times 10^{-19} n^{2/3} \text{ eV}$ --- (2)

further at absolute zero the average energy of an e^- is

$$\bar{E} = \frac{1}{N} \int_0^{E_F} N(E) dE = \frac{4\pi}{Nh^3} (2m)^{3/2} \int_0^{E_F} E^{3/2} dE = \frac{2}{5} \times \frac{4\pi}{Nh^3} (2m)^{3/2} E_F^{5/2}$$

Putting value of N from (1)

$$\bar{E} = \frac{3}{5} E_F \quad \text{--- (3)}$$

- Variation of fermi energy with temp:- fermi energy $\downarrow$ as when the temp. of metal is $\uparrow$ and it can be shown that when $kT \ll E_F$, $E_F \approx E_F(0) \left[1 - \frac{\pi^2}{12} \left(\frac{kT}{E_F(0)} \right)^2 \right]$

The expression (2) for fermi energy is a very useful quantity because it gives the top most energy level at absolute zero from the knowledge of free e^- . E_F is max. energy of the filled state. The corresponding velocity of e^- having KE equal to E_F called fermi velocity & is given by -

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$$\frac{1}{2} m v_f^2 = E_f \Rightarrow v_f = \sqrt{2E_f} \quad \text{--- (4)}$$

& corresponding temp. called fermi temp.

$$kT_f = E_f \quad \left[T_f = \frac{E_f}{k} \right] \quad \text{--- (5)}$$

Ex. for sodium with E_f , 3.2 eV,
 $v_f = 1.1 \times 10^6 \text{ m/s}$ &

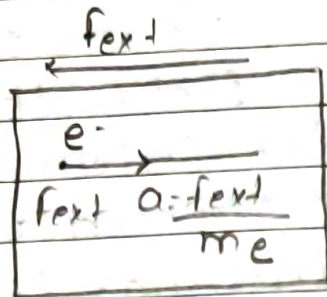
$$T_f = 37100 \text{ K.}$$

* Concept

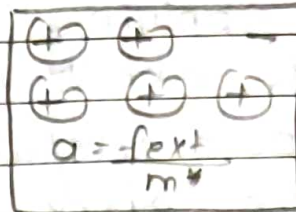
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* Concept of Effective Mass :-

Why is it necessary to talk about concept of effective mass of e^- or hole in solid.



(a)



(b)

Consider 2 situations (a) & (b) in (a) the e^- is moving in vacuum which is an isolated e^- free from any other effect & in fig. (b) the e^- is ~~pro~~ pure inside solid.

For fig (a) $f_{ext} = -e f_{ext} \rightarrow (1)$

Acceleration $a_{vac} = \frac{f_{ext}}{m_e} \rightarrow (2)$

In fig (b) e^- inside the solid & the eq (1) cannot be valid because the movement of an e^- in a lattice will in general be diff. from that of an e^- free space. In addition to external force there will be internal force of attraction b/w the e^- & the ions of crystal lattice. These factors influence the motion of e^- in lattice.

Therefore net force :-

Net force, $F_{total} \Rightarrow f_{ext} + f_{in} \rightarrow (3)$

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Force of e^- in solid =

$$F_{\text{solid}} = F_{\text{ext}} + F_{\text{int}} \quad \text{--- (4)}$$

The e^- in solid will be diff. from a free e^- due to diff. environment. To the outside agent applying electric field, the e^- will appear exhibiting diff. internal max^m be more useful to the external agent if the effect of internal forces (F_{int}) counted in a simple way & if acc. could be calculated by F_{ext} along like something in eqⁿ (2)

for this we take into account all the internal forces, so we will write eqⁿ (4) as

$$F_{\text{solid}} \Rightarrow F_{\text{ext}} \quad \text{--- (5)}$$

$\hookrightarrow$ effective mass.

once m^* considered, the particle can be treated as free & we are not bothered at about the medium in which it is moving.

