Free Study Material from All Lab Experiments

B.Sc. => Solid-State Physics
Chapter - 6
Elementary Band Theory

6

Elementary Band Theory

Syllabus: Kronig Penny model. Band Gap. Conductor, Semiconductor (P and N type) and insulator. Conductivity of Semiconductor, mobility, Hall Effect.

Q.1. Discuss the Kronig-Penny model for a linear lattice. How does it lead to the formation of energy band s in solids? Find energy of electron with periodic potential under the cases

(I) Potential approaches infinity

(II) Potential approaches Zero

Ans. For the treatment of our problem, a periodic repetition of the potential well of Fig., i.e., a periodic arrangement of potential wells and potential barriers, is most probably very close to reality and is also best suited for the calculation. Such a periodic is shown in Fig. for the one-dimensional case.

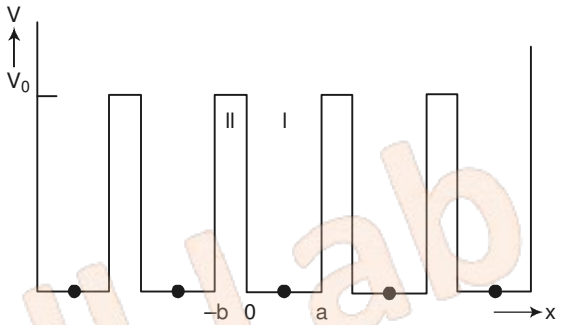


Fig. Ideal periodic square well potential used by Kronig and Penney.

Be calculated by solving Schrodinger equations for the two regions I and II. The time-independent Schrodinger equation takes the following forms for the two regions

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi = 0; \text{ for } 0 < \text{I} < a$$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E - V_0)\psi = 0; \text{ for } -h < x < 0$$

Using Bloch's function then solution can be written as:

$$\psi(x) = u_k e^{ikx} \tag{110}$$

For $E < V_0$

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0; \text{ for } 0 < x < a$$

and $$\alpha^2 = \frac{8\pi^2 mE}{h^2} \text{ and } \beta^2 = \frac{8\pi^2 m}{h^2}(V_0 - E)$$

Using Bluch, solution is;

$$\psi(x) = U_k e^{ikx}$$

On differentiating this eqn two times, and substituting we get,

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

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

The U_1 and U_2 are the values of U_k in $0 < x < a$ and $-b < x < 0$ regions, respectively.

Solution of A is of the term

$$U_1 = e^{mx}$$

On taking double derivative & substituting in we get the solution.

$$m = -ik \pm i\alpha \Rightarrow m_1 = -ik + i\alpha = i(\alpha - k)$$

and $$m_2 = -i(\alpha + k)$$

So $$U_1 = Ae^{m_1 x} + Be^{m_2 x}$$

Similarly eqn B results in

$$U_2 = Ce^{(B-ik)x} + De^{(B+ik)x}$$

Using boundary continuous

$$[U_1]x = o = [U_2]_{x=0} \text{ and } \left[\frac{dU_1}{dx}\right]_{x=0} = \left[\frac{dU_2}{dx}\right]_{x=0}$$

$$[U_1]_{x=a} = [U_2]_{x=-b}, \left[\frac{dU_1}{dx}\right]_{x=a} = \left[\frac{dU_2}{dx}\right]_{x=-b}$$

Using theses we get

$$(A + B) = (C + D) \quad \ldots(1)$$

$$i(\alpha - k)A - i(\alpha + k)B = (\beta - ik)C - (V - ik)D \quad \ldots(2)$$

$$Ae^{i(\alpha k)a} + Be^{-i(\alpha+k)a} = Ce^{-(\beta-ik)h} + De^{(\beta+ik)b} \quad ...(3)$$

$$Ai(\alpha-k)e^{i(\alpha-k)a} - Bi(\alpha+k)e^{-i(\alpha+k)a} = C(\beta-ik)e^{i(\beta-ik)b} - D(\beta+ik)e^{-(v+ik)b} \quad ...(4)$$

