MODULE – 2

ELECTRICAL PROPERTIES OF MATERIALS

2.7.The origin of energy band in a solid.

Energy Bands in Solids

According to the energy band theory of solids, the free electrons move in a periodic potential produced by positive ion cores. The electrons are treated as weakly perturbed by the periodic potential.

In solid solution, the electrons experience a periodic potential since the atomic arrangement is periodic.

A simple qualitative explanation of the formation of energy bands in a solid is given below.

A solid contains an enormous number of atoms packed closely together. Each atom when isolated has a discrete set of electron energy level, 1s, 2s, 2p, …

If we imagine has N atoms on the solid to be isolated from one another, they would have completely coinciding schemes of energy levels.

The energies of electrons within any one isolated atom obey the following conditions.

(i) There are specific electronic energy levels in each atom (fig.). Electrons cannot occupy space.

(ii) Electrons fill the lowest energy levels first; A specific quantity of energy, called a quantum of energy must be supplied to move an electron to the next higher level.

(iii) Pauli's exclusion principle states that no two electrons can occupy the same quantum state. Not more than two electrons can occupy any one energy level.

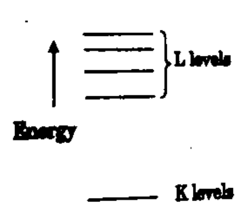


Fig. (a)

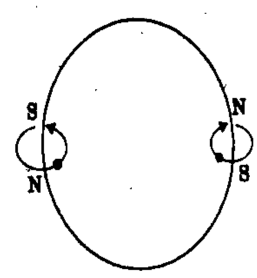


Fig. (b)

Two electrons shall occupy the same energy level because they have opposite electron spins (fig. (b)).

When the atoms are brought in close proximity to form a solid, the valance electrons of adjacent atoms interact and constitute a simple system of electrons common to the entire crystal, and their outermost electronic orbits overlap.

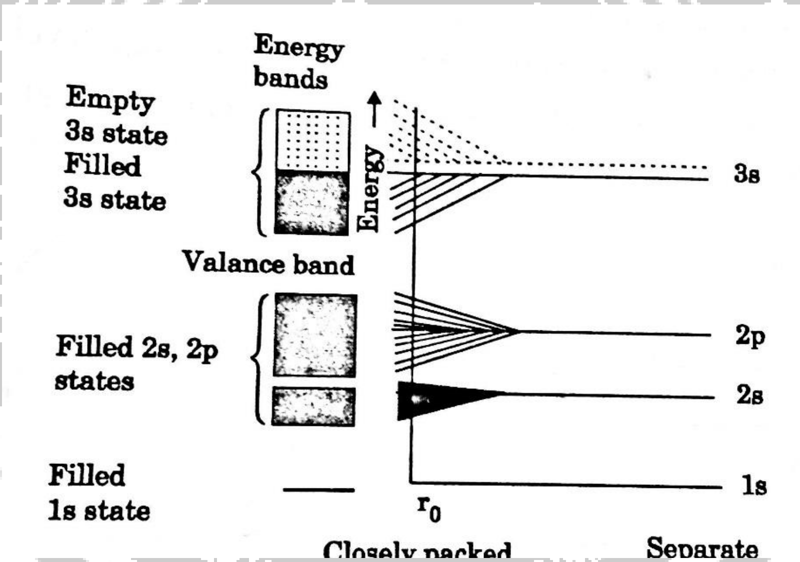
Therefore, N electrons will now have to occupy different energy levels, which may be brought about by the electric forces exerted on each electron by all N nuclei.

As a result of these forces, each atomic energy level is split up into a large number of closely spaced energy levels.

A set of such closely spaced energy levels is called an energy band.

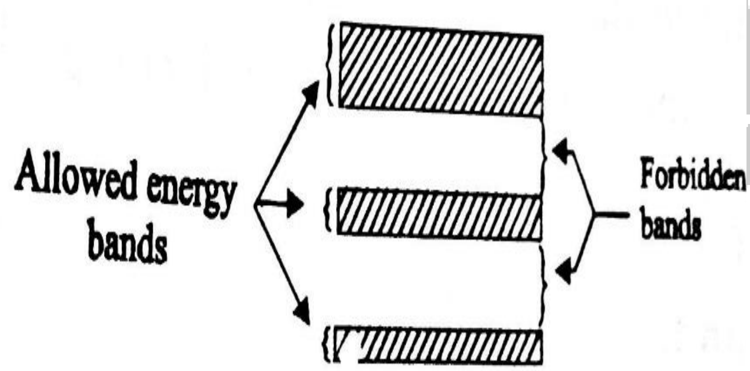
Consider 11 electrons of a neutral sodium atom, each occupying a specific energy level as indicated in fig. The energy levels of sodium become bands when the atoms lie close together.

In figure, r_o represents the spacing between atoms in solid sodium. When the atoms are part of a solid, they interact with each other, and the electrons have slightly different energies.



In an energy band, allowed energies are almost continuous. These energy bands are separated by ranges of energies that have no allowed energy levels.

