❖ **Kronig Penny Model:**

According to quantum free electron theory of metals, a conduction electron in metal experinces constant or zero potential and free to move inside the crystal but will not come out of the metal beacause an infinite potential exists at the surface. This theory successfully explains electrical conductivity, specific heat, thermionic emission and paramagnetism. This theory is fails to explain many other physical properties, for example: (i) it fails to explain the difference between conductors, insulators and semiconductors and (ii) positive Hall coefficient of metals

To overcome such problems, the potential experience by the electrons due to the presence of positive ions is considered as periodic which is shown in Fig. 3. If an electrons moves through these ions, it experiences varying potentials. The potential of an electron at the positive ions site is zero and is maximum in between two ions which is shown in Fig. 3 (b) Kronig and Penny model illustrates the behavior of electrons in a periodic potential by assuming a relatively simple one dimensional model of periodic potential. It is not easy to solve Schrodinger equation with these potential, so they approximated these potential inside the crystal to the shape of rectangular steps as shown in Fig. 3 (c). This model is called Kronig Penny model of potential.

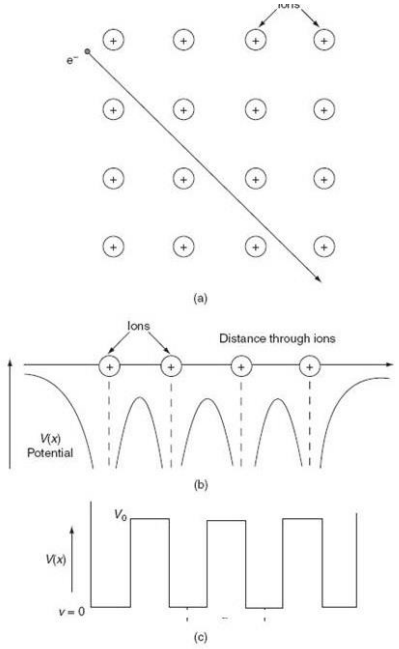


Fig. 3: (a) electron passing through positive ions lattice sites (b) variation of potential after interaction with positive ions and (c) rectangular shape square potential well.

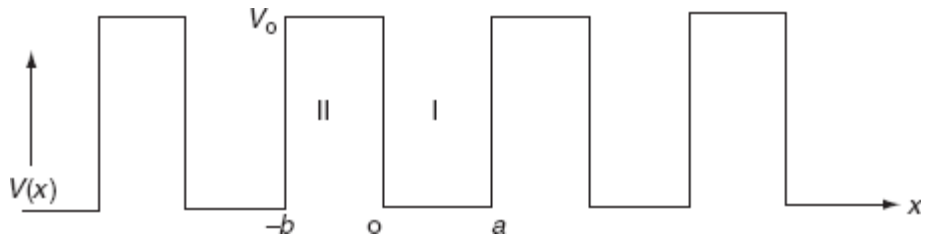


Fig 4: One dimensional periodic potential used by Kronig and Penny

The energies of electrons can be known by solving Schrodinger equation in such lattice. The Schrodinger time-independent wave equation for the motion of an electron along X-direction is given by:

$$\frac{\delta^2\Psi}{\delta x^2} + \frac{2m}{\hbar^2}[E - V(x)]\Psi = 0 \qquad \text{…….. (i)}$$

The energies and wave functions of electrons associated with this model can be calculated by solving time-independent one dimensional Schrodinger's wave equations for the two regions I and II as shown in Fig. 4

The Schrodinger equations are:

$$\frac{\delta^2\Psi}{\delta x^2} + \frac{2m}{\hbar^2}E\Psi = 0 \qquad \text{for } 0 < x < a \qquad \text{……(ii)}$$

$$\frac{\delta^2\Psi}{\delta x^2} + \frac{2m}{\hbar^2}[E - V_0]\Psi = 0 \qquad \text{for } -b < x < 0 \qquad \text{……. (iii)}$$

We define two real quantities α and β such that:

$$\alpha^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad \beta^2 = \frac{2m}{\hbar^2}(V_0 - E) \qquad \text{……. (iv)}$$

Equation (ii) and (iii) becomes

$$\frac{\delta^2\Psi}{\delta x^2} + \alpha^2\Psi = 0 \qquad \text{for } 0 < x < a$$

$$\frac{\delta^2\Psi}{\delta x^2} - \beta^2\Psi = 0 \qquad \text{for } -b < x < 0$$

According to Bloch's therorem, the wave function solution of the Schrodinger equation when the potential is periodic and to make sure the function *u(x)* is also continuous and smooth, can be written as

$$\Psi(x) = e^{ikx}u(x) \qquad \text{……. (v)}$$

Where u (x) is a periodic function which satisfies u (x+a) = u(x)

Using Bloch theorem and all the boundary conditions for the continuity of the wave function the solution of Schrodinger wave equation obtained as

$$P\frac{sin\alpha}{\alpha a} + \cos \alpha a = coska \qquad \ldots\ldots\ldots\ldots\ldots\ldots \text{ (vi)}$$

Where, $P = \frac{mabV_0}{\hbar^2}$ which is a measure of the potential barrier area V_0b.

