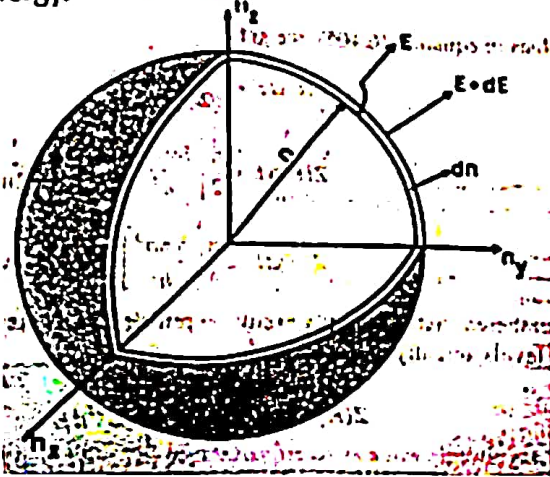


Density of states

The density of states (DOS) is essentially the number of different states at a particular energy level that electrons are allowed to occupy, i.e. the number of electron states per unit volume per unit energy.

Now that we have seen the distribution of modes for waves in a continuous medium, we move to electrons. The calculation of some electronic processes like absorption, emission, and the general distribution of electrons in a material require us to know the number of available states per unit volume per unit energy.



The density of states is once again represented by a function $g(E)$ which this time is a function of energy and has the relation $g(E)dE =$ the number of states per unit volume in the energy range: $(E, E+dE)$.

The number of states with energy less than E_f is equal to the number of states that lie within a sphere of radius $|n_f|$ in a region of K-space where n_x, n_y , and n_z are positive.

$$\therefore N = 2 \times \frac{1}{8} \times \frac{4}{3} \pi n_f^3$$

$$\therefore N = 2 \times \frac{1}{8} \times \frac{4}{3} \pi n_f^3 = \frac{3N}{\pi} \Rightarrow n_f = \left(\frac{3N}{\pi} \right)^{\frac{1}{3}}$$

So the Fermi energy

$$E_f = \frac{\hbar^2 \pi^2 n_f^2}{2ma^2} = \frac{\hbar^2 \pi^2}{2ma^2} \left(\frac{3N}{\pi} \right)^{\frac{2}{3}}$$

$$E_f = \frac{\hbar^2 \pi^2}{2m a^2} \left(\frac{3N}{\pi} \right)^{\frac{2}{3}} = \frac{\hbar^2 \pi^{\frac{2}{3}} (3N)^{\frac{2}{3}}}{2m (a^3)^{\frac{2}{3}}} = \frac{\hbar^2}{2m} \left(\frac{3N\pi^2}{a^3} \right)^{\frac{2}{3}} = \frac{\hbar^2}{2m} \left(\frac{3N\pi^2}{V} \right)^{\frac{2}{3}}$$

$$\therefore N^{\frac{2}{3}} = \frac{2m}{\hbar^2} \left(\frac{V}{3\pi^2} \right)^{\frac{2}{3}} E_f^{\frac{3}{2}}$$

$$\Rightarrow N = \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \left(\frac{V}{3\pi^2} \right) E_f^{\frac{3}{2}}$$

Therefore density of states: $D(E) = \frac{dN}{dE} = \frac{3}{2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \left(\frac{V}{3\pi^2} \right) E_f^{\frac{1}{2}}$

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

Therefore the total number of energy states per unit volume per unit energy range

$$Z(E) = \frac{D(E)}{V} = \frac{1}{V} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} E_f^{\frac{1}{2}} = \frac{1}{2\pi^2} \frac{(2m)^{\frac{3}{2}}}{\hbar^3} 8\pi^3 E_f^{\frac{1}{2}}$$

