UNIT – 1

ELECTRICAL PROPERTIES OF MATERIALS

1.10 Electron in Periodic Potential:

1.10.1 Bloch Theorem

1.11. Tight Binding approximation

1.10 Electron in Periodic Potential:

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

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

Postulates:

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

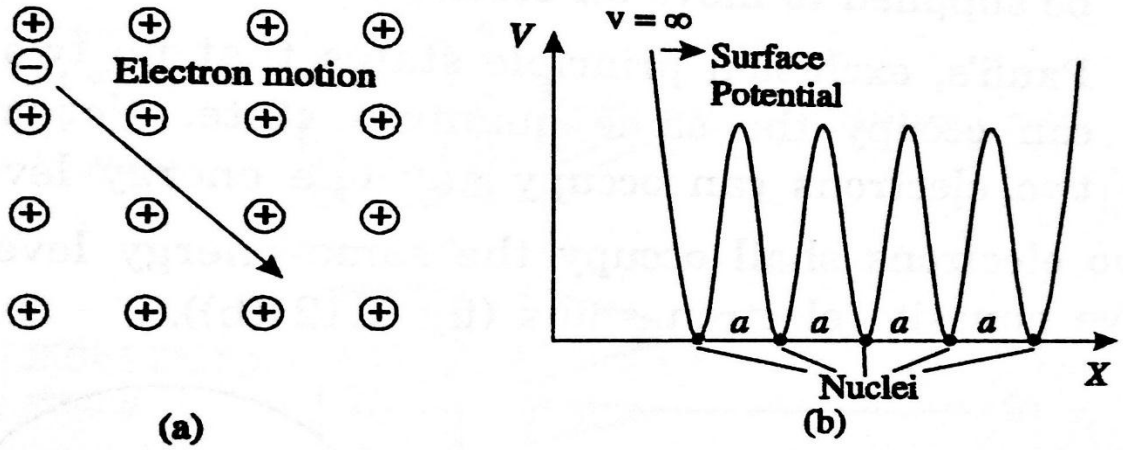

Fig 1.10.1-One dimensional periodic potential distribution for a crystal

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

1.10.1 Bloch Theorem

Bloch theorem is a mathematical statement of an electron wave function moving in a perfectly periodic potential. These functions are called Bloch functions. Let us consider an electron moving in a periodic potential. The Schrodinger equation

is

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\Psi = 0\text{----------(1)}$$

Solution for this equation is

$$\Psi(x) = e^{\pm ikx}u_k(x)\text{---------(2)}$$

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

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

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

1.11 Tight Binding approximation:

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

In free electron approximation

1.The potential of the electron is assumed to be lesser than its total energy.

2.The width of the forbidden bands are smaller than the allowed bands as in fig.

3.Therefore the interaction between the neighboring atoms will be very strong.

4.As the atoms are closer to each other, the inter atomic distance decreases and hence the wave function overlap with each other.

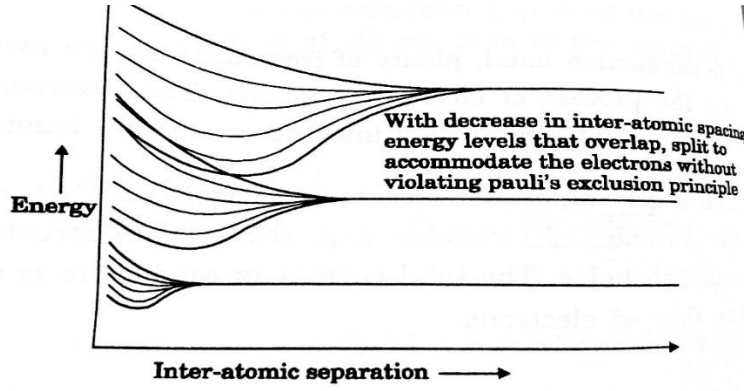

Fig 1.11.1-Tight binding approximation