Eqn. 1, 2, 3 and 4 will have nonvanishing solutions if and only if the determinant of the coefficients A, B, C and D vanishes. This required that

$$\begin{vmatrix} 1 & 1 & 1 & 1 \\ i(\alpha-K) & -i(\alpha-K) & (\beta-iK) & -(\beta-iK) \\ e^{i(\alpha-K)a} & e^{-i(\alpha+k)a} & e^{-(\beta-iK)b} & e^{(\beta+iK)b} \\ i(\alpha-k)e^{i(\alpha-k)a} & -i(\alpha-K)e^{-i(\alpha+k)a} & (\beta-iK)e^{-b(\beta-iK)b} & -(\beta-iK)e^{(\beta+iK)b} \end{vmatrix} = 0$$

Thus the solution of the determinant (Eqn. 4) is

$$\frac{(\beta^2-\alpha^2)}{2\alpha\beta}\sin\alpha a \sin h\beta b \cos\alpha a = \cos K(a+b) \quad ...(5)$$

Eqn. (5) is complicated but a simplification is possible. Kronig and Penney considered the possibility that $V_0 a$ remains finite. Such a function is called delta function. Under these circumstances,

$$\sin h\beta b \to \beta b \text{ and } \cos h\beta b \to 1 \text{as } b \to 0.$$

Hence Eqn. (26) becomes

$$\frac{(\beta^2-\alpha^2)}{2\alpha\beta}\beta b \sin\alpha a + \cos\alpha a = \cos Ka$$

$$(\beta^2-\alpha^2) = \frac{8\pi^2 m}{h2}(V_0-E) - \frac{8\pi^2 m}{h^2}E = \left(\frac{8\pi^2 m}{h^2}\right)[V_0-2E]$$

Since $V_0 >> E$,

$$\beta^2-\alpha^2 = \frac{8\pi^2 m}{h^2}(V_0)$$

Substituting this in the above equation, we get

$$\left(\frac{8\pi^2 m V_0}{2\alpha\beta h^2}\right)\beta h \sin\alpha a + \cos\alpha a = \cos Ka$$

$$P = \frac{mV_o ab}{h^2}$$

Where

$$\left(\frac{mV_0ab}{h^2}\right)\frac{\sin\alpha a}{\alpha a}+\cos\alpha a = \cos Ka$$

i.e., $$P\frac{\sin\alpha a}{\alpha a}+\cos\alpha a = \cos Ka \quad ...(6)$$

The term V_0b is called the barrier strength. The term $P=\frac{mV_0\alpha b}{\hbar^2}$ in Eqn. (6) is sometimes referred as the scattering of the potential barrier. It is a measure of the strength with which electrons in a crystal are attracted to the crystal lattice sites. Also

$$\alpha^2 = \frac{8\pi^2mE}{\hbar^2}, \text{ or } E=\frac{\alpha^2\hbar^2}{8\pi^2m}$$

and $$K=\frac{2\pi}{\lambda} \quad ...(7)$$

Eqn. (6) is a condition of the existence of a solution for the electron wave function.

There are only two variables in Eqn. (6), namely α and K. The right hand side of Eqn. (6) is bounded since it can only assume values between +1 and –1. If we plot the left-hand side of this equation against α a, it will be possible to determine those value of α (and hence).

Reason for Formation Energy Bands:

The wave function at the point $K=\pm\pi/a$ do not have traveling instead standing waves. The standing waves are formed when wave is Bragg reflected; is direction of travel is opposite to its incident direction and subsequent reflection reverses the direction again there by producing standing waves since the wave by itself should be time independent. The two different forms of standing waves in terms of travelling waves $e^{i\pi x/a}$ and $e^{-i\pi x/a}$ are.

$$\psi(+) = e^{i\pi x}+e^{-i\pi x/a}=2\cos\left(\frac{\pi x}{a}\right) \text{ (real part)}$$

$$\psi(-) = e^{i\pi x/a}-e^{-i\pi x/a}=2i\sin\left(\frac{\pi x}{a}\right) \text{ (imaginary part)}$$

These two different standing waves $\psi(+)$ and $\psi(-)$ group electron at different region with different potential energy. This gives raise to the formation of forbidden energy gap.