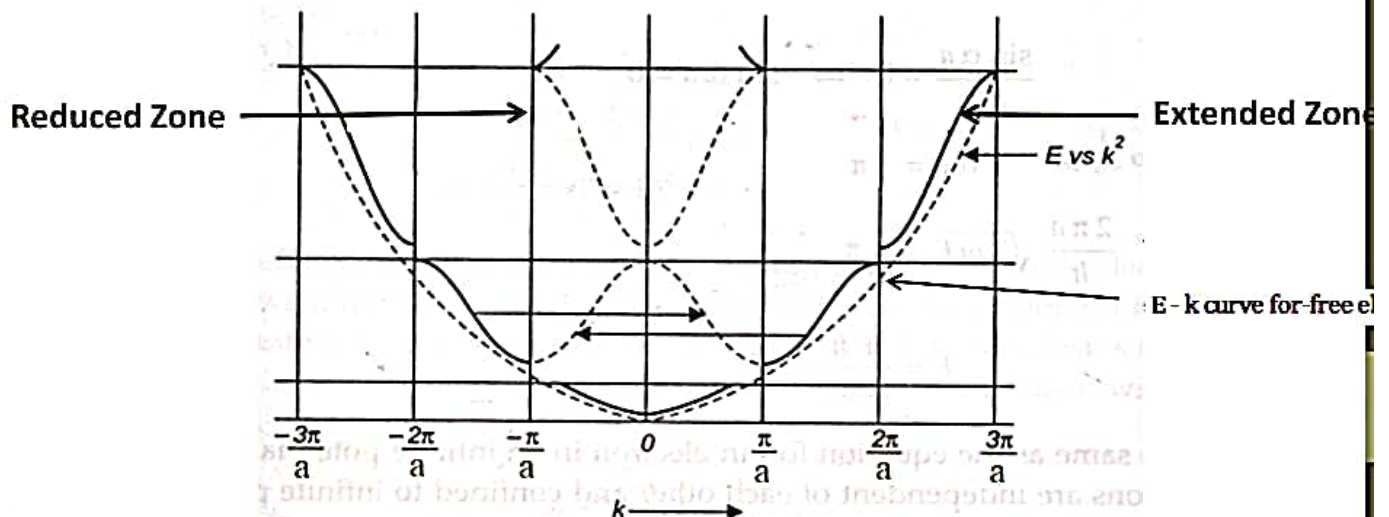
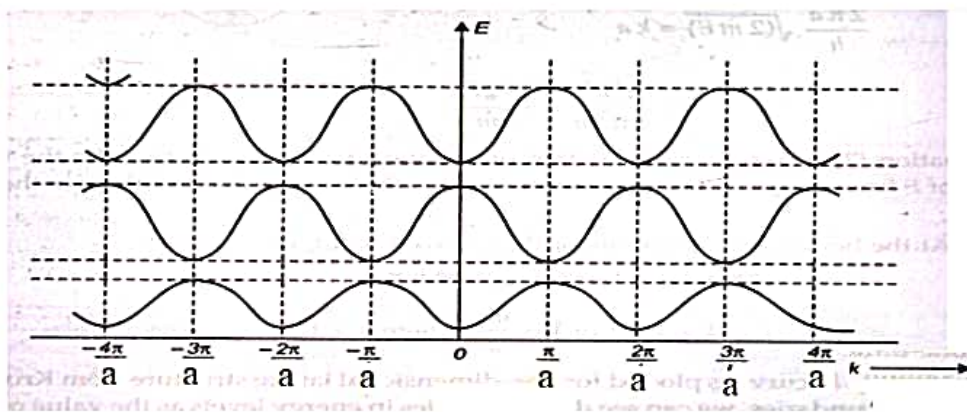
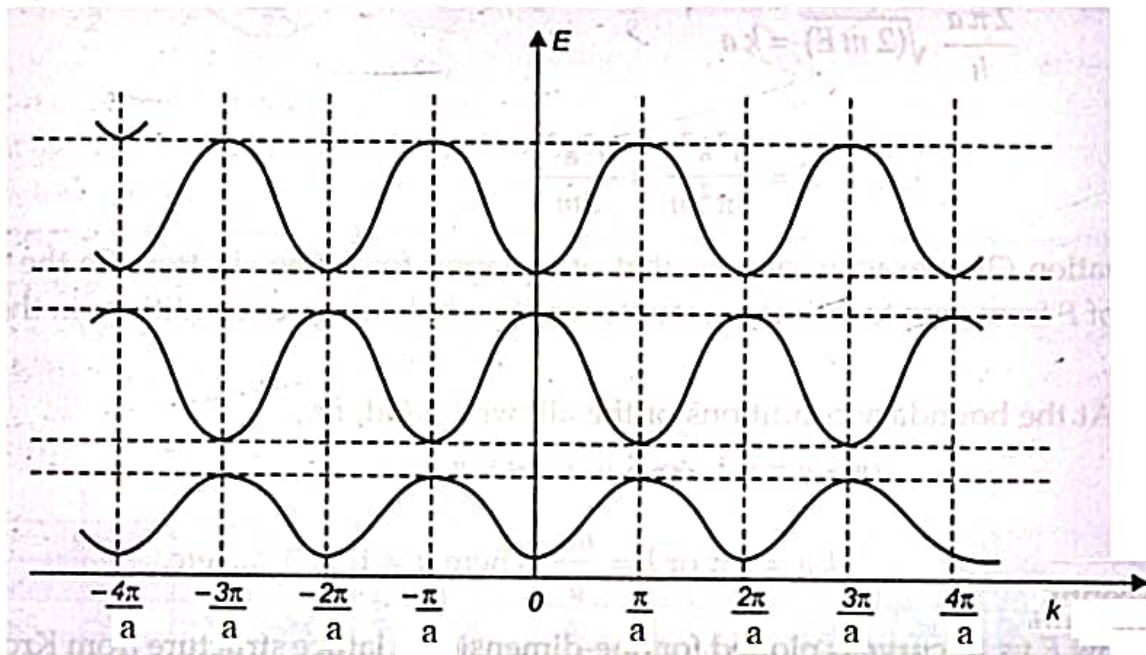
$$Z(E) = \frac{4\pi}{h^3} (2m)^{\frac{3}{2}} E_f^{\frac{1}{2}}$$

