1 Free electron theory-introduction

Free electron theory was developed to explain the electric properties of materials.

1.1 Classical free electron theory

1. Classical free electron theory is following *kinetic theory of gases.*

2. This theory assumes that a piece of material consists of positive ions and *free electrons.*

3. The free electrons are the valance electrons of the atoms which constitute the piece of material.

4. The valance electrons are assumed to have broken their bonds with their parent atoms and become free to move throughout the volume of the material. However, such free electrons are bound to the volume of material and cannot escape from the material.

5. The collection of free electrons is called as free electron gas which obey kinetic theory of gases. [Refer kinetic theory of gases]

6. The free electrons which are assumed to be classical particles obey Maxwell-Boltzmann distribution law which is given by The MB law is given by

$$f(E) = \frac{1}{exp[(E - E_f)/KT]}, \tag{1}$$

   where f(D) is the probability of occupancy of an energy level by an electron. E and E_f stands for energy of a given energy level and Fermi level respectively. K is the Boltzmann constant and T is the temperature.

7. When an electric field is applied to the material, the free electrons are accelerated and achieve a velocity which is called as *drift velocity.*

8. The current which occur due the movement of external electric field is called as **drift current.**

1.2 Quantum free electron theory

1. In quantum theory of free electron gas, the free electrons obey Fermi-Dirac statistics and not Maxwell-Boltzmann statistics.

2. The Coulomb force of repulsion among the negatively charged free electrons is also neglected.

1.3 Fermi-Dirac distribution function

1. The FD distribution function is given by

$$f(E) = \frac{1}{exp[(E - E_f)/KT] + 1} \tag{2}$$

2. The particles which obey FD statistics are called as Fermions. Ex: electrons.

3. Fermions have half integer spin and obey Pauli's exclusion principle.

4. According to Pauli's exclusion principle, no two electrons can occupy same energy level which is given by same set of quantum numbers.

5. Fermi level is defined as the top most filled level at 0 K temperature.

6. Electrons start to occupy energy levels from lowest level. Gradually, they fill higher energy levels. The maximum level which is filled by electrons at 0 K temperature is defined as Fermi level. The corresponding energy is called as Fermi energy.

7. Different cases of FD function:

   Case 1: At 0 K temperature, if $E < E_F$ (Energy level is located below Fermi level), we will get $f(E) = \frac{1}{1+exp[-\infty]}$.
   Since $exp[-\infty] = 0$, we get $f(E) = 1$

   Hence, at 0 K temperature, all the energy levels below the Fermi levels are completely occupied.

   Case 2:
   At 0 K temperature, if $E > E_F$ (Energy level above Fermi level), we will get $f(E) = \frac{1}{1+exp[\infty]}$.
   Since $exp[\infty] = \infty$, we get $f(E) = \frac{1}{\infty}$ which equal to zero.

   Hence, all the energy levels above the Fermi level are completely unoccupied.

   Case: 3

   At any other temperature and at $E = E_F$, we get $f(E) = \frac{1}{1+exp[\frac{0}{KT}]} = \frac{1}{1+1}$, since $exp(0) = 1$. Hence, at Fermi level ($E = E_F$), the probability of occupancy is equal to 0.5. This serves another definition of Fermi level.

2 Band theory of solid

1. Electronic band: A range of continuum of energy levels which can either allow electrons to occupy or forbidden electrons.

2. Electronic structure of an atom is shown in the figure.

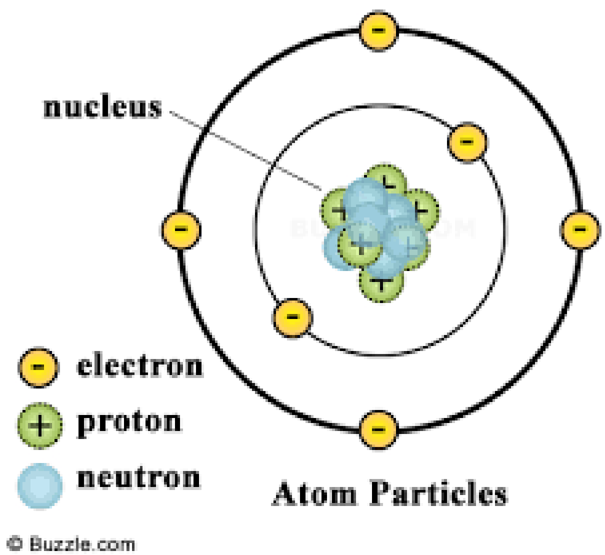


Figure 1: Structure of an atom

3. Two electrons are brought together in the following figure.

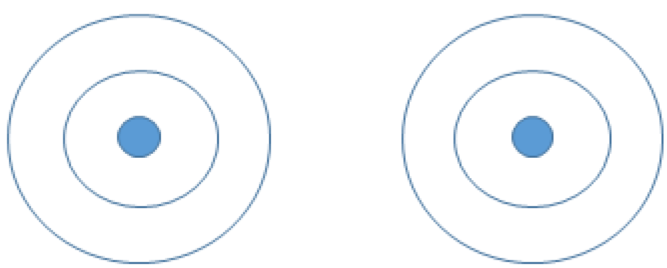


Figure 2: Two atoms separated at a particular distance

4. In Fig. 2, if the two atoms are sufficiently closer, the energy orbit will start to overlap and energy level will interact with each other.

5. **Example:**

(a) In a shell which correspond to a particular energy, maximum two electrons can be accommodated (UP spin and DOWN spin). If two atoms are brought together, energy shells of same energy from both atoms will be interacting.

(b) Quantum mechanically, we have only one energy shell for both the atoms. But we have four atoms.