From equation $P = \frac{mV_0ab}{h^2}$

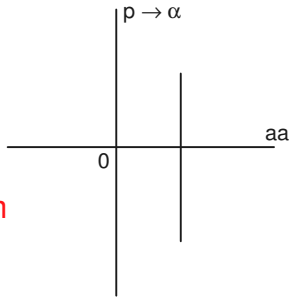
$V_o \to \infty$ when $P \to \infty$

and $V_o \to 0$ when $P \to 0$

Case (i): At one of the extremities, $P \to \infty$

$$\sin \alpha a = 0; \text{ or } \alpha a = \pm n\pi \Rightarrow \alpha^2 = \frac{n^2\pi^2}{a^2} = \frac{2mE}{\hbar^2}$$

on rearranging,



$$E = \frac{n^2\pi^2\hbar^2}{a^2 2m} = \frac{n^2\pi^2\hbar^2}{a^2 2m(2\pi)^2} = \frac{n^2\hbar^2}{8ma^2} \quad ...(8)$$

Here the energy depends on the width of the potential rather than any other parameter. The energy level of electron in the crystal lattice is discrete and is similar to the particle in a potential box with an atomic dimension. This is because with a large value of potential strength barrier the tunneling effect is explicitly improbable.

Case (ii): When $p \to 0$, with the same equation cos αa = cos Ka = > $a = k$

Substituting the values $K^2 = \alpha^2 = \frac{2mE}{\hbar^2}$ on rearranging,

$$E = \left(\frac{\hbar^2}{2m}\right)k^2 \quad ...(9)$$

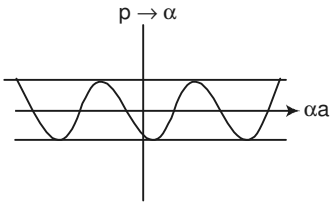
$$= \frac{\hbar^2}{8\pi^2 m}\left(\frac{2\pi}{\lambda}\right)2 = \frac{\hbar^2}{2m\lambda^2}$$

λ here refers to the wave nature of the electron and is equated as de Broglie's wavelength

$$E = \frac{\hbar^2}{2m}\frac{P^2}{\hbar^2} = \frac{P^2}{2m} \quad ...(10)$$

$$= \frac{m^2v^2}{2m} = \frac{1}{2}mv^2$$

The energy obtained above corresponds to the completely free particles



Q.2. what are Conductor, insulators and Semi conductors?

Ans. (a) Metals: Metals are good conductors of electricity. The energy band structure in case of metals is such that either the valency and conduction band overlap as in case of zinc [Fig. (*a*))] or the conduction band is partly filled as in case of sodium [Fig. (*b*)]. Even in the former case, it may considered that conductor has a single energy band which is partly filled and partly empty.

Thus there are empty levels just above the highest filled level. When an electric field is applied, the electrons at the top of the filled portion of the band get accelerated, i.e., gain energy and move into the empty part of the energy band. These electrons behaves as free electrons and some of them start moving in a direction opposite to that of electric field. In other words, a current begins to flow in the solid Hence the metals behave as good conductors.

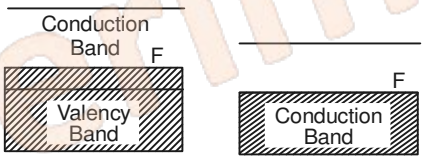


Figure: Energy bands in metals (*a*) conduction and valence bands overlap each other, (*b*) partly filled conduction band.

The highest energy level in the conduction band occupied by electrons at absolute zero temperature is called fermi level (F) and the energy corresponding to the demi level is called Fermi energy.