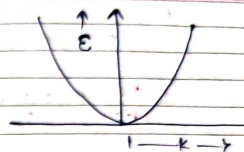
* Interpretation of effective mass from $E-k$ diagram.

consider the free e^- case where E v/s k curve is shown :-

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Energy & Momentum are related as



$$E = \frac{p^2}{2m_0} = \frac{\hbar^2 k^2}{2m_0}$$

$$p = \frac{\hbar^2 k^2}{2m_0} \quad \text{--- (7)}$$

$$\frac{dE}{dk} = \frac{\hbar^2}{2m_0} \times 2k$$

$$\frac{dE}{dk} = \hbar \times \frac{h \times k}{m_0} \rightarrow p \quad \text{--- (8)}$$

$$\left[\frac{dE}{dk} = \frac{\hbar p}{m_0} \right] \quad \text{--- (9)}$$

$$p = m_0 v$$

$$\Rightarrow \frac{dE}{dk} \Rightarrow \hbar v$$

$$\left[\frac{1}{\hbar} \frac{dE}{dk} \Rightarrow v \right] \quad \text{--- (10)}$$

Taking 2nd derivatives of eqⁿ (8)

$$\frac{d^2 E}{dk^2} = \frac{d}{dk} \left(\frac{dE}{dk} \right) \Rightarrow \frac{d}{dk} \left(\frac{\hbar^2 k}{m_0} \right)$$

$$\left[\frac{d^2 E}{dk^2} = \frac{\hbar^2}{m_0} \right]$$

$$\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} = \frac{1}{m_0}$$

$$\left[m_0 \Rightarrow \frac{\hbar^2}{\left(\frac{d^2 E}{dk^2} \right)} \right] \quad \text{--- (11)}$$

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the 2nd derivative of E at k is inversely proportional to mass of particle.

$\frac{d^2E}{dk^2} \rightarrow$ curvature of the energy band in which particle or e^- or hole moving.

Mass of particle is of curvature of the energy band.

for the case of free e^- the mass is a constant. so, the second derivative is also the constant.

In the external electric field e^- acquire accⁿ given in previous eqn & moves in the direction opp. to the applied field because of its -ve charge.

* Normally, we say that the effective mass of an e^- in solid is equal to its mass in the free space.

However, experimentally it is determined that measured value of some e^- of some solids is larger than free e^- mass & in some solids it is slightly less than free e^- mass.

The experimentally determine mass is also called effective mass (m^*). The cause of deviation is the interaction b/w the drifting e^- & the atom in a solid. It is observed that m^* is inversely proportional to the curvature of allowed energy band.

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This implies that m^* depends on the location of e^- in allowed energy band.

for an e^- model when E vs k has a parabolic relationship.

As the mass of e^- is considered to be constant $\therefore \frac{d^2E}{dk^2}$ can also be considered const.

But when e^- moves in a periodic pot. of the crystal lattice, the parabolic relation b/w E and k no longer exists there is breakup in the curve at various zones leading to the forbidden formation allowed & forbidden bands. Near the forbidden band, the curvature of E vs k change & can become -ve (as k approaches zone boundary $\frac{d^2E}{dk^2}$ 1st reduce to 0 & then become -ve).

$\frac{d^2E}{dk^2}$ is no longer constant & also the mass of e^- , actually both of them are a functⁿ of k .

Thus, under periodic pot. mass of e^- given by eqn, $m = \frac{h^2}{4\pi^2} \left(\frac{d^2E}{dk^2} \right)^{-1}$ is known as effective mass & change k .

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Bloch Theorem

Periodic potential:- when e⁻s in 1-D or 3-D in a crystal lattice it consist of regular arrays of atoms arranged in a crystal lattice. An essential prop. of a crystal that is has translational invariance. Means if we pick up the crystal & move it by lattice const. it would look exactly same as before we move it

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

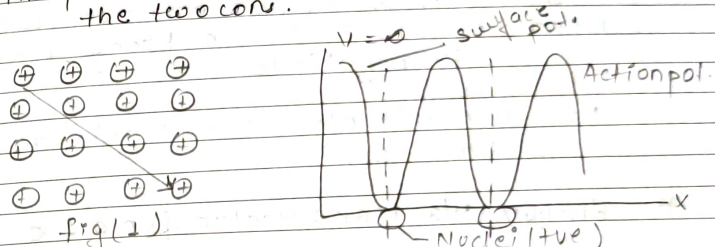
if the pot. is invariant under a translation then the physical prop. of any wave fⁿ that is a soln to the schrodinger eqⁿ must have the same prop. In particular, the probability density must be invariant.

Bloch Theorem

The free e⁻ theory explained some phenomena such as conductivity etc. But it fails to explain why some materials are good conductor, while some are good insulator, & some are semiconductor?

