

# Free Electron Theory of Conduction in Metal

## Crystalline Structure

A solid of definite shape which is formed due to regular repetition of its atoms, ions or molecules in three dimension patterns is called a *crystal*. The location of each atom is well known by periodicity. The periodic arrangement of atoms in a crystal is called *crystal lattice*. The crystal lattice without having atoms in it is called *space lattice or lattice array*.

The most convenient small cell in the crystal structure that carries the property of the crystal is called unit cell. The repetition of unit cell in three dimensions generates the whole crystal. A *basis* is defined as an assembly or group of atoms which when associated with lattice form a crystal. i.e. basis + lattice = crystal. In a crystal the number of nearest neighbors to an atom in a given structure is called *co-ordination number*. In a unit cell the *atomic concentration* is defined as the number of atoms in that unit cell to the volume of unit cell.

### Simple Cubic Unit Cell (SC)

An unit cell having same dimension in all direction and containing only corner atoms is called simple cubic unit cell. The side of the cube is equal to distance between the two atoms.

Each corner atom is shared by eight unit cell so only  $\frac{1}{8}$  th of each corner atom belongs to unit cell.

$$\text{Therefore, number of atoms per unit cell} = 8 \times \frac{1}{8} = 1$$

If 'a' be the side of unit cell and 'r' be the radius of an atom then from figure  $a = 2r$ .

Packing density or Packing fraction is define as.

$$\text{p.f.} = \frac{\text{volume of atoms in unit cell}}{\text{volume of unit cell}}$$

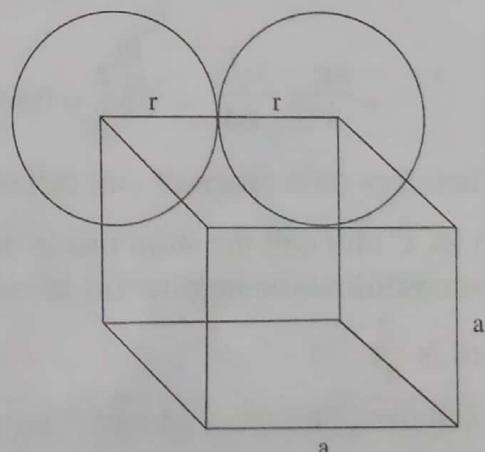


Figure : Simple cubic unit cell

$$= \frac{(4\pi/3)r^3 \times 1}{a^3} = \frac{(4\pi/3)r^3}{(2r)^3} = \frac{\pi}{6} = 0.52 = 52\%$$

Therefore 52% space of unit cell is occupied by the atoms.

In simple cubic unit cell an atom has a close neighbour along  $+x$ -axis and another along  $-x$  axis. The same is true of  $y$  and  $z$  axis. Thus the co-ordination number for each corner atom is six (6).

The atomic concentration for SC unit cell is  $\frac{1}{a^3}$ .

Example: Polonium

### Body Centered Cubic Unit Cell (BCC)

A cubic unit cell with corner atoms and an atom at body centered position (i.e. the point at which body diagonal meets) is called B.C.C unit cell. Each corner atom is shared by eight unit cells, so only  $\frac{1}{8}$  th of each corner atom belongs to unit cell. The atom at body centered position cannot be shared by any other unit cell.

$$\text{Therefore, number of atoms per unit cell} = 8 \times \frac{1}{8} + 1 = 2$$

$$\text{From figure, } \sqrt{(\sqrt{2}a)^2 + a^2} = r + 2r + r$$

$$\sqrt{3}a = 4r$$

$$a = \frac{4}{\sqrt{3}}r$$

$$\text{packing fraction} = \frac{2 \times (4\pi/3)r^3}{a^3} = \frac{2 \times (4\pi/3)r^3}{\left(\frac{4}{\sqrt{3}}r\right)^3}$$

$$= \frac{8\pi}{3} \times \frac{3\sqrt{3}}{64} = \sqrt{3} \frac{\pi}{8} = 0.68 = 68\%$$

Therefore 68% space of unit cell is occupied by the atoms.

In BCC unit cell the atom inside the cell has all the corner atoms as its close neighbours. Thus the co-ordination number for interior atom is eight (8). The atomic concentration for BCC unit cell is  $\frac{2}{a^3}$ .

Examples: Sodium, Lithium, Chromium

### Face Centered Cubic Unit Cell (FCC)

A cubic unit cell formed by corner atoms along with atom in each face centered position [i.e. at a point at which face diagonal meets] is called FCC unit cell. Each corner atom is shared by eight unit cell, so only  $\frac{1}{8}$  th of each corner atom belongs to unit cell. Each atom at face centered position is shared by two unit cell so one half of each face centered atom belongs to unit cell.

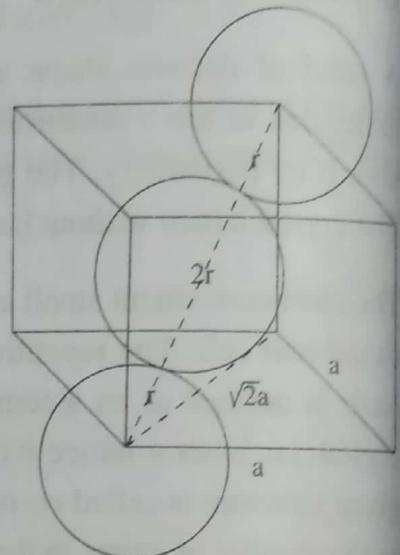


Figure : BCC unit cell

$$\text{Therefore, number of atoms per unit cell} = 8 \times \frac{1}{8} + 6 \times \frac{1}{2} \\ = 4$$

from figure  $\sqrt{2} a = 4r$

$$\Rightarrow a = \frac{4}{\sqrt{2}} r = 2\sqrt{2} r$$

$$\text{Packing fraction} = \frac{4 \times (4\pi/3) r^3}{a^3}$$

$$= \frac{(16\pi/3) r^3}{(2\sqrt{2} r)^3} = \frac{16\pi}{3 \times 8 \times 2\sqrt{2}} = \frac{\pi}{3\sqrt{2}} = 0.74$$

$$\text{Packing fraction (p.f)} = 74\%$$

Therefore 74% space of fcc unit cell is occupied by atoms.

For a FCC unit cell, each corner atom is having four close neighbours in each of three xy, yz and zx planes. Thus the co-ordination number in this case is  $4 \times 3 = 12$ . The atomic concentration for FCC unit cell is  $\frac{4}{a^3}$ .

Examples: Aluminum, Copper, Lead, Silver

### Bravais Lattice

In three dimensional space lattices, there exist only fourteen different distinct lattices. All these are known as Bravais space lattices.

From these fourteen types of lattices the crystals have been classified into seven systems.

In figure a, b, c are called lattice parameter or primitives. The angles between (a, b), (b, c) and (c, a) are denoted by  $\gamma$ ,  $\alpha$  and  $\beta$  respectively. Different specifications for a, b and c as well as  $\alpha$ ,  $\beta$  and  $\gamma$  generate different crystal systems as listed in table below.

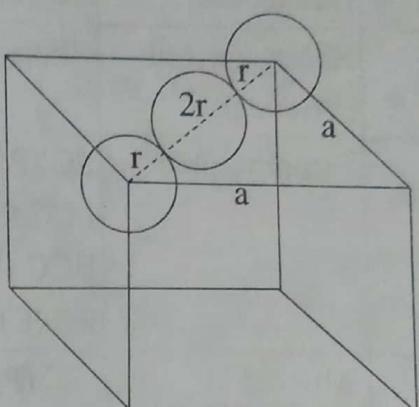
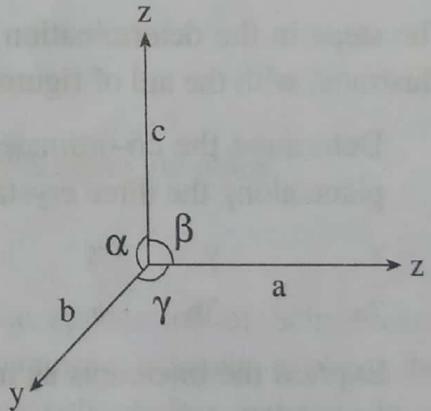


Figure : FCC unit cell



S.N.	Class of crystal	Type of Lattices	Number of Lattices	Angle between axes	Length of primitives
1	Cubic	SC (P) FCC (F) BCC (I)	3	$\alpha = \beta = \gamma = 90^\circ$	$a = b = c$

2.	Tetragonal	SC (P) BCC (I)	2	$\alpha = \beta = \gamma = 90^\circ$	$a = b \neq c$
3.	Hexagonal	SC (P)	1	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	$a = b \neq c$
4.	Rhombohedral (Trigonal)	Rhombohedral (R)	1	$\alpha = \beta = \gamma \neq 90^\circ < 120^\circ$	$a = b = c$
5.	Orthorhombic	SC (P) FCC (F) BCC (I) BC (C)- base centered	4	$\alpha = \beta = \gamma = 90^\circ$	$a \neq b \neq c$
6.	Monoclinic	SC (P) BC (C)	2	$\alpha = \gamma = 90^\circ \neq \beta$	$a \neq b \neq c$
7.	Triclinic	SC (P)	1	$\alpha \neq \beta \neq \gamma$	$a \neq b \neq c$

Where, P = Primitive SC (simple cubic), F = FCC (face centered cubic), I = BCC (body centered cubic), C = BC (base centered), R = Rhombohedral.