(b) Insulators: These are very poor conductors of electricity. In case of insulators, the valency band is completely filled and the conduction band completely empty. The energy gap between valency band and conduction band is very large, e.g., for diamond it is 6 eV, as shown in fig. Therefore, a very large amount of energy has to be supplied to the electron to move it from valency band to conduction. When an electric field is applied across such a solid, electrons in the valency band do not gain such a large amount of energy so as to jump in to the conduction band. The conduction band, therefore, continues to remain almost empty. Thus no electron flow takes place, i.e., no current flows through such a solid. Hence the solid behaves like an insulator.

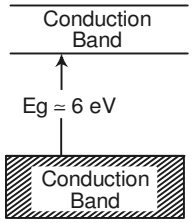


Figure. Energy band in insulators.

At any non-zero temperature, some electrons can be excited to the conduction band, which is now no longer fully empty. These electrons, therefore, can conduct electricity with a conductivity proportional to p, which lis indeed very small.

$$p \propto \exp\left(-\frac{E_g}{kT}\right)$$

In the expression E_g is the energy gap, k is Boltzman's constant and T is the,

(c) Semi-conductors: These have conductivity between metals and in sulators. The energy band structure of a semiconductor is shown in fig. In this case, the energy gap between valency band and conduction band is small and is of the order of 1.1 eV in silicon. At absolute zero temperature the valence band is completely filled and conduction band is totally empty. Hence they are insulators at low temperatures.

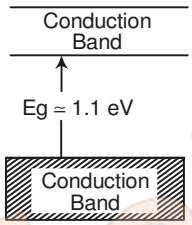


Figure: Energy band in semi-conductors.

At room temperature, some electrons in valency band acquire sufficient thermal energy to jump over the energy gap E_g into the conduction band. In the conduction band, these electrons are free to move under the influence of even a small electric field. As mentioned in insulators, the fraction p of electrons which can be excited to the conduction band is proportional to exp. $\left(-\frac{E_g}{kT}\right)$, where letters have their usual meanings. As E_g, in case of semiconductors is quite small, this fraction is sizeable for semi-conductors. This accounts for small conductivity of semi-conductors at room temperature. It is important to note that unlike metal, the resistance of semi-conductors decreases with the rise in temperature. It is because with rise in temperature more and mor e electrons jump from valency band into conduction band and therefore, conductivity of semi-conductor increases.

Q.3. Discuss about *P-N* type extrinsic semiconductor.

Ans. The Doping of Semiconductors

The addition of a small percentage of foreign atoms in the regular crystal lattice of silicon or germanium produces dramatic changes in their electrical properties, producing *n*-type and *p*-type semiconductors.

Pentavalent impurities: Impurity atoms with 5 valence electrons produce *n*-type semiconductors by contributing extra electrons.

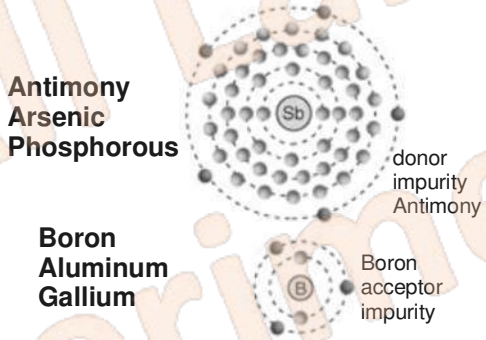
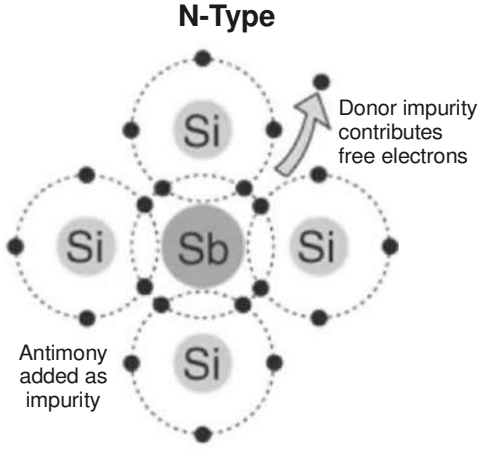
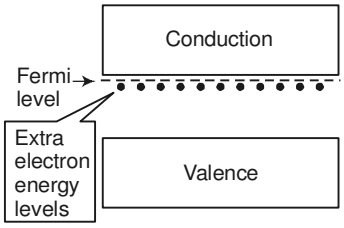