In order to understand the diff. b/w conductor & insulator, it is necessary to incorporate the variation of pot.

Inside a metallic crystal, e⁻s periodic is periodic with periodicity of the lattice. The pot. is min at the site & max b/w the two con.



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

$$\psi = 0 \quad (1)$$

where,

$$V(x) = V(x+a) \quad (2)$$

thus eqⁿ takes the form of

$$\psi(x) = e^{ikx} u_k(x) \quad (3)$$

$u_k(x)$ & $u_k(x+a)$ are the e⁻ wave modulated by periodic functⁿ

After solving we get,

$$k = \frac{2\pi n}{L}$$

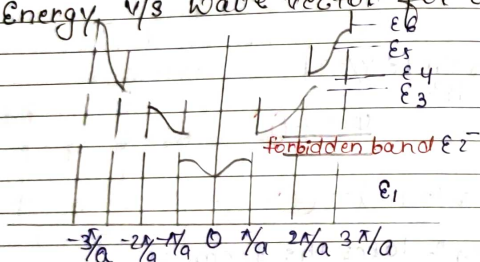
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→ K.P model & E-k diagram,

Here, we discussed about E-k characteristics in an undefined pot. zone. However, to know the exact relationship b/w E v/s k in a defined pot. zone, we need to construct the Kronig-Penney Model.

Pot. is max^m b/w 2 ions & min. at the ion site.

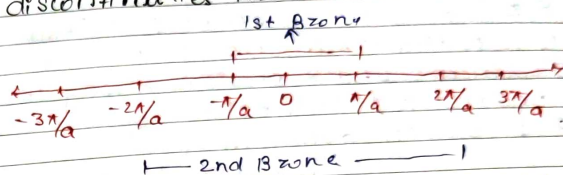
* Energy v/s wave vector for a 1-D



Allowed Band.

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discontinuities in E occurs at $ka = \pm 2\pi n$



At these values of $k = \frac{n\pi}{a}$ a small (res) in momentum will (res) the energy of e^- so that it can jump discontinuously from the top of one allowed band to the bottom of the next region b/w 1st Brillouin zone values of k. for which discontinuities occur called 2nd Brillouin zone & so on above fig. shows B-zones for 1-dimensional lattice.

- ① Near the bottom of band from E-k curve doesn't differ much from E-k curve for free e^- in the these regions $m^* \rightarrow m$.
- ② At point of inflection B the $\frac{d^2E}{dk^2} \rightarrow 0$. In these region $m^* \approx 0$. It means $\frac{d^2E}{dk^2}$ that an external field can not exert any action on the motion of e^- in the region.
- ③ Near the top of allowed band, the $\frac{d^2E}{dk^2} < 0$. m^* of e^- occupying levels near the top of band is -ve. The concept of effective mass provides description of the charge carrier in crystals.

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Brillouin Zones:-

B.Z is a representation of permissive value of k of the e^- s in one, two or 3-D. The concept of BZ provides a way to understand the orig. of allowed & forbidden bands in solids.

The effective mass arises because of interaction of e^- wave packet with periodic lattice. If the interaction b/w them is very large or in other words if there is a strong binding force b/w e^- s the lattice it will be difficult for e^- s to move meaning there by that e^- has acquired a large effective mass.

* Fermi level & carrier concn in Semiconductors:-

We know that Fermi Dirac distribution given by:-

$$f(E) = \frac{1}{\exp\left(\frac{E - E_F}{kT}\right) + 1} \quad (1)$$

In general for semiconductivity, we say that the E_F corresponds to level that has occupancy of $1/2$. This means that E_F is greater than

E_V (valence band energy level) if the conduction band is completely empty & hence E_F must be less than E_C .

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Therefore, $E_V < E_F < E_C$. But its exact portion depends upon temp.

