

UNIT- 2

ELECTRICAL PROPERTIES OF MATERIALS

CONTENTS

2.5. 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 $E+dE$.

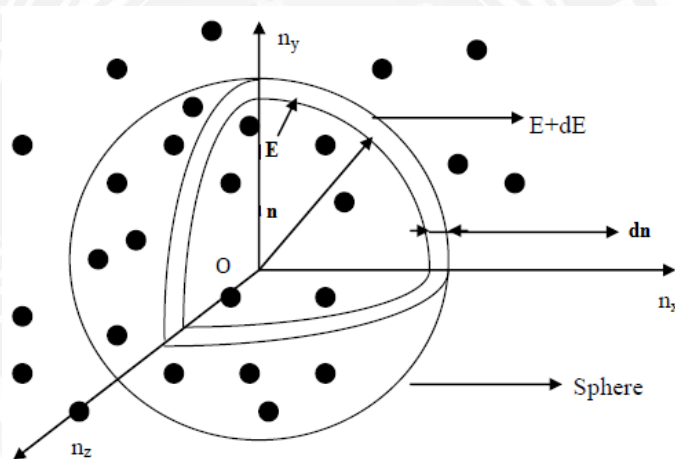


Fig2.5.1-Density of States

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

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 within a sphere of radius 'n'

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

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

Number of available energy states within one octant of sphere of radius 'n' corresponding to energy 'E'

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

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

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

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

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

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

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

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

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

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

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

$$E = \frac{n^2 h^2}{8ma^2}$$

$$n^2 = \frac{8mEa^2}{h^2} \dots \dots \dots (7)$$

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,

$$2ndn = \frac{8ma^2}{h^2} dE$$

$$ndn = \frac{8ma^2}{2h^2} dE \dots \dots \dots (9)$$

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

$$N(E) dE = \frac{\pi}{2} \left(\frac{8ma^2E}{h^2}\right)^{\frac{1}{2}} \left(\frac{8ma^2 dE}{2h^2}\right)$$

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

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,

$$N(E) dE = 2 \times \frac{\pi}{4} \left(\frac{8ma^2}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}} dE$$

$$= \frac{\pi}{2} (8m)^{\frac{3}{2}} \left(\frac{a^3}{h^3}\right) E^{\frac{1}{2}} dE$$

$$= \frac{\pi}{2} 8(2m)^{\frac{3}{2}} \left(\frac{a^3}{h^3}\right) E^{\frac{1}{2}} dE \quad (\because (8m)^{\frac{3}{2}} = 8(2m)^{\frac{3}{2}})$$

$$N(E) dE = \frac{4\pi}{h^3} a^3 (2m)^{\frac{3}{2}} E^{\frac{1}{2}} dE \dots \dots \dots (11)$$

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

$$Z(E) dE = \frac{N(E) dE}{V}$$

$$= \frac{\frac{4\pi}{h^3} a^3 (2m)^{3/2} E^{1/2} dE}{a^3}$$

$$Z(E) dE = \frac{4\pi}{h^3} (2m)^{3/2} E^{1/2} dE \dots \dots \dots (12)$$

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

2.5.1. 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 $F(E)$.

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

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.

2.5.2. Calculation of Fermi Energy

Fermi energy is calculated from the expression of carrier concentration.

$$\begin{aligned} n_c &= \frac{8\pi}{3h^3} (2mE_F)^{3/2} \\ (E_F)^{3/2} &= \frac{3h^3 n_c}{8\pi (2m)^{3/2}} \end{aligned}$$

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

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

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.