Fig. Trivalent impurities

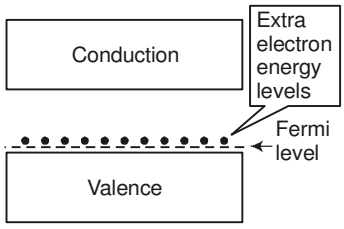
Impurity atoms with 3 valence electrons produce *p*-type semiconductors by producing a "hole" or electron deficiency.

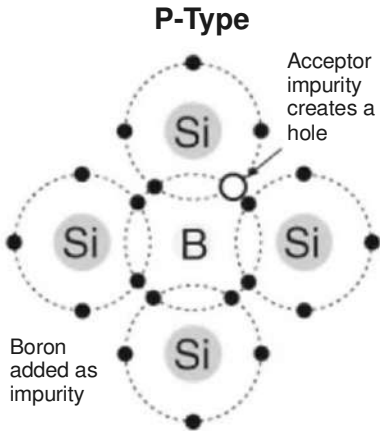
N-Type Semiconductor: The addition of pentavalentimpurities such as antimony, arsenic or phosphorous contributes free electrons, greatly increasing the conductivity of the intrinsic semiconductor. Phosphorous may be added by diffusion of phosphine gas (PH_3).





P-Type Semiconductor: The addition of trivalent impurities such as boron, aluminum or gallium to an intrinsic semiconductor creates deficiencies of valence electrons, called "holes". It is typical to use B_2H_6 diborane gas to diffuse boron into the silicon material.





Q.4. Define and derive for mobility of semiconductors. Also Discuss Hall effect.

Ans. Consider a block of semiconductor of length l and area of cross-section A, as shown in Fig. Let ne and nh be number densities of electrons and holes respectively. Let us further suppose that a current l flows through the semiconductor block, when a potential difference V is applied across it. Since flow of current in a semiconductor is due to the motion of both electrons and holes, so we have

$$l = l_e + l_h \qquad ...(1)$$

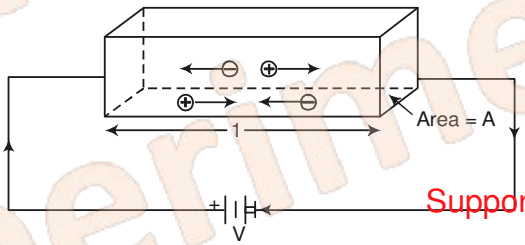


Figure. Carrier Mobilities of semi conductors.

where le and lh are current due to motion of electrons and current due to motion of holes respectively. In terms of number densities ne and nh and drift velocities v_e and v_h of electrons and holes, eq. (1) becomes

$$l = n_e A e v_e + n_h A e v_h \qquad ...(2)$$

or
$$l = eA(n_e v_e + n_h v_h) \qquad ...(3)$$

Now
$$l = \frac{V}{R}$$

where R is the resistance offered by the semiconductor block to the flow of current. Therefore, Eq. (3) becomes

$$\frac{V}{R} = eA(n_e v_e + n_h v_h) \qquad ...(4)$$

Now if E is the electric set up across the semiconductor block, then

$$E = \frac{V}{l} \text{ or } V = El.$$

Substituting this value of V in eq. (4), we get

$$\frac{El}{R} = eA(n_e v_e + n_h v_h) \text{ or } \frac{E}{\frac{RA}{l}} = e(n_e v_e + n_h v_h 0$$

But $\frac{RA}{l} = \rho$, the resistivity (specific resistances) of the material of the conductor, therefore,

$$\frac{E}{\rho} = e(n_e v_e + n_h v_h) \quad ...(5)$$

The above equation can be further modified in terms of an important quantity called the 'mobility of the carriers'.

