

**UNIT- 1****ELECTRICAL PROPERTIES OF MATERIALS****1.4. Density of Energy States**

A parameter of interest in the study of conductivity of metals and semiconductors is the density of states. The Fermi function  $F(E)$  gives only the probability of filling up of electrons in a given energy state. It does not give the information about the number of electrons that can be filled in a given energy state, to know that we should know the number of available energy states called density of state

Density of states  $Z(E)dE$  is defined as the number of states per unit volume in an energy interval  $E$  and  $E+dE$ .

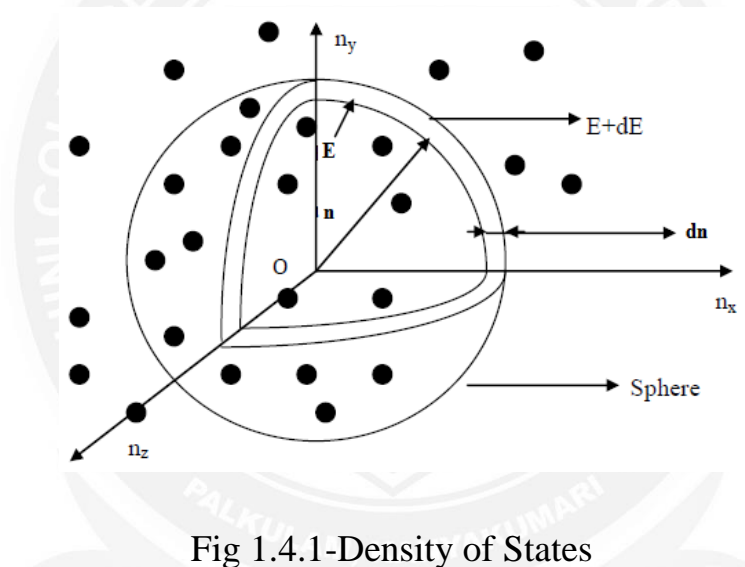


Fig 1.4.1-Density of States

$$\text{Density of states } Z(E) dE = \frac{N(E)dE}{\text{Volume of the metal piece (V)}}$$

The number of available energy levels can be obtained for various combinations of quantum numbers  $n_x, n_y$  and  $n_z$ .

$$i.e. \quad n^2 = n_x^2 + n_y^2 + n_z^2$$

Let us construct a three dimensional space of points which represents the quantum numbers  $n_x, n_y$  and  $n_z$  as shown in above figure. Each point in this space represents an energy level. Let us consider a cubical sample with side ' $a$ '. A sphere is constructed with the quantum numbers  $n_x, n_y$  and  $n_z$  as three coordinate axes in three dimensional space, as shown in above figure. A radius ' $n$ ' is drawn from the origin ' $O$ ' to a point  $n_x, n_y$  and  $n_z$  in space and all the points on the surface of the sphere will have the same energy ' $E$ '. Thus,  $n^2 = n_x^2 + n_y^2 + n_z^2$  denotes the radius ' $n$ '. Any change in  $n_x, n_y$  and  $n_z$  will change ' $E$ ' and hence the radius ' $n$ '.

Therefore, the number of energy states with in a sphere of radius ‘ $n$ ’

$$n = \frac{4}{3}\pi n^3 \quad \dots \dots \dots (1)$$

Since the quantum numbers  $n_x, n_y$  and  $n_z$  can have only positive integer value, we have totake only one of the sphere, (*i.e*)  $(1/8)^{\text{th}}$  of the spherical volume.

Number of available energy states within one octant of sphere of radius ‘ $n$ ’ corresponding to energy ‘ $E$ ’

$$n = \frac{1}{8}\left(\frac{4}{3}\pi n^3\right) \quad \dots \dots \dots (2)$$

Hence, the number of available energy states between the spheres of radius  $n+dn$  corresponding to energy  $E+dE$  is

$$= \frac{1}{8}\left(\frac{4}{3}\pi(n+dn)^3\right) - 3)$$

The number of available energy states between the shell of radius ‘ $n$ ’ and ‘ $n+dn$ ’ corresponding energy between ‘ $E$ ’ and ‘ $E+dE$ ’ is determined by subtracting equation (2) from equation (3), we have

$$\begin{aligned} N(E)dE &= \frac{1}{8}\left(\frac{4}{3}\pi(n+dn)^3\right) - \frac{1}{8}\left(\frac{4}{3}\pi n^3\right) \\ &= \frac{1}{8}\left(\frac{4}{3}\pi\right) [(n+dn)^3 - n^3] \\ N(E) dE &= \frac{1}{8}\left(\frac{4}{3}\pi\right) (dn^3 + 3n^2dn + 3ndn^2) \quad \dots \dots (4) \end{aligned}$$

Since  $dn$  is very small, the higher powers  $dn^2$  and  $dn^3$  terms are neglected. Equation (4) becomes,

$$N(E)dE = \frac{1}{8}\left(\frac{4}{3}\pi\right) 3n^2dn \quad \dots \dots (5)$$

Number of available energy states between interval  $E$  and  $E+dE$  is given by

$$\begin{aligned} N(E) dE &= \frac{\pi}{2} n^2 dn \\ N(E) dE &= \frac{\pi}{2} n(ndn) \quad \dots \dots \dots (6) \end{aligned}$$