Therefore the number of energy states in the energy interval E and $E + dE$ are

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

E-K diagrams: Energy is periodic in K

1) Periodic Zone

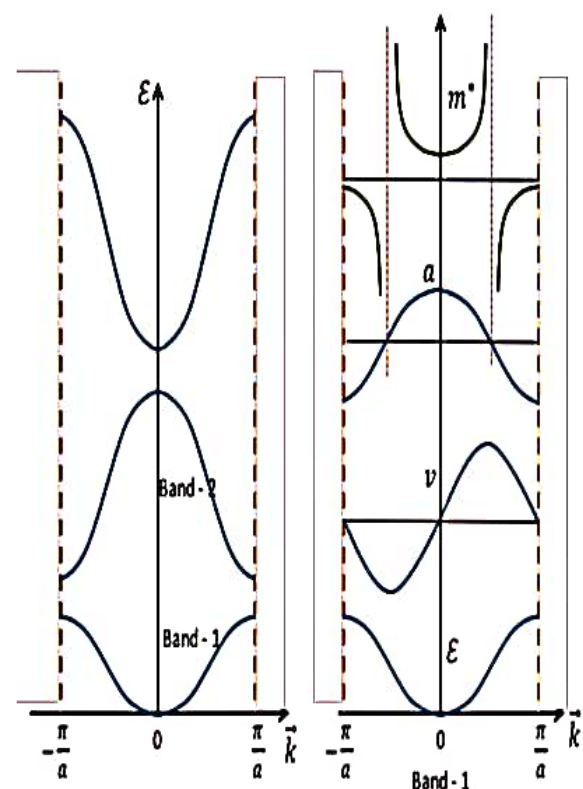
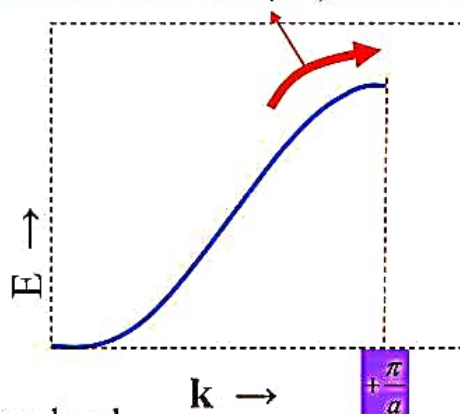