(c) According to Pauli principle, only two electrons can be accommodated in a shell.

(d) In order to accommodate all four electrons, a new energy shell will be created with slightly different energy.

6. Addition of more and more atoms would create more energy levels which can form a continuum of energy level (Energy band).

7. Such an energy band is called allowed band.

8. Shells which are located interior can also make an allowed band gap.

9. The outermost allowed band in metals is called as conduction band and the interior inner allowed band is called as valance band.

10. The gap between conduction band and valance band is called as energy band and is a forbidden band.

3 Effective mass

1. The energy of an electron is given by

$$E = \frac{1}{2} m v^2, \tag{3}$$

which can be written as

$$E = \frac{P^2}{2m}, \tag{4}$$

where P is the momentum which is related to wave vector as $P = \hbar K$.

$$E = \frac{\hbar^2 K^2}{2m} \tag{5}$$

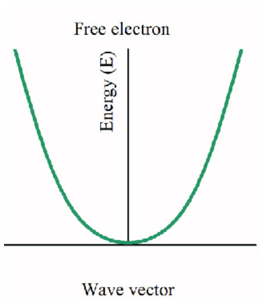
differentiating E twice with respect to K, we get

$$\frac{d^2 E}{dK^2} = \frac{\hbar^2}{m} \tag{6}$$

$$m = \frac{\hbar^2}{\left(\frac{d^2 E}{dK^2}\right)} \tag{7}$$

2. From Eq. 7, we can observe that m which is the mass of electron is not a constant and a variable of $\left(\frac{d^2E}{dK^2}\right)$

3. $\left(\frac{d^2E}{dK^2}\right)$ is the radius of curvature of a parabola which describes the variation of E with respect to K. E-K diagram is shown in the figure.

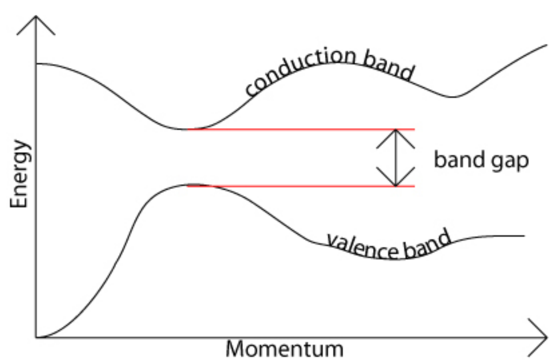


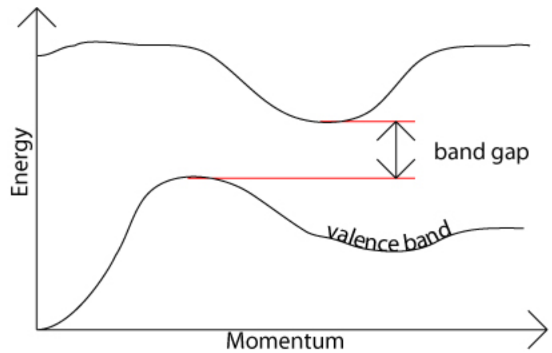
4. Effective mass is different from actual rest mass. It can be zero or even negative for electrons depends on its position in the band.

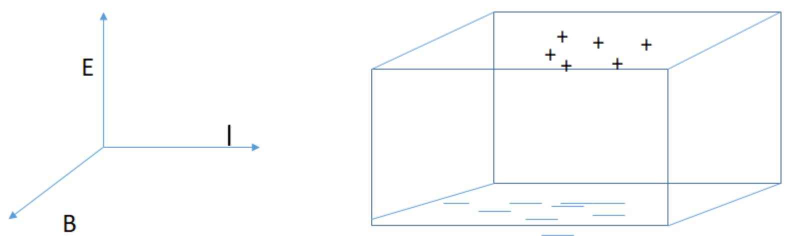
4 Direct and indirect bandgap semiconductor

In direct bandgap semiconductor, the top of valance band and the bottom of conduction band are at same momentum. So that the transition between conduction band and valance band takes place directly.

In indirect bandgap semiconductor, the top of valance band and bottom of conduction band occur at different momentum. Hence direct transition is not possible.







5 Hall effect

If a magnetic field (B) is applied perpendicular (transverse) to a current (I) carrying conductor (current and magnetic field are perpendicular to each other), an electric field (voltage) which is perpendicular to both current and magnetic field is produced. This effect is known as Hall effect.

Consider a current carrying conductor as shown in the figure. The electrons move in negative x direction. A magnetic field is applied in z direction. Because of this movement of charge carriers and perpendicular magnetic field Lorentz force will be created. The Lorentz force on electrons is given by

$$F = -qv \times B, \tag{8}$$

where q is the charge of electron and the -ive sign represent negative charge. v is the velocity of electron and B is the magnetic field. Since v is in the x direction and B is in the y direction, the F vector (force acting on electrons) will be in -z direction. Because of this force, electron will be oriented towards -z direction. Hence a potential will be created between +z side and -z side. If holes are present in the conductor, then they will be oriented towards positive y direction. The voltage created in this manner is called Hall voltage. The Hall electric field can be given as

$$E_H = \frac{V_H}{d}. \tag{9}$$

This electric field is in the opposite direction to that of the Lorentz force and under stable condition both of them are equal. The force due to the Hall electric field is given by

$$F_E = qE_H \tag{10}$$

Since the Hall force is equal to the Lorentz force,

$$\begin{aligned} qvB &= qE_H \\ vB &= E_H \\ vB &= \frac{V_H}{d} \end{aligned}$$

$$vBd = V_H \tag{11}$$

The above expression gives Hall voltage