Also, we know that the no. of e^- occupying energy state given by:-

$$n(E) dE \Rightarrow f(E) Z(E) dE \quad (2)$$

$$-E(E) = C E^{1/2} \quad (3)$$

→ Intrinsic Semiconductor:-

$$Z(E) = C(E - E_C)^{1/2} \quad (4)$$

To obtain density of energy states in conduction band is obtained by integrating the energy values from E_C to E to p for

$$n = \int_{E_C}^{\infty} C \frac{\exp\left(\frac{E - E_C}{kT}\right) dE}{\exp\left(\frac{E - E_F}{kT}\right) + 1} \quad (5)$$

Now if we assume that $E_C - E_F \gg 4kT$ then 1 can be ignored

$$n = \int_{E_C}^{\infty} C (E - E_C)^{1/2} \exp\left(-\frac{E - E_F}{kT}\right) dE \quad (6)$$

Now, if $\exp(-E/kT)$ (ves) very rapidly as E grows therefore it is possible to substitute ∞ for E to p & assume that $(E - E_C)/kT = x$.

$$n = C (kT)^{3/2} \exp\left[-\frac{(E_C - E_F)}{kT}\right] \int_0^{\infty} x^{1/2} e^{-x} dx$$

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On simplifying

$$n \rightarrow N_c \exp \left[-\frac{(E_c - E_F)}{kT} \right]$$

$$n \rightarrow 2 \left(\frac{2\pi m^* kT}{h^2} \right)^{3/2}$$

$$n \rightarrow N_c \exp \left(\frac{-E_g}{2kT} \right)$$

condn
↑
band.

$E_F - E_c \rightarrow \frac{E_g}{2}$
↓
fermi level

→ Density of holes near valance band

$$p \rightarrow \int_{E_v}^{\infty} z(E) [1 - f(E)] dE$$

$$z(E) \rightarrow C (E_v - E)^{1/2}$$

Assumed, $1 - f(E) \approx \exp \left(\frac{E - E_F}{kT} \right)$
by approx

Density of holes,

$$p \rightarrow C \int_{E_v}^{\infty} (E_v - E)^{1/2} \exp \left(\frac{E - E_F}{kT} \right) dE$$

$$p \rightarrow N_v \exp \left(-\frac{(E_F - E_v)}{kT} \right) \therefore N_v = 2 \left(\frac{2\pi m^* kT}{h^2} \right)^{3/2}$$

In intrinsic semiconductor, $n \rightarrow p$

$$E_F = \frac{E_c + E_v}{2} + \frac{kT}{2} \ln \frac{N_v}{N_c}$$

→ for intrinsic, $n_i p_i \rightarrow n_i^2$

$$N_c N_v \exp \left(-\frac{(E_c - E_v)}{kT} \right) \Rightarrow n_i \rightarrow \sqrt{N_c N_v} \exp \left(\frac{-E_g}{2kT} \right)$$

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Thus, $n_i p_i \rightarrow n^2$ - for any semiconductor at thermal eqⁿ the product of e⁻ & holes is const.

→ Electrical Conductivity of Semiconductor as a functⁿ of tempⁿ :-

The conductivity of purest int. semiconductor at any temp. is due to intrinsic charge carriers, e⁻ & holes called intrinsic conductivity the general exp is :-

$$\sigma_i \rightarrow e(n_i e + p_i h), \text{ for semi, } n \rightarrow p \rightarrow n_i \left\{ \begin{array}{l} E_c + \frac{E_g}{2} \Rightarrow n_{e,e} \\ E_v \Rightarrow n_{h,h} \end{array} \right.$$

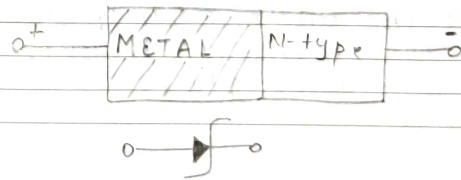
$$\sigma_i = 2e \left(\frac{2\pi kT}{h^2} \right)^{3/2} (m_e^* m_h^*)^{3/4} \exp \left(\frac{-E_g}{kT} \right)$$

$\mu_e \rightarrow \frac{V_e}{E}, n_{e,e}$

* Schottky Diode :- is a metal-semiconductor junction diode.

construction -

consists of a junction b/w metal like Pt, Au, Ag, tungsten etc & N-type semiconductor. most common semiconductor material used is silicon. GaAs can also be used which has lower rised higher operating freq. SO has no depletion layer.



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(Saathi)

Operation :- Metals have work fn which is defined as the minimum energy required for an electron to escape into vacuum.