Effective mass of electron

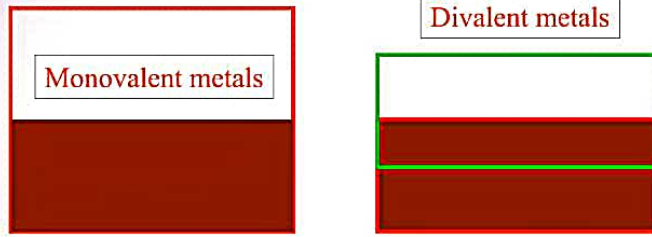
- ❑ The magnitude of the Energy gap between two bands is the difference in the potential energy of two electron locations.
- ❑ The effective mass of an electron (m^*) in a solid could be different from the rest mass (m_0). The effective mass can be larger or smaller than the rest mass.
- ❑ Collisions with atoms increases the rest mass, while enhanced propagation in the crystal gives a reduced effective mass.
- ❑ From the concept of group velocity the effective mass can be deduced. It is related to the curvature of the E-k curve. Close to band edges, m^* can be negative.

$$m^* = \frac{h^2}{4\pi^2} \frac{1}{\left(d^2E / dk^2\right)}$$

K.E of the electron increasing
 Decreasing velocity of the electron
 -ve effective mass (m^*) of the electron



Energy band diagram: METALS



- ❑ Monovalent metals: Ag, Cu, Au → 1 e⁻ in the outermost orbital
⇒ outermost energy band is only half filled
- ❑ Divalent metals: Mg, Be → overlapping conduction and valence bands
⇒ they conduct even if the valence band is full
- ❑ Trivalent metals: Al → similar to monovalent metals!!!
⇒ outermost energy band is only half filled !!!

Energy band diagram: SEMICONDUCTORS

Semiconductor

Conduction Band

Valence Band

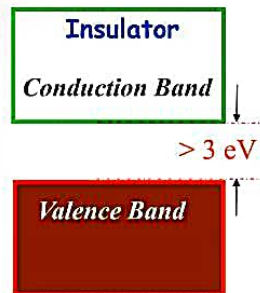
2-3 eV

Band Gaps of some intrinsic semiconductors							
Material	Si	Ge	GaP	GaAs	InSb	CdS	ZnTe
Band Gap (eV)	1.11	0.67	2.25	1.42	0.17	2.4	2.26

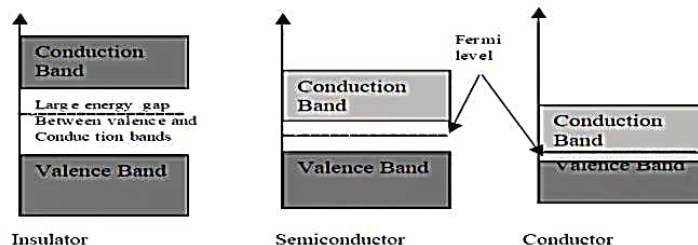
Energy Band Diagram at 0K

- ❑ Elements of the 4th column (C, Si, Ge, Sn, Pb) → valence band full but no overlap of valence and conduction bands
- ❑ Diamond → PE as strong function of the position in the crystal
⇒ Band gap is 5.4 eV
- ❑ Down the 4th column the outermost orbital is farther away from the nucleus and less bound ⇒ the electron is less strong a function of the position in the crystal ► reducing band gap down the column

