BAND THEORY

Bloch Theorem

In order to study the electronic structure of molecules and solids Bloch used one electron equation. For free electron theory, an electron is assumed to move in a constant potential V_0 and hence for a one dimensional case the Schrödinger's wave equation for electron is given by

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V_0)\psi = 0 \quad \text{---} \quad (1)$$

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

where $$k = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

The solution of equation (1) is

$$\psi(x) = e^{\pm ikx}$$

and, $$\frac{d^2\psi}{dx^2} = -k^2 e^{\pm ikx}$$

using these results in eq^n (1), we get

$$-k^2 e^{\pm ikx} + \frac{2m}{\hbar^2}(E-V_0)e^{\pm ikx} = 0$$

or $$-k^2 + \frac{2m}{\hbar^2}(E-V_0) = 0 \quad \text{as } e^{\pm ikx} \neq 0$$

or $$k^2 = \frac{2m}{\hbar^2}(E-V_0)$$

$$\therefore E - V_0 = \frac{\hbar^2 k^2}{2m}$$

$\therefore$ kinetic energy, $E_{kin} = E - V_0 = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}$

where $p = \hbar k$ = momentum of electron

If an electron is moving in one dimensional periodic potential, the potential energy of an electron can be written as

$$V(x) = V(x+a) \quad \text{———} \quad (2)$$

where a is the period. Hence $V(x)$ is the periodic potential.

The Schrödinger's wave equation in this case can be written as

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi = 0 \qquad \text{---(3)}$$

For the solution of eqn.(3), there is an important theorem which states that there exist solutions of the form:

$$\psi(x) = e^{\pm ikx}\, u_k(x) \qquad \text{---(4)}$$

Where $u_k(x) = u_k(x+a)$ ---(5)

Hence the solutions of eqn.(3) are plane waves having type $e^{\pm ikx}$ modulated by the function $u_k(x)$ which has the same periodicity as the lattice constant. This statement is known as Bloch-Theorem. The wave functions of type (4) are known as Bloch function. The Bloch function $\psi(x) = e^{ikx} u_k(x)$ has the property.

$$\psi(x+a) = e^{\pm ik(x+a)}\, u_k(x+a) = e^{\pm ikx}\, u_k(x+a)\, e^{\pm ika}$$

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

$\therefore \psi(x+a) = e^{\pm ika}\, \psi(x)$

Thus, the Bloch function has the property:

$$\psi(x+a) = Q\,\psi(x), \quad \text{where } Q = e^{\pm ika}$$