The physical significance of the quantity P is that if P is increased the area of the potential barrier is increased and the given electrons is bound more strongly to a particular potential well. When P→0, the potential barrier becomes very weak which mean that the electrons are free electrons.

Equation (vi) is the condition which must be satisfied for the solution to the wave equation to exist. Since *coska* lies between +1 and -1, the left hand side should assume only those values of αa for which its value lies between +1 and -1. Such values of *αa*, therefore represents wave like solution of the type of equation *(vi)* and are allowed. The other values of not allowed. Figure 5. Shows the plot of left hand side and versus *αa* of equation *(vi)* for P = 3π/2. The vertical axis lying between -1 and +1 as indicated by the horizontal lines, represents the values acceptable to the left hand side. It may be noted that since α^2 is proportional to the energy E, the abscissa is a measure of the energy. The following conclusions may be drawn from Figure 5.

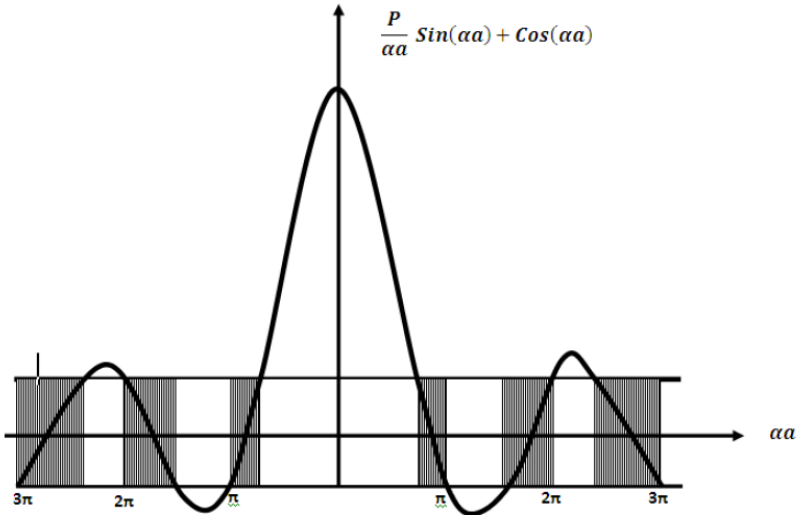


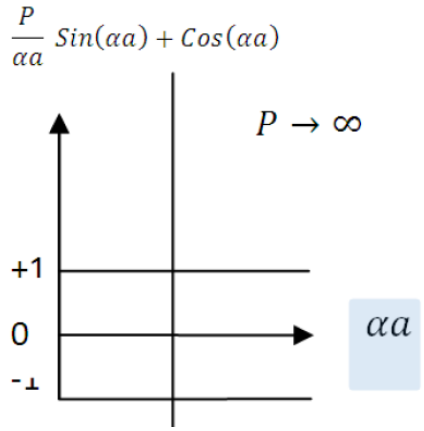
Figure 5: Plot of left hand side of equation (vi) as a function of *αa* using $P = \frac{3\pi}{2}$. The shaded and transparent portions referred to as allowed and forbidden bands respectively.

The following conclusions can be made from the Figure 5.

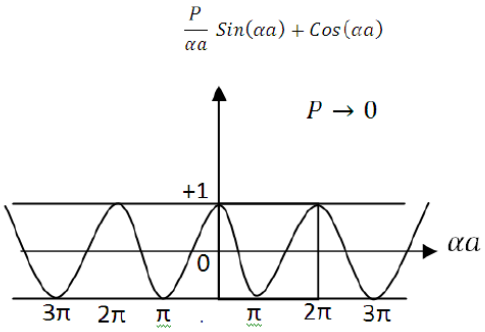
(i) The energy spectrum of the electron consists of a large number of allowed energy bands and forbidden energy bands.

(ii) The width of the allowed energy bands increases with increasing of o i.e. with increases energy.

(iii) As p → ∞ the allowed regions becomes infinity narrow and the energy spectrum becomes a line spectrum as shown in figure



(iv) For, P = 0, the energy spectrum is continuous as shown in Figure 7.