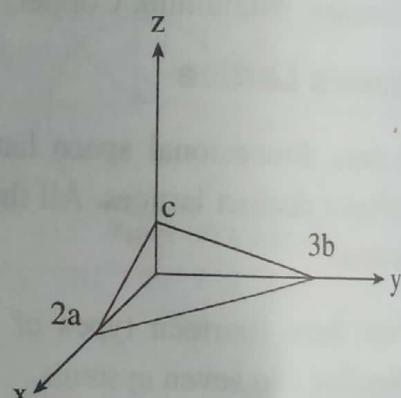
## Miller Indices

Miller indices are a set of three numbers denoted as  $(h, k, l)$  used to represent a lattice plane in a crystal.

The steps in the determination of miller indices of a plane are illustrated with the aid of figure.

- Determine the co-ordinates of the intercepts made by the plane along the three crystallographic axes (x, y, z axes)

$$\begin{array}{ccc} x & y & z \\ 2a & 3b & c \end{array}$$



- Express the intercepts as multiples of the unit cell dimensions, or lattice parameters along axes. i.e.

$$\begin{array}{ccc} 2 & 3 & 1 \end{array}$$

- Get the reciprocals of these numbers

$$\begin{array}{ccc} \frac{1}{2} & \frac{1}{3} & \frac{1}{1} \end{array}$$

- Reduce these reciprocals to the smallest set of integral numbers and enclose them in bracket. [Multiply each with the L.C.M ]

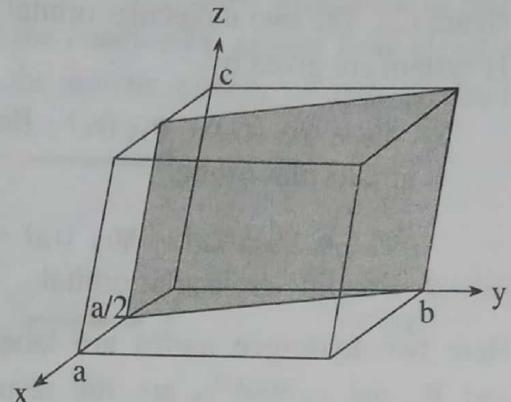
$$6 \times \frac{1}{2} \quad 6 \times \frac{1}{3} \quad 6 \times \frac{1}{1}$$

$$\begin{array}{ccc} 3 & 2 & 6 \end{array}$$

Therefore, the miller indices for the plane (2a, 3b, c) are given by  $(h, k, l) = (3, 2, 6)$ . If a plane cuts an axis on the negative side of the origin, the index is negative and denoted as  $(h, \bar{k}, l)$  by placing a minus (-) sign above the corresponding index. For an intercept at infinity the corresponding index is zero.

The six faces of a cubic crystal are  $(1, 0, 0)$ ,  $(0, 1, 0)$ ,  $(0, 0, 1)$ ,  $(\bar{1}, 0, 0)$ ,  $(0, \bar{1}, 0)$  and  $(0, 0, \bar{1})$ . From a crystallographic point of view many planes

in lattice are equivalent i.e. a plane with given miller indices can be shifted about in the lattice by a choice of the position and orientation of the unit cell. The indices of such equivalent planes are enclosed in braces {} instead of in parenthesis ( ). For example, all the six cube faces are crystallographically equivalent because the unit cell can be rotated in various directions and still appear the same. The six equivalent faces are collectively designated as {1, 0, 0}.



For example, for the plane shown in figure (2).

$$\text{Here, } (x, y, z) = \left(\frac{a}{2}, b, \infty\right)$$

$$\text{Intercepts} = \left(\frac{1}{2}, 1, \infty\right)$$

Their reciprocals are  $(2, 1, 0)$

There are no fraction so  $(2 1 0)$  are required Miller indices for crystallographic plane.

## Modern Theory of Solid

One of the great successes of quantum mechanics has been the application of Schrödinger equation to the behavior of molecules and solid. For example, quantum mechanics explains the nature of the bond between atoms and its consequences. An intuitively obvious outcome from quantum mechanics is that the energy of the electron is still quantized in the molecule. In addition, the application of quantum mechanics to large number of atoms as in solid, leads to energy bands with in which the electron energy levels are almost continuous. It is nearly impossible to understand the principles of operation of modern solid state electronic devices without good knowledge of the band theory of solids.

## Molecular Orbital Bonding Theory

The bond formation between two H-atoms can easily explained by describing the behaviour of electrons with in the molecule. Each H-atom is associated with an atomic orbital  $\psi_{1s}$ . As two atoms approach each other as shown in figure (1) the atomic wave functions overlap. This

overlapping of wave functions produces two new wave functions with different energies and hence different quantum number. The two wave functions can overlap either in phase forming *bonding molecular orbital* or in out of phase forming *anti-bonding orbital* as shown in figure (2). The two molecular orbital in H-H system are given by.

$$\Psi_{\sigma} = \Psi_{1s}(r_A) + \Psi_{1s}(r_B) - \text{Bonding molecular orbital}$$

$$\Psi_{\sigma^*} = \Psi_{1s}(r_A) - \Psi_{1s}(r_B) - \text{Anti Bonding molecular orbital}$$

Here two hydrogen atoms are labeled A and B, and  $r_A$  and  $r_B$  are the respective distances of the electrons from their parent nucleus. Here to find molecular orbital we have used *linear combinations of atomic orbital (LCAO) method*.

Here,  $\Psi_{\sigma}$  is symmetric and  $\Psi_{\sigma^*}$  is anti-symmetric and has node between the nuclei, as in hydrogenic wave functions. Since  $\Psi_{\sigma^*}$  has a node so it has higher energy than the  $\Psi_{\sigma}$  orbital.

The atomic energy level  $E_{1s}$  splits into two energy levels  $E_{\sigma}$  and  $E_{\sigma^*}$  corresponds to  $\Psi_{\sigma}$  and  $\Psi_{\sigma^*}$ . The splitting is due to interaction (overlap) between the atomic orbital. The two energies  $E_{\sigma}$  and  $E_{\sigma^*}$  are widely different and can be calculated from Schrödinger wave equation by using potential energy function of the system.  $E_{\sigma^*}$  lies above  $E_{1s}$  and  $E_{\sigma}$  lies below  $E_{1s}$  as shown in figure (3).

As interatomic separation ( $R$ )

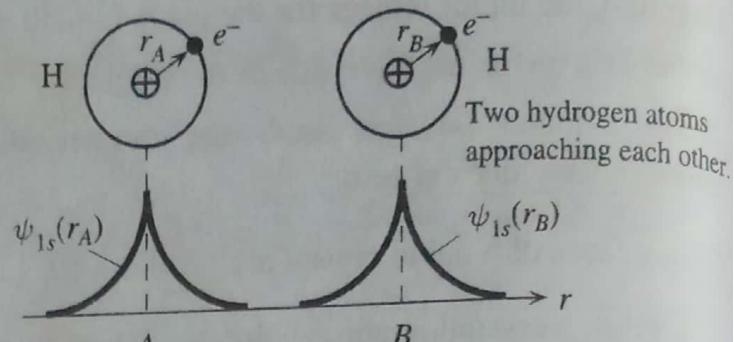


Figure 1: Two hydrogen atoms approaching each other

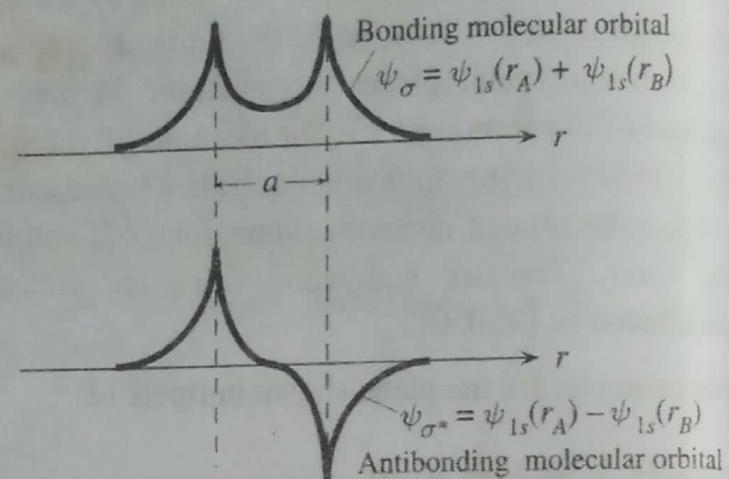


Figure 2: Formation of molecular orbitals when two H-atoms approach each other

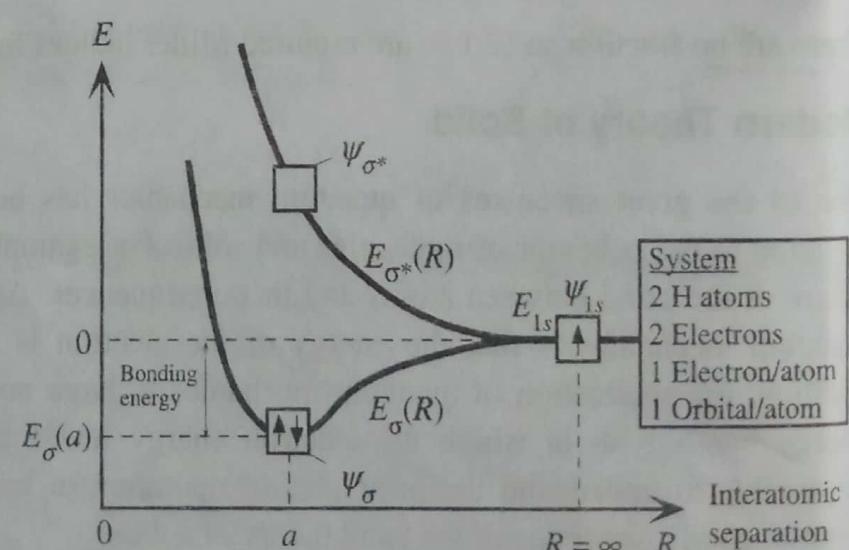


Figure 3: Energy of  $\Psi_{\sigma}$  and  $\Psi_{\sigma^*}$  versus the inter atomic separation ( $R$ )

decreases and the two atom get closer, the energy of  $\Psi_{\sigma}$  orbital became minimum at  $R = a$  (where  $a$  = closest interatomic distance).