From the application of Schrodinger wave equation, the energy of the electron in a cubical metal piece of side ‘ $a$ ’ is given by

$$\begin{aligned} E &= \frac{n^2 h^2}{8ma^2} \\ n^2 &= \frac{8mEa^2}{h^2} \quad \dots \dots \dots (7) \end{aligned}$$

Take the square root of the above equation we get,

$$n = \left( \frac{8ma^2E}{h^2} \right)^{1/2} \dots \dots \dots (8)$$

Differentiate the equation (7), we get,

$$\begin{aligned} 2n dn &= \frac{8ma^2}{h^2} dE \\ n dn &= \frac{8ma^2}{2h^2} dE \dots \dots \dots (9) \end{aligned}$$

Substitute eqn. (8) and (9) in eqn. (6) we have

$$\begin{aligned} N(E) dE &= \frac{\pi}{2} \left( \frac{8ma^2E}{h^2} \right)^{\frac{1}{2}} \left( \frac{8ma^2 dE}{2h^2} \right) \\ N(E) dE &= \frac{\pi}{4} \left( \frac{8ma^2}{h^2} \right)^{\frac{3}{2}} E^{1/2} dE \dots \dots \dots (10) \end{aligned}$$

Pauli's exclusion principle states that the two electrons of opposite spins can occupy each state. Hence, the number of energy states available for electron occupancy is given by,

$$\begin{aligned} N(E) dE &= 2 \times \frac{\pi}{4} \left( \frac{8ma^2}{h^2} \right)^{\frac{3}{2}} E^{\frac{1}{2}} dE \\ &= \frac{\pi}{2} (8m)^{\frac{3}{2}} \left( \frac{a^3}{h^3} \right) E^{\frac{1}{2}} dE \\ &= \frac{\pi}{2} 8(2m)^{\frac{3}{2}} \left( \frac{a^3}{h^3} \right) E^{\frac{1}{2}} dE \quad (\because (8m)^{\frac{3}{2}} = 8(2m)^{\frac{3}{2}}) \\ N(E) dE &= \frac{4\pi}{h^3} a^3 (2m)^{\frac{3}{2}} E^{\frac{1}{2}} dE \dots \dots \dots (11) \end{aligned}$$

The density of states is equal to the number of states per unit volume in the energy range in  $E$  and  $E+dE$

$$\begin{aligned} Z(E) dE &= \frac{N(E) dE}{V} \\ &= \frac{\frac{4\pi}{h^3} a^3 (2m)^{3/2} E^{1/2} dE}{a^3} \\ Z(E) dE &= \frac{4\pi}{h^3} (2m)^{3/2} E^{1/2} dE \dots \dots \dots (12) \end{aligned}$$

This is the expression for the density of states and it is used to calculate the carrier concentration of metals and semiconductors.

#### 1.4.1. Calculation of Carrier Concentration at 0 K

The number of electrons per unit volume is called carrier concentration. It is calculated by summing up the product of the density of states  $Z(E)$  and Fermi distribution function  $F(E)$ .

Carrier concentration  $n_c = \int Z(E) F(E) dE$

Substituting  $Z(E)$  and  $F(E)$  in the above equation, we get,

$$n_c = \int \frac{4\pi}{h^3} (2m)^{3/2} E^{1/2} \frac{1}{1 + e^{(E-E_F)/KT}} dE \quad \dots (1)$$

For metals at  $T = 0$  K, the upper most occupied level is  $E_F$  and  $F(E) = 1$ . Now the equation (1) becomes,

$$\begin{aligned} n_c &= \int_0^{E_F} \frac{4\pi}{h^3} (2m)^{3/2} E^{1/2} dE \\ &= \frac{4\pi}{h^3} (2m)^{3/2} \int_0^{E_F} E^{1/2} dE \\ n_c &= \frac{4\pi}{h^3} (2m)^{3/2} \left[ \frac{E^{3/2}}{3/2} \right]_0^{E_F} \\ n_c &= \frac{8\pi}{3h^3} (2mE_F)^{3/2} \quad \dots \dots \dots (2) \end{aligned}$$

This equation is the carrier concentration or density of charge carrier at 0 K in terms of Fermi energy.

#### 1.4.2. Calculation of Fermi Energy

Fermi energy is calculated from the expression of carrier concentration.

$$n_c = \frac{8\pi}{3h^3} (2mE_F)^{3/2}$$

$$(E_F)^{3/2} = \frac{3h^3 n_c}{8\pi (2m)^{3/2}}$$

Multiply the power of  $2/3$  on both sides of the above equation, we have

$$E_F = \left[ \frac{3h^3 n_c}{8\pi (2m)^{3/2}} \right]^{2/3}$$

$$E_F = \left[ \frac{3h^3 n_c}{\pi (8m)^{3/2}} \right]^{2/3} \quad (\because (8m)^{3/2} = 8(2m)^{3/2})$$

Rearrange the above equation, we get

$$E_F = \frac{h^2}{8m} \left( \frac{3n_c}{\pi} \right)^{2/3}$$

This is the expression for Fermi energy of electrons in solids at absolute zero temperature. It is depends only on the density of electrons of metals.