- It is basically the energy diff. b/w fermi level vacuum levels.
- for semiconductor the diff. b/w vacuum level known as electron affinity.
- When a junction formed between a metal & semiconductor the fermi levels of both get aligned & a barrier is formed due to energy diff. b/w work function of metal & electron affinity of semiconductor.
- When diode is unbiased electrons on N-side have lower energy levels than electrons in metal. Hence, electron on N-semi cond. side can not surmount the junction barrier (Schottky barrier.) for going over to metal.
- When diode is F.B the electron on N-side gain enough energy to cross the barrier and enter the metal. Hence, e⁻s pt placing into metal with very large energy & they are called hot electron. Hence the diode is called hot carrier diode.
- If R.B the diode, e⁻s in metal can not over come the barrier. Hence no condⁿ take place.

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- The metal semiconductor junction is thus unidirectional and behaves as a diode.
- V-I characteristics of S.O. are similar to PN junction diode when F.B. Since there is no charge storage in the metal-semiconductor junction, the diode would switch off as soon as R.B. pot. applied.

Advantage over P-N junction Diode :-

- P-N diode is bipolar device because it has both e⁻ & holes as magnitude carrier.
- S.O. has e⁻s majority carrier as both side of electron junction. Thus S.O. are unipolar device because there are no minority carrier in reverse direction i.e., no significant current from metal to semiconductor when diode is R.B.
- The delay due to e-hole recombination present in PN diode is absent in S.O.
- The junction contact area between semicond. & metal is larger than in point contact diode hence F.B. resistance is lower (i.e., noise is comparatively lower). low noise fig. is highly important in communication receivers & radar units.
- Since no holes are available in metal there is no depletion layer or charge store. The delay due to e-hole recombination thus absent so S.O. can switch off faster than a bipolar diode.

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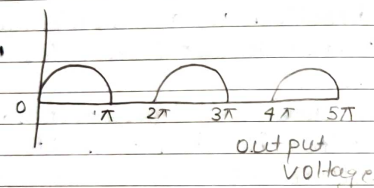
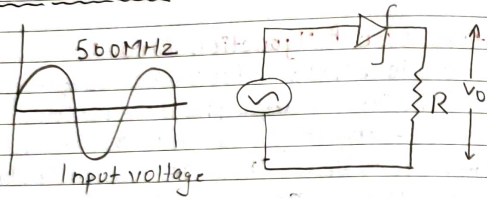
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Applications

- SD can easily rectify signals of freq. exceeding 300 MHz. The output will be perfect.

Sine wave as



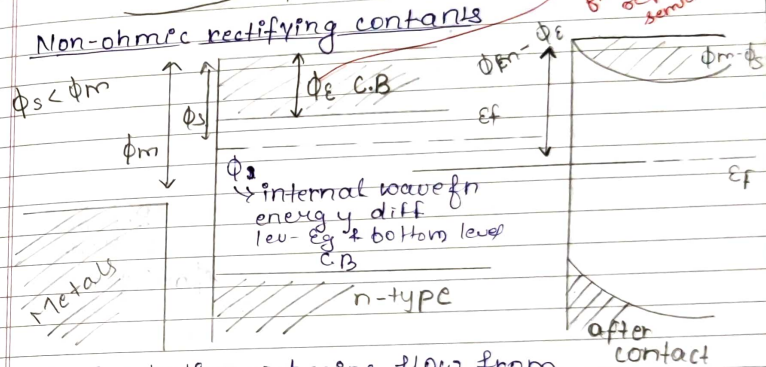
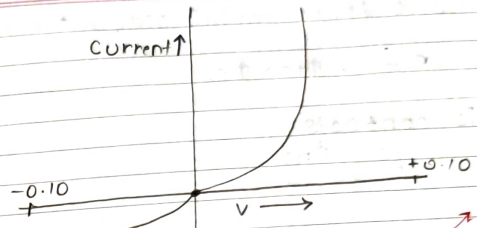
- (i) It finds applications in very high freq & fast digital circuit.
- (ii) Used as microwave detection & mixing.
- (iv) Used in clipping & clamping circuit.

ohmic if $\phi_s > \phi_m$ (ohmic)
 & if $\phi_p < \phi_m$ (ohmic)
 $\phi_s < \phi_m$
 $\phi_p > \phi_m$ } non-ohmic (rectifying)