Each orbital state can hold two electrons with spin paired, and within the two hydrogen atoms we have two electrons. If these two electrons enter the  $\psi_{\sigma}$  orbital and pair their spins then this new configuration is energetically more favorable than two isolate H-atoms and  $\psi_{\sigma^*}$  orbital. It is responsible to form  $H_2$  molecule. The energy difference between that of two isolated H-atoms and the  $E_{\sigma}$  minimum energy at  $R = a$  is called *bonding energy*.

When two electrons in the  $H_2$  molecule occupy the  $\psi_{\sigma}$  orbital, their probability distribution (or the negative charge distribution) is such that the negative PE arising from attractions of these two electrons and two proton is larger in magnitude than the positive PE arising from electron-electron repulsion and proton - proton repulsion and the kinetic energy of two electrons. Therefore the  $H_2$  molecule is energetically stable.

Figure (4) illustrates the change in the electron energy levels as two isolated H atom are brought together to form the  $H_2$  molecule.

When we bring three hydrogen atoms (labeled A, B and C) together it generates three separate molecular orbital states  $\psi_a$ ,  $\psi_b$  and  $\psi_c$  from three  $\psi_{1s}$  orbital of different atom.

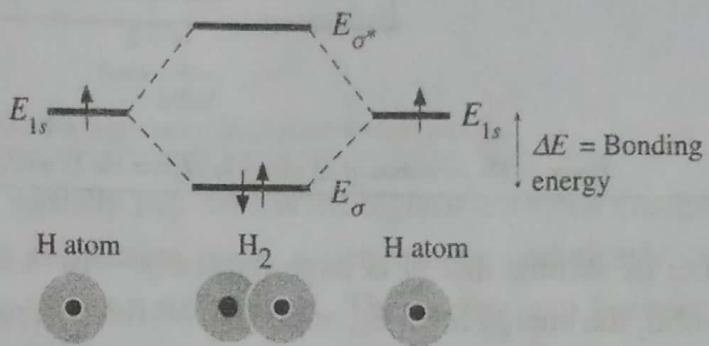


Figure 4: Schematic diagram showing the changes in the electron energy as two isolated H-atoms, far left and far right, come together to form a hydrogen molecule

The energies  $E_a$ ,  $E_b$  and  $E_c$  of  $\psi_a$ ,  $\psi_b$  and  $\psi_c$  can be calculated from Schrödinger wave equation by using PE function of this system. As in the case of  $H_2$ , the molecular wave functions having more nodes have higher energy and other have lower energy. There are three electrons in the three hydrogen system. The first two pair their spins with function  $\psi_a$  and energy  $E_a$ . The third one enter orbital  $\psi_b$  at energy  $E_b$ . Here  $H_3$  has an extra electron (unpaired) at the higher energy level ( $E_b$ ), which tends to increase the net energy of the atom. Thus  $H_3$  is much less stable than the  $H_2$  molecule.

## Band Theory of Solids

In the formation of solid, the identical orbital of different atoms interact with each other to form the large number of energy levels equal to the number of atoms. The separation between the energy levels is so small that for very large numbers of atoms require to form a solid, it can be assumed continuous. So that the continuous energy levels is regarded an *energy band*.

Consider the formation of Lithium metal from N atoms of Li. Li has configuration  $1S^2, 2S^1$ . We assume that the atomic energy levels will split into N separate energy levels. Since  $1S$  shell is full and is close to the nucleus, it will not be affected much by interatomic interaction.

In the system of N isolated Li atoms, we have N electrons in N  $\psi_{2s}$  orbitals at the energy  $E_{2s}$  as shown in figure (1).

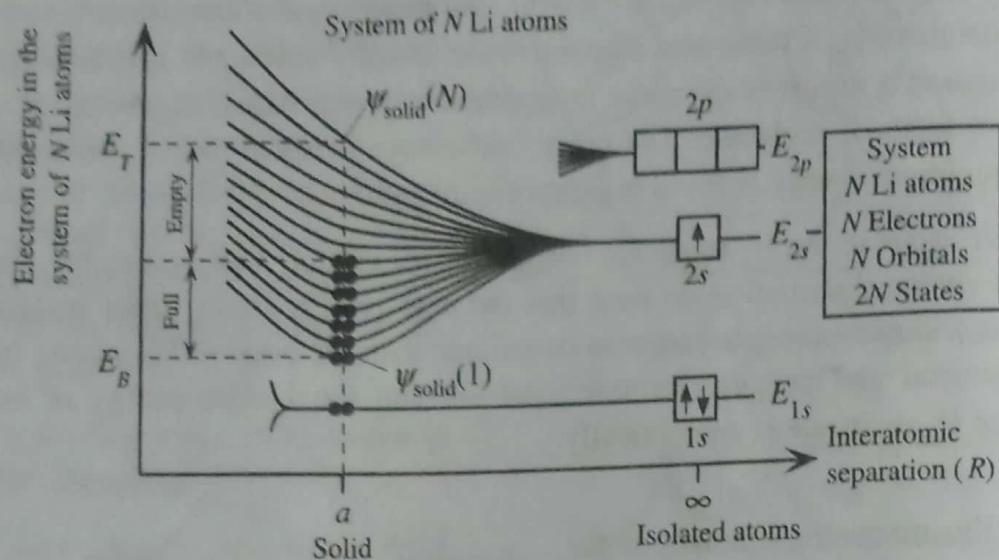


Figure 1: The formation of 2S energy band from the 2S orbitals when  $N$  Li atoms come together to form the Li solid

Let us assume that  $N$  is large (typically  $\sim 10^{23}$ ). As  $N$  atoms are brought together to form the solid, the energy level  $E_{2s}$  splits into  $N$ - finely separated energy levels.

The interatomic interactions between  $N \psi_{2s}$  orbital thus spread the  $N$  energy levels between the bottom and top levels,  $E_B$  and  $E_T$ , respectively which are determined by the closest inter atomic distance 'a'. It is obvious that with  $N$  very large, the energy separation between two consecutive energy level is very small; indeed it is almost infinitesimal as shown in figure (1).

Remember that each energy level  $E_i$  in Li metal of figure (1) is the energy of an electron wave function  $\psi_{\text{solid}(i)}$  in the solid. Where  $\psi_{\text{solid}(i)}$  is one particular combination of the  $N$  atomic wave functions  $\psi_{2s}$ . There are  $N$  different ways to combine  $N$  atomic wave functions  $\psi_{2s}$ , since each can be added in phase or out of phase. The phase combination has lowest energy ( $E_B$ ) and the out of phase combination have highest energy ( $E_T$ ). Other combination of  $\psi_{2s}$  give rise to different energy values between  $E_B$  and  $E_T$ .

The single 2S energy level  $E_{2s}$  therefore splits into  $N$  finely separated energy levels, forming an energy band as shown in figure (1). The  $N/2$  separate energy levels are filled because each can take two electrons with opposite spins. Therefore the band is half full. The energy band formed by atomic energy levels are termed as their respective band such as 1S band, 2S band etc as shown in figure (2). It must be emphasized that the electrons with in a band do not belong to any specific atom but to the whole solid.