Energy band diagram: INSULATORS

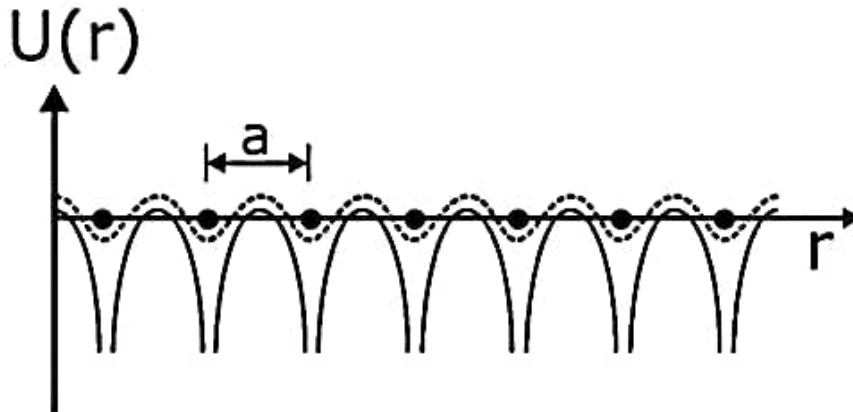


Insulators does not have any free electron. Therefore, transition of electron from valence band to conduction band is not possible.



BAND THEORY OF SOLIDS

BLOCH THEOREM:



Metals and alloys are crystalline in nature. When the electron move into the periodic ion core, it enters into the periodic potential i.e. potential is minimum at the positive ion sites and maximum between the two ions.

The one dimensional Schrödinger wave for this case is

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

The periodic potential $V(x)$ may be defined as

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

Bloch has shown that the one dimensional solution of the form

$$\psi(x) = e^{ikx} u_k(x) = e^{ika} u_k(a)$$

$$\text{Where } u_k(x) = u_k(x + a)$$

$$\psi(x + a) = e^{ik(x+a)} u_k(x + a)$$

$$= e^{ikx} e^{ika} u_k(x + a)$$

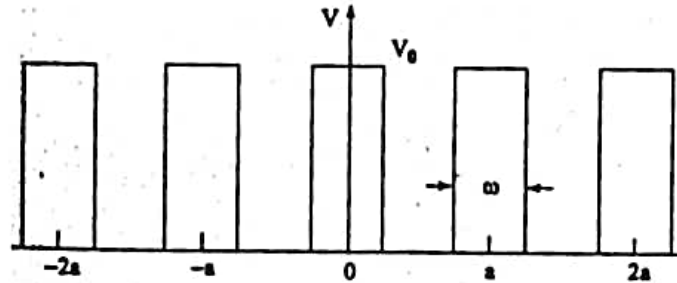
$$= e^{ika} e^{ikx} u_k(x)$$

$$\boxed{\psi(x + a) = e^{ika} \psi(x)}$$

This is referred as Bloch condition.

KRONIG-PENNEY MODEL:

The free electrons in a metal move under a periodic potential due to regularly arranged positive ions. The nature of the energies of the electron is determined by solving Schrödinger wave equation. For simplicity, the periodic potential is taken in the form of regular one dimensional array of square well potentials.



Within the well the electron has potential energy

$$V = 0, 0 < x < a$$

Outside the well the electron has the PE

$$V = V_0, -a < x < 0$$

∴ the Schrödinger wave equation for the two regions are

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m E}{h^2} \psi = 0, 0 < x < a \text{ ----- (1)}$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m (E - V_0) \psi}{h^2} = 0, -a < x < 0 \text{ ----- (2)}$$