Mobility of carriers, be it of electrons or holes, is defined as the drift velocity of the carriers per unit electric field. We can, therefore, write the mobilities of electrons and holes expressed by symbols μ_e and μ_h as,

$$\mu_e = \frac{v_e}{E} \text{ and } \mu_h = \frac{v_h}{E} \quad ...(6)$$

Incorporating (6) in (5), we get

$$\frac{1}{\rho} = e[n_e \mu_e + n_h \mu_h] \quad ...(7)$$

But

$$\frac{1}{\rho} = \sigma \quad ...(8)$$

where σ is the conductivity of semiconductor. So, we get

$$\sigma = e[n_e \mu_e + n_h \mu_h] \quad ...(9)$$

Equation (9) tells us that the conductivity of a semi-conductor depends upon the mobilities of electrons and holes as well as their number densities. Now, as far as the increase in temperature is concerned, the mobilities μ_e and μ_h are not much affected by it. We, therefore, note that rise in conductivity with rise in temperature of a semi-conductor is chiefly due to increase in carrier concentrations.

Hall's Effect: If a metal or a semi-conductor carrying current I is placed in a magnetic field acting at right angle to the direction of flow of current, an electric field is set up at right angle to both the directions of the current as well as that of the magnetic field. This phenomenon is known as Hall's effect.

It was discovered by *E.H.* Hall. The existence of the transverse e.m.f. can be shown by the following experiment. Consider a cuboid strip *OAB' CDEFG* of metal or semi-conductor with its three edges parallel to the three axes *OX*,

OY and *OZ* as shown. Let the strip be provided with terminals T_1 and T_2 on opposite faces parallel to *Z*-axis. Let a current *I* be passed through the strip along +ve *X*-direction. If we connect, the terminals T_1 and T_2 to a sensitive galvanometer, no deflection will be seen. On applying magnetic field along +ve *Z*-direction, the galvanometer shows some deflection. On reversing the direction to the magnetic field, the direction of current in the galvanometer is also reversed. This indicates, on applying magnetic field, a potential difference exists between the terminals T_1 and T_2, which were at same potential, when the magnetic field was not applied. This transverse e.m.f., set up is known as Hall's Voltage or Hall potential difference.

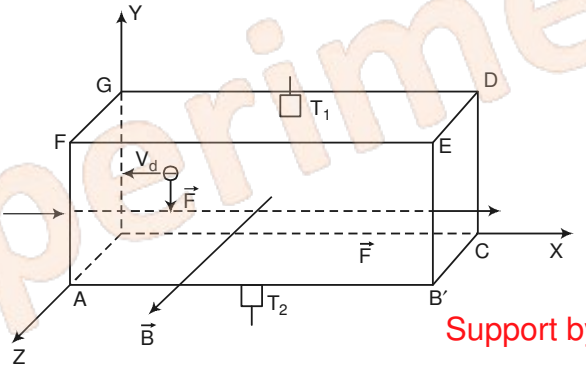


Figure. Hall's Effect

Theory: Let us suppose the strip is metallic and the charge carrier are electrons, moving along – ve *X*-direction. A charge (*q*) moving at right angle to the magnetic field experiences a force of magnitude $qvB\,[\vec{F} = q(\vec{v} \times \vec{B})]$. Thus a force $F = -ev_dB$ will act on the electron, where *e* is the charge, v_d is the drift velocity and B is the magnitude of magnetic field. Applying Flaming's left hand rule, we find the force is directed downwards and thus electron will move towards face *OAB′C*. The same will be true for all other free electrons. This will make *T*1 at positive and *T*2 at negative potential. This process will continue, till the negative potential of *T*2 stops the further movement of electrons. At this stage, the forces acting on the electron due to two fields are equal and opposite and

$$eE_t = ev_dB \qquad ...(10)$$

or $$E_t = v_dB$$

If d is the depth of the strip, measured parallel to *Y*-axis, the transverse electric field E_t is given by

$$E_t = \frac{V_H}{d} \qquad ...(11)$$

when V_H is Hall's potential difference.