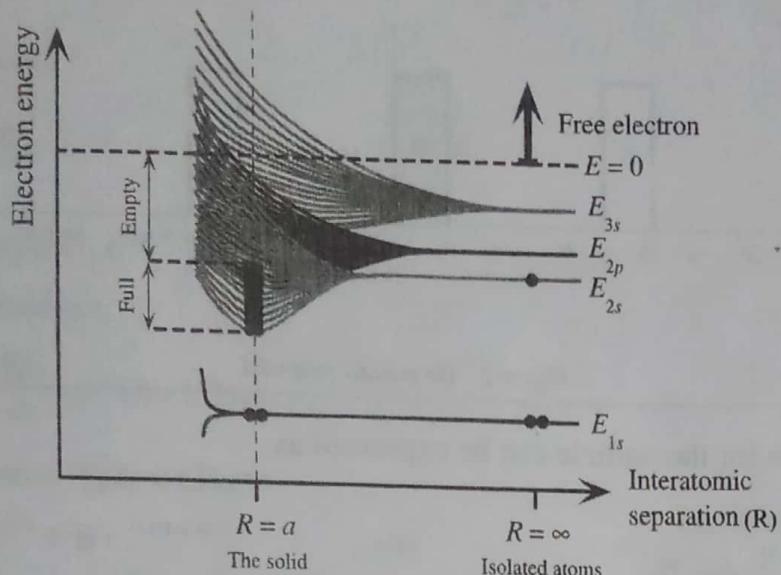


Figure 2: Formation of different energy bands when large number of Li-atoms brought together

In solid, valence band is either completely or partially full. This is the highest occupied energy band. The next higher energy band is called conduction band, which can be completely or partially filled band. Conduction band is the lowest unfilled band. The energy gap between valence band and conduction band is called forbidden gap where no states are available and so no electrons.

All the materials are classified on the basis of energy band gap. According to which they are basically conductors, semiconductors and insulators. In conductor, there is virtually no energy gap between valence band and conduction bond. They overlap with each other. The valence electrons can be readily assumed as conduction electron.

In insulators, the energy band gap between valence band and conduction band is of the order of 10 eV. All the states in valence band are completely filled and in conduction band all states are empty.

In semi conductors the energy gap between valence band and conduction band is in average 1eV. Here also at absolute zero all the states in valence band are occupied and all the states in conduction band are empty. But at room temperature the number of electrons in semiconductor is fairly higher than that of insulators as less energy is required to excite valence electrons to conduction band in semiconductor.

### Kroning - Penny Model

It is the treatment of energy levels of an electron experiencing one dimensional periodic potential. Consider a periodic potential with period  $L = a + b$  as shown in figure. Where 'a' is the width of well and 'b' is width of barrier.

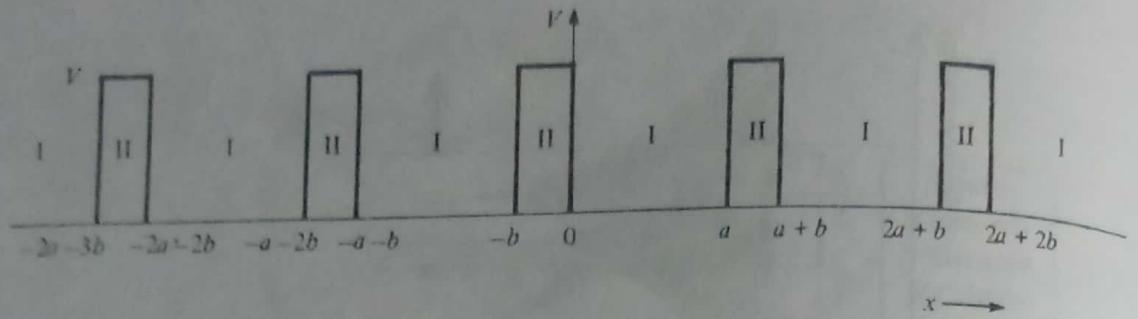


Figure 1 : The periodic potential

The potential function for the particle can be expressed as

$$V(x) = 0 \text{ for region I}$$

$$V(x) = V \text{ for region II}$$

For region (I) Schrödinger wave equation can be written as

$$\frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2} \psi_1 = 0$$

$$\frac{d^2\psi_1}{dx^2} + \alpha^2 \psi_1 = 0 \quad \dots(1)$$

$$\text{Where } \alpha^2 = \frac{2mE}{\hbar^2}$$

Since the potential is periodic, its' solution can be written as,

$$\psi_1 = U_1 e^{ikx}$$

$$\frac{d\psi_1}{dx} = e^{ikx} \frac{dU_1}{dx} + ikU_1 e^{ikx}$$

$$\frac{d^2\psi_1}{dx^2} = e^{ikx} \frac{d^2U_1}{dx^2} + ike^{ikx} \frac{dU_1}{dx} + ike^{ikx} \frac{dU_1}{dx} + (ik)^2 U_1 e^{ikx}$$

$$= e^{ikx} \left( \frac{d^2U_1}{dx^2} + 2ik \frac{dU_1}{dx} - k^2 U_1 \right)$$

Substituting the value of  $\frac{d^2\psi_1}{dx^2}$  in equation (1)

$$e^{ikx} \left( \frac{d^2U_1}{dx^2} + 2ik \frac{dU_1}{dx} - k^2 U_1 \right) + \alpha^2 U_1 e^{ikx} = 0$$

$$\frac{d^2U_1}{dx^2} + 2ik \frac{dU_1}{dx} - k^2 U_1 + \alpha^2 U_1 = 0 \quad \dots(2)$$

For region (II), Schrödinger wave equation can be written as

$$\frac{d^2\psi_2}{dx^2} + \frac{2m(E-V)}{\hbar^2} \psi_2 = 0 \Rightarrow \frac{d^2\psi_2}{dx^2} - \frac{2m(V-E)}{\hbar^2} \psi_2 = 0$$

$$\frac{d^2\psi_2}{dx^2} - \beta^2 \psi_2 = 0$$

$$\beta^2 = \frac{2m(V-E)}{\hbar^2}$$

And its solution is,  $\psi_2 = U_2 e^{ikx}$

Proceeding as above we get,

$$\frac{d^2U_2}{dx^2} + 2ik \frac{dU_2}{dx} - \beta^2 U_2 - k^2 U_2 = 0 \quad \dots(3)$$

The solution of equation (2) and (3) are

$$U_1 = A e^{i(\alpha - k)x} + B e^{-i(\alpha + k)x} \quad \dots(4)$$

$$U_2 = C e^{(\beta - ik)x} + D e^{-(\beta + ik)x} \quad \dots(5)$$

We have the boundary conditions,

$$U_1(x=0) = U_2(x=0)$$

$$U'_1(x=0) = U'_2(x=0)$$

Since the potential is periodic with period,  $L = a + b$  i.e.  $U(x+L) = U(x)$

For,  $x = -b$ ,  $U(-b+a+b) = U(-b)$

$$U(a) = U(-b)$$

$$\therefore U_1(a) = U_2(-b)$$

$$U'_1(a) = U'_2(-b)$$

Using these boundary conditions and solving equation (4) and (5) we get

$$\frac{\beta^2 b}{2\alpha} \sin \alpha L + \cos \alpha L = \cos k L$$

$$\frac{P}{\alpha L} \sin \alpha L + \cos \alpha L = \cos k L \quad \dots(6)$$

$$\text{Here, } P = \frac{\beta^2 b L}{2} = \frac{2m(V-E)}{\hbar^2} \cdot \frac{bL}{2} = \frac{m(V-E)}{\hbar^2} bL$$

$$\text{Therefore, } P = \frac{mVbL}{\hbar^2} \text{ ( for } V \gg E).$$

Here in equation (6) the right side has limit of  $\pm 1$  whereas left side does not. The allowed solution occurs for ranges of  $\alpha$  such that left side is between  $+1$  and  $-1$  as shown in figure (2). For other value of energy there are no traveling waves to the wave equation so that the forbidden gaps in the energy spectrum are formed.

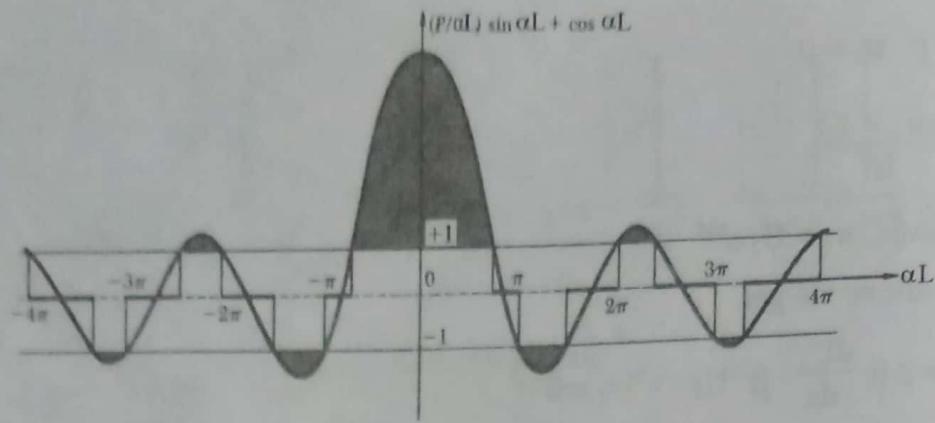


Figure 2: The plot of  $\frac{P}{\alpha L} \sin \alpha L + \cos \alpha L$  for  $P = \frac{3\pi}{2}$

### Case - I

When  $P \rightarrow 0, V \rightarrow 0$ , from (6)

$$\cos \alpha L = \cos k L \Rightarrow \alpha L = k L \Rightarrow \alpha = k$$

$$\sqrt{\frac{2mE}{\hbar^2}} = k$$

$$E = \frac{\hbar^2 k^2}{2m}$$

Then the E versus K curve becomes continuous parabola, the same as that of free electron. This case applies to crystal where the electrons are almost free of their nuclei. (Conductor).