$$\text{Let } \alpha^2 = \frac{8\pi^2 m E}{h^2}$$

$$\text{And } \beta^2 = \frac{8\pi^2 m (V_0 - E)}{h^2}$$

Then (1) and (2) becomes

$$\frac{\partial^2 \psi}{\partial x^2} + \alpha^2 \psi = 0, \text{----- (3)}$$

$$\frac{\partial^2 \psi}{\partial x^2} - \beta^2 \psi = 0, \text{----- (4)}$$

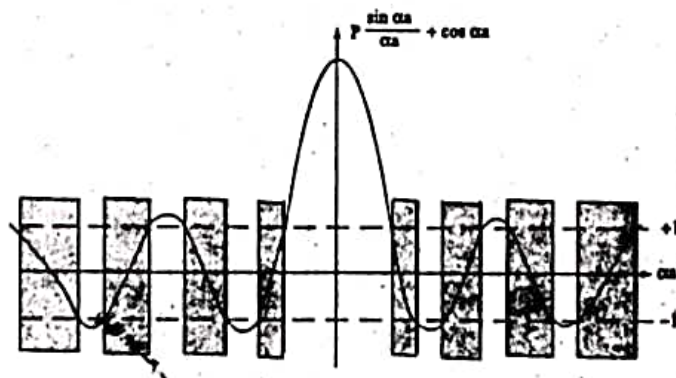
On solving equations (3) and (4) and by applying Bloch Theorem we get

$$\boxed{P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka} \text{ ----- (5)}$$

$$\text{Where } P = \frac{mabV_0}{h^2}$$

$$\text{and } \alpha^2 = \frac{8\pi^2 mE}{h^2} \Rightarrow E = \frac{h^2 \alpha^2}{8\pi^2 m}$$

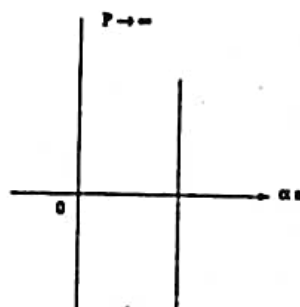
The nature of the equation is illustrated by the plot i.e. drawn between $P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$ and αa and at the same time the RHS having the value between +1 and -1



In the above graph only some of the range of αa values are allowed indicating the a limiting range of energies are allowed. Allowed energy region is indicated by dark region and the forbidden region is indicated by dotted lines.

Special cases:

- (i) If $P \rightarrow \infty$ the allowed band reduces to single energy level. This is the special case of electron trapped.



- (ii) If $P \rightarrow 0$

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

$$k = \alpha$$

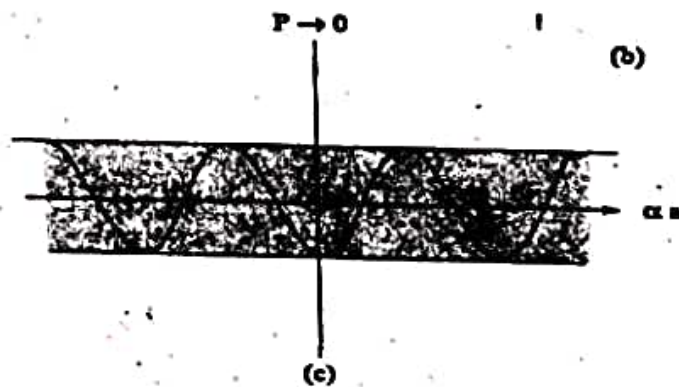
$$k^2 = \alpha^2 = \frac{8\pi^2 mE}{h^2} \Rightarrow E = \frac{h^2 k^2}{8\pi^2 m} = \frac{h^2}{8\pi^2 m} \frac{4\pi^2}{\lambda^2}$$

$$\Rightarrow E = \frac{h^2}{2m} \frac{m^2 v^2}{h^2} = \frac{1}{2} mv^2$$

Therefore Total energy = KE + PE

$$\Rightarrow \text{Potential Energy } V = 0$$

And this is the case of free electron.



Finally we conclude that

- (i) Electrons in solids are permitted to be in allowed energy bands separated by forbidden energy gaps.
- (ii) Allowed energy band width increases with αa
- (iii) $P \rightarrow \infty$ is the case of electron trapped and $P \rightarrow 0$ is the case of classical free particle