UNIT– 1

CONDUCTING 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.

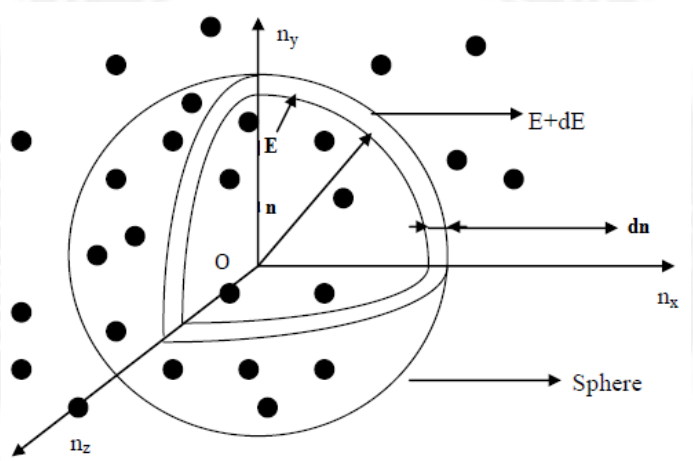

Fig 1.4.1-Density of States

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

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

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

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*'

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

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*) $(1/8)^{th}$of the spherical volume.

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

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

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

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

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

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

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

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

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

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

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

$$N(E)\,dE = \frac{\pi}{2}n^2dn$$

$$N(E)\,dE = \frac{\pi}{2}n(ndn) \quad \ldots\ldots\ldots\ldots\ldots\ldots (6)$$

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

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

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

Take the square root of the above equation we get,

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

Differentiate the equation (7), we get,

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

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

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

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

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

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,

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

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

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

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

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

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

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

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

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,

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

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

$$n_c = \int_0^{E_F} \frac{4\pi}{h^3}(2m)^{3/2}E^{1/2}\,dE$$

$$= \frac{4\pi}{h^3}(2m)^{3/2}\int_0^{E_F} E^{1/2}\,dE$$

$$n_c = \frac{4\pi}{h^3}(2m)^{3/2}\left[\frac{E^{3/2}}{3/2}\right]_0^{E_F}$$

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

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.

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

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

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

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

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

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.