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Conduction e^- begins flow from SC to metal until Fermi energies of both sides equal. Surface of metal becomes $-ve$ charged & surface of SC $\rightarrow +ve$ charged & which result in pot. barrier at junction. Since Fermi energy of both sides is same so energy level of bulk semiconductor get lowered by an amount $\phi_m - \phi_s$ as shown.
 If surface is viewed for SC side height of pot. barrier ~~bar~~ b/w SC & metal is
 $V_{sm} = \phi_m - \phi_s$

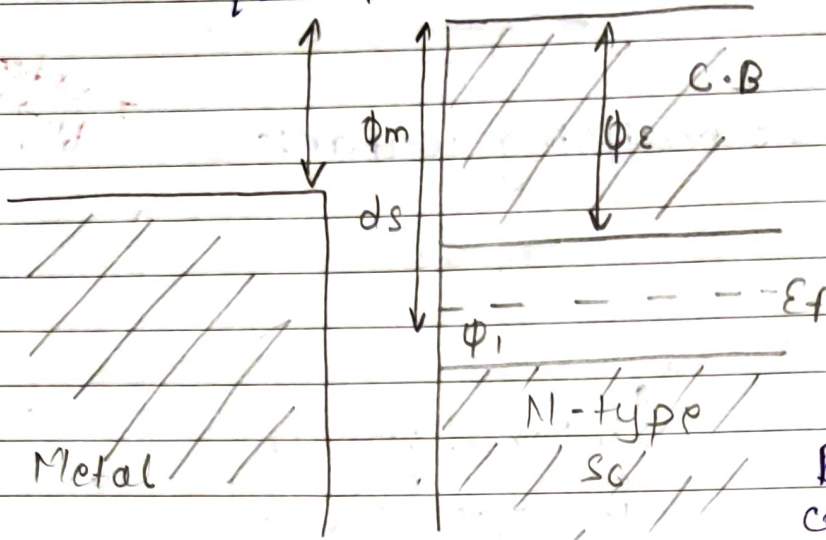
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if viewed from metal side, barrier height

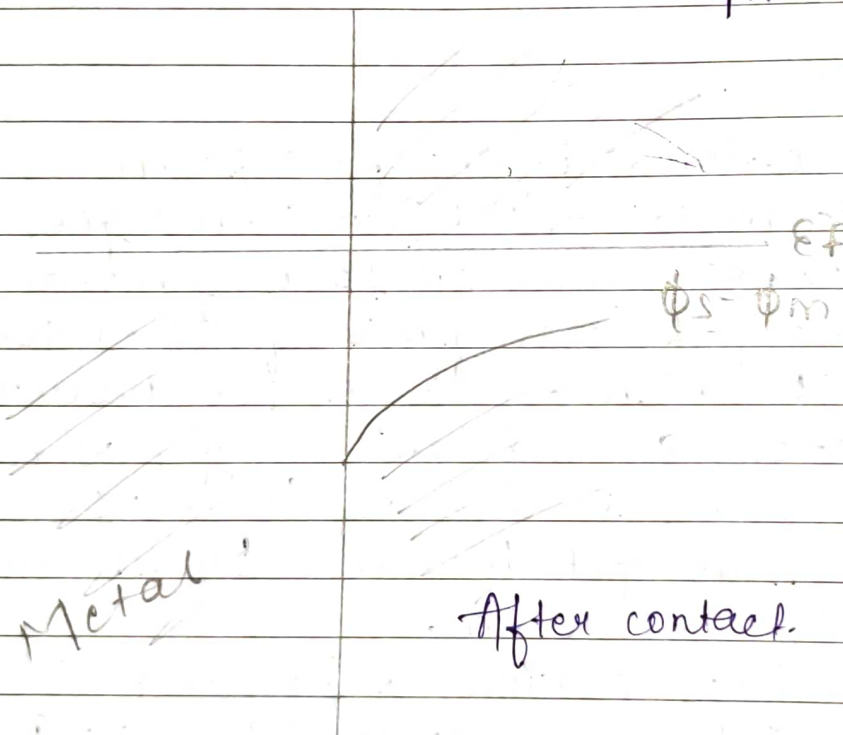
$$eV_{ms} = \phi_m - \phi_s$$

* Ohmic contacts

$\phi_s > \phi_m$ Vacuum level



Before contact
 $\phi_m < \phi_s$



Laser -

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