### Case II

For  $P \rightarrow \infty, V \rightarrow \infty$ , the allowed energy region becomes infinitely narrow and the energy spectrum is a line spectrum. The equation (6) has only solution of,

$$\sin \alpha L = 0$$

$$\sin \alpha L = \sin n\pi$$

$$\alpha L = n\pi$$

$$\alpha = \frac{n\pi}{L}$$

$$\sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{L}$$

$$E = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

This is exactly same as the electron in an infinite potential well of width L. This shows that energy levels are discrete and the electron is completely bound in one shell of width L. This case applies to crystal, where the electrons are tightly bound to their nuclei (insulator).

### Case III

At the boundary conditions of allowed band.

$$\text{i.e. } \cos kL = \pm 1$$

$$\cos kL = \cos n\pi$$

$$k = \frac{n\pi}{L}, n = 1, 2, 3, \dots$$

The E vs. k curve is plotted for one dimensional lattice structure from Kroning - Penny model.

In the graph E versus k discontinuities occur at,  $k = \frac{\pi}{L}, \frac{2\pi}{L}, \frac{3\pi}{L}, \dots, \frac{n\pi}{L}$ . The k values define the

first, second, third etc Brillouin zones. The region between  $+\frac{\pi}{L}$  to  $-\frac{\pi}{L}$  is called first Brillouin

zone. The second Brillouin zone consists of two part, from  $+\frac{\pi}{L}$  to  $+\frac{2\pi}{L}$  and the second from  $-\frac{\pi}{L}$  to  $-2\pi/L$ .

Each portion of the curve is called a bond. The curves are horizontal at the top and bottom, parabolic near the top and the bottom with concave upward in the lower portion and concave downward in the upper portion. From figure (3), we can say that in the middle of the Brillouin zones, the E-K curve is identical to that of the free electron. But at the

boundaries of the zones i.e. at  $k = \frac{n\pi}{L}$ , their behaviour is totally different.

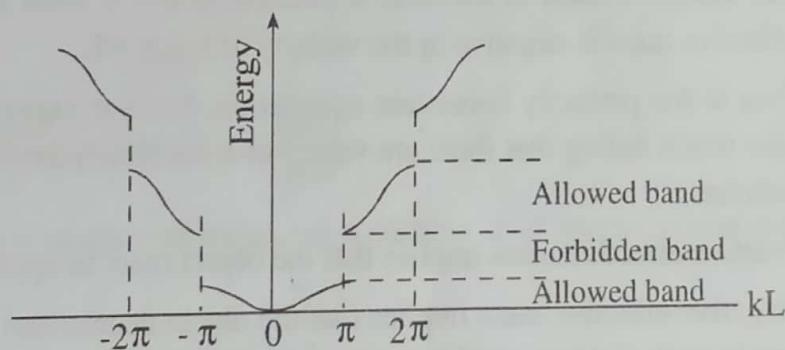


Figure 3: Showing allowed and forbidden bands

### Effective Mass of an Electron

For a free particle, the relationship between energy

$$\text{and momentum is given by } E = \frac{P^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m} = \hbar \cdot \frac{\hbar k}{m}$$

$$= \frac{\hbar P}{m} = \frac{\hbar m v}{m} = \hbar v$$

$$v = \frac{1}{\hbar} \frac{dE}{dk} \quad \dots(1)$$

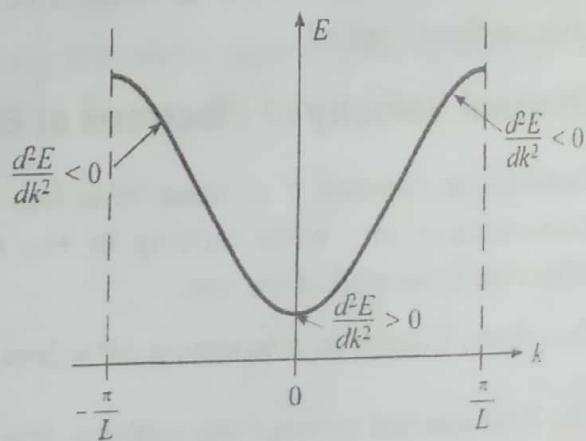


Figure : Electron motion in the conduction band of a conductor

$$\text{Here, } \frac{dE}{dk} = \frac{\hbar^2 k}{m} \Rightarrow \frac{d^2 E}{dk^2} = \frac{\hbar^2}{m}$$

$$\text{Therefore, } m = \frac{\hbar^2}{d^2 E / dk^2}$$

This shows that  $E$  versus  $k$  plot is parabolic. For a free particle this curvature  $d^2 E / dk^2$  is constant. But for electron in solid the curvature  $d^2 E / dk^2$  is not always constant and hence mass is also not constant.

For solid we can write.

$$m^* = \frac{\hbar^2}{d^2 E / dk^2} \quad \dots(2)$$

Where  $m^*$  represents effective mass of electron in the crystal.

The curvature  $d^2 E / dk^2$  is positive when the  $E$ - $k$  curve is concave upward and is negative when the curve is concave downward as shown in figure.

The effective mass of electron is positive at  $k = 0$  since the curve is concave upward. But the effective mass is negative in the vicinity of  $k = \pm \pi/L$ .

This is the perfectly consistent conclusion, but our experiences are with positive masses. It is also worth noting that there are values of  $k$  for which the curvature is zero, implying the mass is infinite.

Positive effective mass implies that the object react to applied external force in the normal way.

Negative effective mass implies that the object decelerates in the direction of applied force. This can happen if the applied force is overmatched by internal forces due to crystal lattice, when an external force tries to impel a particle into a region dominated by repulsive potential whose magnitude increases as the particle penetrates further into the region.

The infinite effective mass implies that the object cannot be accelerated by external force. This can be due to the internal force of crystal which cancels the effect of applied force.

Hence effective mass allow us to describe the response of crystal to the particles in terms of external force applied.

### **Thermal Velocity of Electrons at Equilibrium**

Consider an electron 'e' of mass 'm' is free to move inside a box of length 'a'. The electron has momentum  $+mv_x$  while moving in +ve  $x$ -direction and  $-mv_x$  in -ve  $x$  - direction after it's reflection from wall of the box.

Therefore, Change in momentum  $\Delta P = 2mv_x$ .

The time interval between the collision  $\Delta t = \frac{2a}{v_x}$ .

Therefore, Force on the wall  $F = \frac{\Delta P}{\Delta t} = \frac{mv_x^2}{a}$

$$\text{Pressure on the wall} = \frac{\text{Force}}{\text{Area}} = \frac{mv_x^2}{a \times a^2} = \frac{mv_x^2}{a^3}$$

$$\text{Total pressure due to } N\text{-electrons, } P = \frac{Nm v_x^2}{a^3}$$

$$\text{The mean square velocity is given by } v^2 = v_x^2 + v_y^2 + v_z^2$$

Since the mean square velocity along x - direction is equal to that along y and z direction.

$$\text{i.e. } v_x^2 = v_y^2 = v_z^2 \Rightarrow v^2 = v_x^2 + v_y^2 + v_z^2 = 3v_x^2$$

$$v_x^2 = v^2/3$$

$$\text{Pressure } P = \frac{Nm v^2}{3a^3}$$

$$\text{Total pressure (P)} = \frac{Nm v^2}{3V} \quad [V = a^3, \text{ volume of box}]$$

$$PV = \frac{Nm v^2}{3} \quad \dots(1)$$

$$\text{From ideal gas equation, } PV = nRT \quad \dots(2)$$

$$\text{Comparing equations (1) and (2), } \frac{Nm v^2}{3} = nRT \Rightarrow v^2 = \frac{3nRT}{Nm}$$

Since, Total number of electron (N) = number of moles (n)  $\times$  number of electrons in one mole ( $N_A$ )

$$\text{Therefore, } v^2 = \frac{3nRT}{nN_A m} = \frac{3RT}{N_A m}$$

$$\text{The velocity of electron } v = \sqrt{\frac{3RT}{N_A m}} = \sqrt{\frac{3KT}{m}} \quad \dots(3)$$

Since,  $K = \frac{R}{N_A} = 1.38 \times 10^{-23} \text{ JK}^{-1}$  is Boltzman constant.

The average kinetic energy per degree of freedom is  $\frac{1}{2} KT$ . So for three degrees of freedom this is  $\frac{3}{2} KT$ . Also kinetic energy of electron is  $\frac{1}{2} mv^2$

$$\text{Therefore, } \frac{1}{2} mv^2 = \frac{3}{2} KT$$

$$v = \sqrt{\frac{3KT}{m}} \quad \dots(4)$$

**Note:**  $R = 8.31 \text{ J mole}^{-1}\text{K}^{-1}$ ,  $N_A = 6.02 \times 10^{23} \text{ mol}^{-1}$

Equation (3) or (4) gives thermal velocity of electron at equilibrium. This equilibrium is maintained by the electron interaction with lattice called lattice vibration. This results to

produce phonon wave. The energy exchange between electron and lattice crystal is called lattice scattering.

## Mean Free Time Between Collision and Drift Velocity of Electron in an Electric Field.

(Electron mobility, Conductivity and Resistivity.)

When a conductor does not have applied electric field across it, its conduction electron move randomly. Since there is no net flow of charge so there is no current. When a potential difference is applied across it, the free electrons tend to move in the direction opposite to that of applied electric field with a speed called drift speed  $v_d$ .