These regions are known as forbidden bands or energy gaps

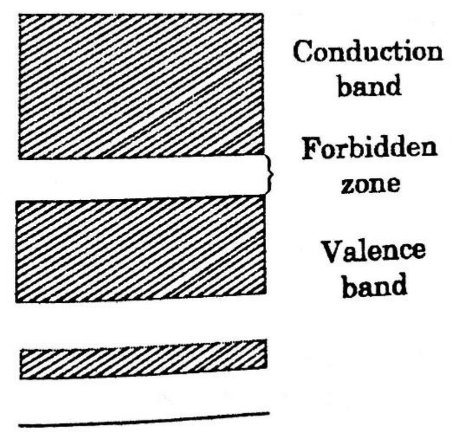


The amount of splitting is not the same for different levels. The levels filled by valence electrons are distributed to a greater extent, while those filled by electrons of inner shells are distributed only slightly.

If there are N atoms in a solid, there are N allowed quantum states in each band. Each quantum state is occupied by a maximum of two electrons with opposite spins. Thus, each energy band can be occupied by 2N electrons.

The valence band consists of a group of states containing the outermost electrons or valence electrons of an atom. The band formed from atomic energy levels containing valence electrons is called valence band.

These electrons have the highest energy. The band is obviously the highest occupied band.



Above the valence band, there exists the band of next higher permitted energies called conduction band. It is separated from the valence band by a gap

The gap represents the range of energy which electrons cannot possess.

The conduction band corresponds to the first excited states and it is normally the lowest unfilled energy band.

In conduction band, the electrons can move freely and they are generally called conduction electrons.

2.7.1.Effective mass of Electron and Hole

The mass acquired by an electron when it is accelerated in a periodic potential is called effective mass of an electron.It is denoted by m^*.

Explanation:

When an electron is accelerated the mass of the electron is not constant,but it varies.This varying mass is called effective mass (m^*).

Derivation of effective mass of electron:

When electric field is applied to a crystal the electron gains velocity described by wave vector k.

Group velocity $v_g = \frac{dw}{dk}$ ----------------------(1)

Where ω – angular frequency of the electron.
k- wave vector

we know that $E = h\nu$

$$E = \frac{h\,\omega}{2\pi}$$

$$= \hbar\,\omega$$

$$\omega = \frac{E}{\hbar} \text{ ----------------------------(2)}$$

Substituting (2) in(1)

$$v_g = \frac{d}{dk}\left(\frac{E}{\hbar}\right)$$

$$v_g = \frac{1}{\hbar}\frac{dE}{dk}$$

The acceleration 'a' is

$$a = \frac{d}{dt}(v_g)$$

$$= \frac{d}{dt}\left[\frac{1}{\hbar}\left(\frac{dE}{dk}\right)\right]$$

$$= \frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{dk}{dt} \text{ -------------------(4)}$$

Momentum 'p' of an electron

$$p = \frac{h}{\lambda}$$

$$= \frac{h}{2\pi}\frac{2\pi}{\lambda}$$

$$= \hbar\,k \text{ ---------------------(5)}$$

Differentiating (5) w.r.t 't'

$$\frac{dp}{dt} = \hbar\frac{dk}{dt}$$

Or

$$F = \hbar\frac{dk}{dt}$$

$$\frac{dk}{dt} = \frac{F}{\hbar} \text{ ----------------(6)}$$

Substituting (6) in (4)

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

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

$$F = \left[\frac{\hbar^2}{\frac{d^2E}{dk^2}}\right] a \text{------------------(7)}$$

When an electrical field is applied ,acceleration is

$$a = \frac{eE}{m^*} = \frac{F}{m^*}$$

$$F = m^* a \text{--------------------(8)}$$

Comparing (7) & (8)

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

$$m^* = \frac{\hbar^2}{\frac{d^2E}{dk^2}}$$

From (9) effective mass is not constant but depends on $\frac{d^2E}{dk^2}$

Special Cases:

Case i :

If $\frac{d^2E}{dk^2}$ is positive then m^* is also positive.

Case ii :

If $\frac{d^2E}{dk^2}$ is negative then m^* is also negative.

Case iii :

If $\frac{d^2E}{dk^2}$ is more then electrons behave as light particles.

Case iv :

If $\frac{d^2E}{dk^2}$ is very small,then the electrons behave as heavy particles.

2.7.2.Concept of hole (or) Effective or Negative mass of electron:

The effective mass $m^{\star}$ is negative near the zone edges of filled valence bands.The electrons in these regions are accelerated in a direction opposite to the direction of the applied field. This is called the negative mass behavior of the electrons.

The electrons with negative effective mass is considered as the same positive mass of that of an electron, but with positive charge. This new entity is given the name “hole”.

The positive hole conduction and effective negative electron mass conduction are in equilibrium. The calculation made on the hole appear to be more convenient and hence the hole concept is retained.

Several phenomena like Hall effect, Thomson Effect etc find explanation on the basis of the hole concept.