Origin of band in solids: According to quantum free electron theory, the free electrons move in constant potential and the atoms have independent energy levels (discrete energy levels). Pauli's exclusive principle is applied in filling the energy levels. According to Kroning and Penney model the free electrons moves in a square well periodic potential and predicts the existence of allowed energy band and forbidden energy gaps.

The origin of an energy gap is explained by considering the formation of energy bands in solids. The concentration of atoms in a gaseous medium is very low compared to the concentrations of atoms in a solid medium. As a result, the interaction between any two atoms in a gaseous substance is very weak, since the interatomic distance is very large.

In case of solid substance interatomic distance is very small, and hence there is an interaction between any two successive atoms. Due to this interaction the energy levels of all atoms overlap with each other and hence bands are formed.

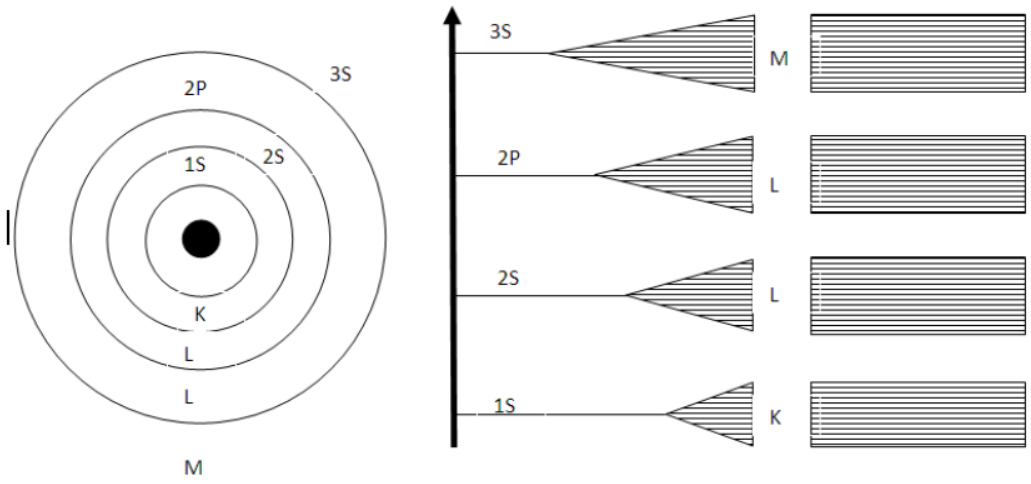


Fig. 6: Band formation in solid

Conductors, Semiconductors and Insulators:

The solids are classified into three types based on the forbidden gap. Those are conductors, semiconductors and insulators.

Conductors: In case of conductors, the valance and conduction bands are overlap to each other as shown in Figure 7 (a). In conduction band plenty of free electrons are available for conduction. The energy gap in conductors is zero. The charge carrier in conductors is electrons. All metals are example of conductors.

Semiconductors: In case of semiconductors the forbidden gap is very small as shown in Figure 7 (b). Germanium and silicon are the best examples of semiconductors. In Germanium the forbidden gap is 0.7 ev. In *Si* the forbidden gap is 1.1 ev. At 0K the valence band is completely fulfilled and the conduction band is totally empty. When a small amount of energy is supplied, the electrons can easily jump from valence band to conduction band. The charge carriers in semiconductors are both electrons and holes.

Insulators: In case of insulators the forbidden energy gap is very wide as shown in Figure 7 (c). In insulators the valence electrons are bound vary tightly to their parent atoms. In case of

insulators the forbidden energy gap is always >6eV. Due to this fact electrons cannot jump from valence band to conduction band.

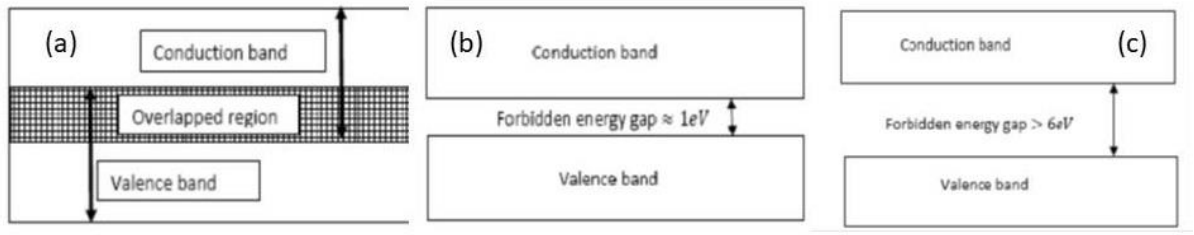


Figure 7: Band diagram of (a) metal, (b) semiconductor and (c) Insulator.