Let an electron of mass 'm' and charge 'e' is placed in an electric field E, The electric force experienced by it is ,  $F = eE$ .

Also from Newton's law,  $F = ma$ .

Hence,  $ma = eE$

$$\Rightarrow a = \frac{eE}{m}$$

The average drift speed of electron is,  $v_d = a\tau$  , where  $\tau$  is average time between collision called mean free time or relaxation time.

$$\text{Therefore, } v_d = \frac{eE\tau}{m} \quad \dots(1)$$

The electron mobility is defined as the drift speed per unit applied electric field.

$$\text{Electron mobility, } (\mu) = \frac{v_d}{E} = \frac{e\tau}{m} \quad \dots(2)$$

$$\text{Since current density, } J = v_d en = \frac{eE\tau}{m} ne = \frac{ne^2\tau}{m} \cdot E \quad \dots(3)$$

$$\text{Also, } J = \sigma E. \quad \dots(4)$$

$$\text{Comparing equations (3) and (4), Electron conductivity, } \sigma = \frac{ne^2\tau}{m} \quad \dots(5)$$

$$\text{Resistivity } \rho = \frac{1}{\sigma} = \frac{m}{ne^2\tau}$$

$$\text{Also from (3), } \sigma = ne \cdot \frac{e\tau}{m} = ne\mu \quad \dots(6)$$

## Diffusion of Electrons

When there is a local concentration of particles (electrons) in a small portion of a volume the particle tend to spread out until they are uniformly distributed through out the available space.

This process is called *diffusion*. During diffusion there is motion of charged particle this give rise to a current called *diffusion current*.

### Fick's Law:

It states that carrier flux (number of particles crossing per unit area per unit time) is proportional to concentration gradient.

$$\text{i.e., } \phi = -D \frac{dn}{dx}$$

Here -ve sign indicates that the diffusion occurs towards the decreasing concentration gradient. D is called diffusion coefficient.

For electron, the diffusion current density is

$$J_{\text{diffusion}} = (-e) \phi = e D \frac{dn}{dx}$$

Therefore, the total current density,  $J = J_{\text{drift}} + J_{\text{diffusion}}$

$$J = ne\mu E + eD \frac{dn}{dx}$$

For holes, the diffusion current density is,

$$J_{\text{diffusion}} = e\phi = -eD \frac{dp}{dx}$$

Therefore, Total current density,  $J = J_{\text{drift}} + J_{\text{diffusion}}$

$$= \sigma E - eD \frac{dp}{dx}$$

$$= pe\mu E - eD \frac{dp}{dx}$$

Here, p = concentration of holes, and  $\mu$  = mobility of holes.

For most materials, the diffusions coefficient is found to vary with temperature as  $D = D_0 e^{-\frac{Q}{kT}}$

Here,  $D_0 = 1/2 a^2 f$  is called pre factor, 'a' is lattice constant, 'f' is vibrational frequency of lattice, and 'Q' is energy of ions for diffusion called activation energy.

### Einstein's Relation between Mobility and Diffusion Coefficient

In the presence of electric field, the total current density in a conductor is given by,

$$\begin{aligned} J &= J_{\text{drift}} + J_{\text{diffusion}} \\ &= \sigma E + eD \frac{dn}{dx} = ne\mu E + eD \frac{dn}{dx} \end{aligned}$$

Under equilibrium condition, The total current must be zero.

$$ne\mu E + eD \frac{dn}{dx} = 0 \Rightarrow eD \frac{dn}{dx} = -ne\mu E$$

$$\text{Therefore, } \frac{dn}{n} = -\frac{\mu E}{D} dx$$

Integrating,

$$\ln(n) = -\frac{\mu Ex}{D} + \ln(A) \text{ (constant)}$$

$$\text{or } \ln\left(\frac{n}{A}\right) = -\frac{\mu Ex}{D}$$

$$n = A e^{-\frac{\mu Ex}{D}} \quad \dots(1)$$

From Boltzmann's statistics, for an electric field we have

$$n = A e^{-\frac{eEx}{KT}} \quad \dots(2)$$

$$\text{Comparing equations (1) and (2)} \frac{\mu Ex}{D} = \frac{eEx}{KT}$$

$$\frac{\mu}{D} = \frac{e}{KT}$$

$$\left[ \frac{D}{\mu} = \frac{KT}{e} \right] \quad \dots(3)$$

Equation (3) is the relation between diffusion coefficient and electron mobility called Einstein's relation.

$$\text{For electron it is given by } \left[ \frac{D_e}{\mu_e} = \frac{KT}{e} \right] \quad \dots(4)$$

$$\text{For holes it is given by } \left[ \frac{D_h}{\mu_h} = \frac{KT}{e} \right] \quad \dots(5)$$

### Solved Examples

- Calculate the root mean square (rms) velocity of nitrogen molecule in atmospheric air at 27°C. Also calculate the root mean square velocity in one direction ( $V_{rms,x}$ ). Given atomic mass of nitrogen is  $M_{at} = 14 \text{ gm mol}^{-1}$ .

*Solution:*

Here  $M_{at} = 14 \text{ gm}$

1 mole of  $N_2$  gas =  $2 \times 14 = 28 \text{ gm}$

Since one mole of  $N_2$  gas contains  $6.022 \times 10^{23}$  molecules

$\therefore$  Mass of  $6.022 \times 10^{23}$  number of  $N_2$  molecule = 28 gm =  $28 \times 10^{-3}$  kg

$$\text{Mass of one molecule of } N_2, (m) = \left( \frac{28 \times 10^{-3}}{6.022 \times 10^{23}} \right) = 4.65 \times 10^{-26} \text{ kg}$$

$$\text{We have, } V_{\text{rms}} = \sqrt{\frac{3KT}{m}} = \sqrt{\frac{3 \times 1.38 \times 10^{-23} \times 300}{4.65 \times 10^{-26}}} = 517 \text{ ms}^{-1}$$

$$\text{Since, } V_{\text{rms}}^2 = V_{\text{rms},x}^2 + V_{\text{rms},y}^2 + V_{\text{rms},z}^2$$

$$\text{Let, } V_{\text{rms},x} = V_{\text{rms},y} = V_{\text{rms},z}$$

$$\Rightarrow V_{\text{rms}}^2 = 3 V_{\text{rms},x}^2$$

$$\Rightarrow V_{\text{rms},x}^2 = \frac{V_{\text{rms}}^2}{3} \Rightarrow V_{\text{rms},x} = \frac{V_{\text{rms}}}{\sqrt{3}} = 298 \text{ ms}^{-1}$$

2. Find the diffusion coefficient of phosphorus (P) atoms in the Silicon (Si) crystal at a temperature of  $1100^\circ\text{C}$ . Given  $D_o = 10.5 \text{ cm}^2\text{s}^{-1}$  and activation energy = 3.69 eV.

*Solution:*

Here,  $D_o = 10.5 \text{ cm}^2\text{s}^{-1}$ ,  $Q = 3.69 \text{ eV} = 3.69 \times 1.6 \times 10^{-19} \text{ J}$ ,  $T = 1100^\circ\text{C} = (1100 + 273)$

K = 1373 K

We have,

$$D = D_o e^{-\frac{Q}{KT}} = 10.5 e^{-\left(\frac{3.69 \times 1.6 \times 10^{-19}}{1.38 \times 10^{-23} \times 1373}\right)} \\ = 3.0 \times 10^{-13} \text{ cm}^2\text{s}^{-1}$$

3. Calculate the drift mobility and the mean scattering time of conduction electrons in copper at room temperature, given that the conductivity of copper is  $5.9 \times 10^5 \Omega^{-1}\text{cm}^{-1}$ . The density of copper is  $8.96 \text{ g cm}^{-3}$  and its atomic mass is  $63.5 \text{ g mol}^{-1}$ . (Assume one free electron per atom)

*Solution:*

Here, conductivity,  $\sigma = 5.9 \times 10^5 \Omega^{-1} \text{ cm}^{-1}$ , density,  $d = 8.96 \text{ g cm}^{-3}$  atomic mass,  $M_{\text{at}} = 63.5 \text{ g mol}^{-1}$ .

$$\text{We have, number of copper atoms per unit volume } n = \frac{dN_A}{M_{\text{at}}} \\ = \frac{8.96 \times 6.02 \times 10^{23}}{63.5} = 8.5 \times 10^{22} \text{ cm}^{-3}$$

Since,  $\sigma = ne\mu$

$$\Rightarrow \mu = \frac{\sigma}{ne} = \frac{5.9 \times 10^5}{1.6 \times 10^{-19} \times 8.5 \times 10^{22}} = 43.4 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$$

$$\text{Again, } \mu = \frac{e\tau}{m}$$

$$\Rightarrow \tau = \frac{\mu m}{e} = \frac{43.4 \times 10^{-4} \times 9.1 \times 10^{-31}}{1.6 \times 10^{-19}} = 2.5 \times 10^{-14} \text{ s}$$

4. The resistivity of copper at 20 degree centigrade is  $0.69 \times 10^{-8} \Omega\text{-m}$  and density of free electron is  $8.5 \times 10^{28} \text{ m}^{-3}$ . Calculate the mean free time of electron in copper lattice. Assume  $m^* = 1.01 \text{ m}$ , where  $m = 9.1 \times 10^{-31} \text{ kg}$ .

**Solution:**

Here Temperature (T) =  $20^\circ\text{C} = 293 \text{ K}$ .

Resistivity, ( $\rho$ ) =  $0.69 \times 10^{-8} \Omega\text{-m}$ , density of free electron,

$$n = 8.5 \times 10^{28} \text{ m}^{-3}, m = 1.01 \times 9.1 \times 10^{-31} = 9.191 \times 10^{-31} \text{ kg.}$$

$$\text{We have conductivity, } \sigma = \frac{ne^2\tau}{m} \Rightarrow \tau = \frac{m\sigma}{ne^2} = \frac{m}{ne^2\rho}$$

$$\therefore \tau = \frac{9.191 \times 10^{-31}}{8.5 \times 10^{28} \times (1.6 \times 10^{-19})^2 \times 0.69 \times 10^{-8}}$$

$$= 6.12 \times 10^{-14} \text{ sec.}$$

5. Calculate the diffusion coefficient of electrons at 300K in n-type semiconductor doped with  $10^{15}$  arsenic atoms per  $\text{cm}^3$  ( $\mu$  for given doping  $1300 \text{ cm}^2 \text{ V}^{-1} \text{ S}^{-1}$ )

**Solution:**

Here, T = 300K , n =  $10^{15}$  per  $\text{cm}^3$ ,  $\mu = 1300 \text{ cm}^2 \text{ V}^{-1} \text{ S}^{-1}$

We have from Einstein relation

$$\frac{D}{\mu} = \frac{KT}{e} \Rightarrow D = \frac{KT\mu}{e} = \frac{1.38 \times 10^{-23} \times 300 \times 1300 \times 10^{-4}}{1.6 \times 10^{-19}}$$

$$D = 3.37 \times 10^{-3} \text{ m}^2 \text{ s}^{-1}$$

6. Electrons in undoped Gallium Arsenide have a mobility of  $8.800 \text{ cm}^2/\text{V.S.}$  calculate average time between collision. Calculate distance travel between two collisions. Use average velocity of electron  $10^7 \text{ m/sec}$ .

**Solution:**

Here,  $\mu = 8.8 \text{ cm}^2/\text{V.S.} = 8.8 \times 10^{-4} \text{ m}^2 \text{ V}^{-1} \text{ S}^{-1}$ ,  $v = 10^7 \text{ m/sec}$

$$\text{Since, } \mu = \frac{e\tau}{m} \Rightarrow \tau = \frac{m\mu}{e} = \frac{9.1 \times 10^{-31} \times 8.8 \times 10^{-4}}{1.6 \times 10^{-19}}$$

$$\tau = 5 \times 10^{-15} \text{ sec}$$

$$\text{Again, mean free path, } \lambda = v \cdot \tau = 10^7 \times 5 \times 10^{-15} = 5 \times 10^{-8} \text{ m}$$

$$= 50 \times 10^{-9} \text{ m} = 50 \text{ nm}$$

7. If electrical conductivity of Potassium is  $1.39 \times 10^5 \text{ Sm/cm.}$  Calculate the drift mobility of electron at room temperature. Molar mass and density of potassium are 39.95 and 0.91 gm/cc.

**Solution:**

Here,  $\sigma = 1.39 \times 10^5 \text{ Sm/cm} = 1.39 \times 10^7 \text{ Sm/m} = 1.39 \times 10^7 \text{ mho/m}$

Molar mass,  $M_{at} = 39.95$  g/mol, density  $d = 0.91$  gm/cc

$$\text{Number of K atoms per unit volume, } n = \frac{d N_A}{M_{at}} = \frac{0.91 \times 6.02 \times 10^{23}}{39.95}$$

$$n = 1.37 \times 10^{22}/\text{cm}^3 = 1.37 \times 10^{28} \text{ m}^{-3}$$

Now the drift mobility is

$$\mu = \frac{\sigma}{ne} = \frac{1.39 \times 10^7}{1.37 \times 10^{28} \times 1.6 \times 10^{-19}} = 6.34 \times 10^{-3} \text{ m}^2 \text{V}^{-1} \text{S}^{-1}$$

$$= 63.4 \text{ cm}^2 \text{V}^{-1} \text{S}^{-1}$$

8. A uniform silver wire has resistivity  $1.54 \times 10^{-8}$  ohm/m at room temperature. For an electric field along the wire of  $1 \text{ V cm}^{-1}$ , compute the average drift velocity of electron assuming there are  $5.8 \times 10^{28}$  conduction electron per  $\text{m}^3$ . Also calculate mobility and relaxation time.

*Solution:*

Here,  $\rho = 1.54 \times 10^{-8}$  ohm-m,  $E = 1 \text{ V cm}^{-1} = 10^2 \text{ V m}^{-1}$ ,  $n = 5.8 \times 10^{28}$  electrons  $\text{m}^{-3}$ .

The current density is given by,  $J = v_d e n = \sigma E$

$$\Rightarrow v_d = \frac{\sigma E}{ne} = \frac{E}{\rho ne} = \frac{10^2}{1.54 \times 10^{-8} \times 5.8 \times 10^{28} \times 1.6 \times 10^{-19}}$$

$$= 7 \times 10^{-1} \text{ m/sec} = 0.7 \text{ m/sec}$$

$$\text{Mobility, } \mu = \frac{Vd}{E} = \frac{7 \times 10^{-1}}{10^2} = 7 \times 10^{-3} \text{ m}^2 \text{V}^{-1} \text{S}^{-1}$$

9. Drift mobility of conduction electron is  $43 \text{ cm}^2 \text{V}^{-1} \text{S}^{-1}$  and mean speed is  $1.2 \times 10^6 \text{ m s}^{-1}$ . Calculate mean free path of electrons between collisions.

*Solution:*

Here,  $\mu = 43 \text{ cm}^2 \text{V}^{-1} \text{S}^{-1} = 43 \times 10^{-4} \text{ m}^2 \text{V}^{-1} \text{S}^{-1}$ , means speed  $v = 1.2 \times 10^6 \text{ ms}^{-1}$ ,

$$\text{We have, } \mu = \frac{e\tau}{m} \Rightarrow \tau = \frac{m\mu}{e}$$

$$\text{Mean free path, } \lambda = v\tau = \frac{mv\mu}{e} = \frac{9.1 \times 10^{-31} \times 1.2 \times 10^6 \times 43 \times 10^{-4}}{1.6 \times 10^{-19}}$$

$$= 2.935 \times 10^{-8} \text{ m} = 29.35 \times 10^{-9} \text{ m} = 29.35 \text{ nm}$$

10. A copper wire of cross-sectional area of  $5 \text{ mm}^2$  carries a steady current of  $50 \text{ A}$ . Calculate density of free electrons and average drift velocity of electrons. Assume one free electron per atom, Given mass and density of copper are  $63.5 \text{ g/mol}$  and  $8.93 \text{ g/cm}^3$ .

*Solution:*

$$A = 5 \text{ mm}^2 = 5 \times 10^{-6} \text{ m}^2, I = 50 \text{ A}$$

$$n = \frac{dN_A}{m_{at}} = \frac{8.93 \times 6.02 \times 10^{23}}{63.5} = 8.5 \times 10^{22}/\text{cm}^3 = 8.5 \times 10^{28} \text{ m}^{-3}$$

$$\text{Again, } I = v_d e n A \Rightarrow v_d = \frac{I}{neA} = \frac{50}{8.5 \times 10^{28} \times 1.6 \times 10^{-19} \times 5 \times 10^{-6}}$$

$$\therefore v_d = 7.35 \times 10^4 \text{ ms}^{-1}$$

11. Show that for cubic lattice, the lattice constant 'a' is given by  $a = \left[ \frac{NM}{\rho N_A} \right]^{1/3}$ . Where,  $N$  is the number of atoms per unit cell,  $M$  is atomic weight;  $N_A$  is Avogadro's number, and  $\rho$  is density of the crystal material.

*Solution:*

$$\text{We have, density } \rho = \frac{\text{mass of unit cell}}{\text{volume of unit cell}}$$

$$\Rightarrow \rho = \frac{\text{number of atoms per unit cell} \times \text{mass of one atom}}{a^3}$$

$$\rho = \frac{N \times \text{mass of one atom}}{a^3}$$

The mass of  $N_A$  (Avogardo's number) number of atoms = Atomis mass ( $M$ )

$$\therefore \text{Mass of one atom} = \frac{\text{atomic mass (M)}}{N_A} = \frac{M}{N_A}$$

$$\text{Therefore, } \rho = \frac{N \times M}{a^3 \times N_A}$$

$$a^3 = \frac{NM}{\rho N_A}$$

$$a = \left[ \frac{NM}{\rho N_A} \right]^{1/3}$$

12. Molybdenum has the BCC crystal structure, a density of  $10.22 \text{ g cm}^{-3}$ , and an atomic mass of  $95.94 \text{ g mol}^{-1}$ . What is atomic concentration, lattice parameter  $a$  and atomic radius of molybdenum?

*Solution:*

Here density,  $\rho = 10.22 \text{ gm cm}^{-3}$ ,  $M_{at} = 95.94 \text{ gm mol}^{-1}$

$$\text{Since, } \rho = \frac{\text{mass of unit cell (or mass of all atoms in unit cell)}}{\text{volume of unit cell}}$$

$$= \frac{\text{number of atoms per unit cell} \times \text{mass of one atom}}{a^3}$$

$$= \frac{\text{number of atoms per unit cell} \times \left( \frac{M_{at}}{N_A} \right)}{a^3}$$

For BCC crystal, number of atoms per unit cell = 2

$$\therefore \rho = \frac{2 \times M_{at}}{N_A \times a^3} \Rightarrow a^3 = \frac{2 \times M_{at}}{\rho N_A}$$

$$a^3 = \frac{2 \times 95.94 \times 10^{-3}}{6.022 \times 10^{23} \times 10.22 \times 10^{-3} \times 10^6} = 3.12 \times 10^{-29}$$

$$\Rightarrow a = 3.15 \times 10^{-10} \text{ m}$$

$\therefore$  Lattice parameter,  $a = 3.15 \times 10^{-10} \text{ m}$

For BCC crystal structure we have,  $4r = \sqrt{3} a$

Here,  $r$  = radius of the atom

$$\Rightarrow r = \frac{\sqrt{3}}{4} a = 1.36 \times 10^{-10} \text{ m}$$

$$\text{Atomic concentration} = \frac{\text{Number of atoms in unit cell}}{\text{Volume of unit cell}}$$

$$= \frac{2}{a^3} = 6.41 \times 10^{28} \text{ atoms/m}^3$$

13. Calculate the number of atoms per unit cell of a metal having lattice parameter of  $2.9 \text{ \AA}$  and density of  $7.87 \text{ gm/cc}$ . Atomic weight of the metal is  $55.85 \text{ g/mol}$  and  $N_A = 6.023 \times 10^{23}/\text{mol}$ .

*Solution:*

$$\text{We know, density, } \rho = \frac{\text{mass of unit cell}}{\text{volume of unit cell}}$$

$$\Rightarrow \rho = \frac{\text{number of atoms per unit cell} \times \text{mass of one atom}}{a^3}$$

$$\rho = \frac{N \times \text{mass of one atom}}{a^3}$$

The mass of  $N_A$  (Avogadro's number) number of atoms = Atomic mass

$$\text{Mass of one atom} = \frac{\text{Atomic mass}}{N_A} = \frac{M_{at}}{N_A}$$

$$\text{Therefore, } \rho = \frac{N \times M_{at}}{N_A \times a^3}$$

$$N = \frac{\rho \times N_A \times a^3}{M_{at}} = \frac{7.87 \times 10^{-3} \times 10^6 \times 6.023 \times 10^{23} \times (2.9 \times 10^{-10})^3}{55.85 \times 10^{-3}} = 2$$

14. What is applied electric field that will impose a drift velocity equal to  $0.1\%$  of the mean speed ( $v = 10^6 \text{ ms}^{-1}$ ) of conduction electron in copper. Given,  $\mu = 43.4 \text{ cm}^2 \text{V}^{-1} \text{S}^{-1}$  and conductivity,  $\sigma = 5.9 \times 10^7 \Omega^{-1} \text{m}^{-1}$ . What is the corresponding current density and current through a copper wire of diameter 1mm? With reference to this example, explain how mean speed remains unaffected by drifting of electrons.

*Solution:*

Here  $\mu = 43.4 \text{ cm}^2 \text{V}^{-1} \text{S}^{-1}$ ,  $v_d = 0.1\% \text{ of } 10^6 = 10^3 \text{ m/sec}$

$$\text{Since, } \mu = \frac{v_d}{E} \Rightarrow E = \frac{v_d}{\mu}$$

$$\therefore E = \frac{10^3}{43.4 \times 10^{-4}} = 2.3 \times 10^5 \text{ V/m}^{-1}$$

Which is an unattainably large electric field in a metal.

$$\text{We have, } J = \sigma E = 5.9 \times 10^7 \times 2.3 \times 10^5$$

$$= 1.4 \times 10^{13} \text{ A/m}^2 = 1.4 \times 10^7 \text{ A/mm}^2$$

This means a current of  $1.4 \times 10^7 \text{ A}$  through a 1mm diameter wire! It is clear from this example that for all practical purposes, even under the highest working current and voltage the drift speed is much smaller than the mean speed of electrons (means speed lies in the order of  $10^6 \text{ m/s}$ ). Consequently when an electric field is applied to a conductor, the mean speed is unaffected.

Reversely seeing the example. If we apply current of  $1.4 \times 10^7 \text{ A/mm}^2$  or an electric field of  $2.3 \times 10^5 \text{ Vm}^{-1}$  the drift velocity of electron will be  $10^3 \text{ m/sec}$  only. However, in practice we need not to apply such larger amount of current and voltage. So drift velocity come to even lesser value than  $10^3 \text{ m/sec}$ . But mean speed is in the order of  $10^6 \text{ m/sec}$ . So mean speed remains unaffected due to drifting of electrons.

- 15. The resistivity of copper is  $1.70 \times 10^{-6} \Omega \cdot \text{cm}$  at room temperature. Assuming that there is one electron per atom contributing to conduction, calculate the mobility. Given number of atoms per unit volume,  $n = 8.5 \times 10^{22}/\text{cm}^3$ .**

**Solution:**

$$\rho = 1.7 \times 10^{-6} \Omega \cdot \text{cm}, \mu = ?, n = 8.5 \times 10^{22}/\text{cm}^3$$

$$\text{We have, } \sigma = ne\mu$$

$$\mu = \frac{\sigma}{ne} = \frac{1}{\rho ne}$$

$$\begin{aligned}\mu &= \frac{1}{1.7 \times 10^{-6} \times 10^{-2} \times 8.5 \times 10^{22} \times 10^6 \times 1.6 \times 10^{-19}} \\ &= 4.325 \times 10^{-3} \text{ m}^2/\text{V-S} \\ &= 43.25 \text{ cm}^2/\text{V-S}.\end{aligned}$$

- 16. Calculate  $V_{th}$  at room temperature (300K). Assume  $m$  is the rest mass of an electron.**

**Solution:** Here,  $T = 300\text{K}$ ,  $m = 9.1 \times 10^{-31} \text{ kg}$

$$\begin{aligned}\text{Since, } V_{th} &= \sqrt{\frac{3KT}{m}} = \sqrt{\frac{3 \times 1.38 \times 10^{-23} \times 300}{9.1 \times 10^{-31}}} \\ &= 1.17 \times 10^5 \text{ m/sec}\end{aligned}$$

17. What should be the electric field in a sample cube 3 mm side of silver having resistivity  $1.62 \times 10^{-8} \Omega\text{-m}$  carrying current of 80A. Also calculate drift velocity at mobility  $0.0056 \text{ m}^2/\text{V.S.}$

*Solution:*

$$\text{We have, } \sigma = ne\mu \Rightarrow n = \frac{\sigma}{e\mu} = \frac{1}{\rho e\mu}$$

$$n = \frac{1}{1.62 \times 10^{-8} \times 1.6 \times 10^{-19} \times 0.0056} = 6.9 \times 10^{28}/\text{m}^3$$

$$\text{Since, } I = v_d enA \Rightarrow v_d = \frac{I}{neA}$$

$$v_d = \frac{80}{6.9 \times 10^{28} \times 1.6 \times 10^{-19} \times 3 \times 3 \times 10^{-6}}$$

$$v_d = 8 \times 10^{-4} \text{ m/sec}$$

$$\text{We have, } \mu = \frac{v_d}{E} \Rightarrow E = \frac{v_d}{\mu} = \frac{8 \times 10^{-4}}{0.0056} = 0.144$$

$$E = 0.144 \text{ V/m}$$

18. The specific gravity of Tungsten is  $18.8 \text{ g/cm}^3$  and its atomic weight is  $184 \text{ g/mol}$ . Assuming that there are two free electrons per atom, calculate the mobility of free electrons in the Tungsten metal (Given: conductivity =  $0.29 \times 10^8 \text{ mho/m}$ ).

*Solution:*

Here density  $d = 18.8 \text{ g/cm}^3$ ,  $M_{\text{at}} = 184 \text{ g/mol}$

$$\text{Therefore, } n = \frac{dN_A}{M_{\text{at}}} = \frac{18.8 \times 6.02 \times 10^{23}}{184} = 6.15 \times 10^{22}/\text{cm}^3$$

Therefore,  $n = 2 \times 6.15 \times 10^{22}/\text{cm}^3$  [Since, There are two free electrons per atom]

$$\text{We have, } \sigma = ne\mu \Rightarrow \mu = \frac{\sigma}{ne}$$

$$\text{Therefore, } \mu = \frac{0.29 \times 10^8}{2 \times 6.15 \times 10^{22} \times 1.6 \times 10^{-19}}$$

$$\mu = 1.47 \times 10^{-3} \text{ m}^2/\text{V.S.}$$

### Exercise

1. Define lattice and basis of a crystal and draw a neat diagram of body centered cubic structure of chromium and determine its packing density and state its co-ordination number.
2. Calculate the lattice constant, face diagonal, body diagonal and packing density of body centered cubic (BCC) crystal unit cell.