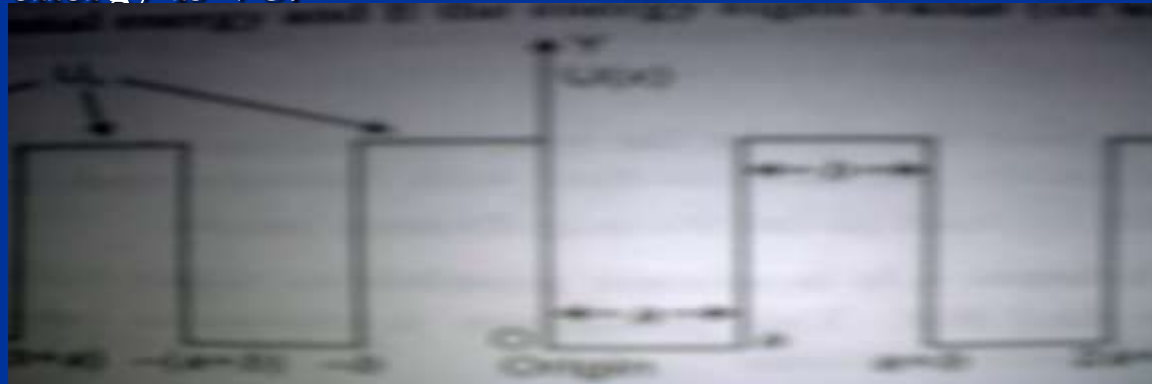


Band theory of solids

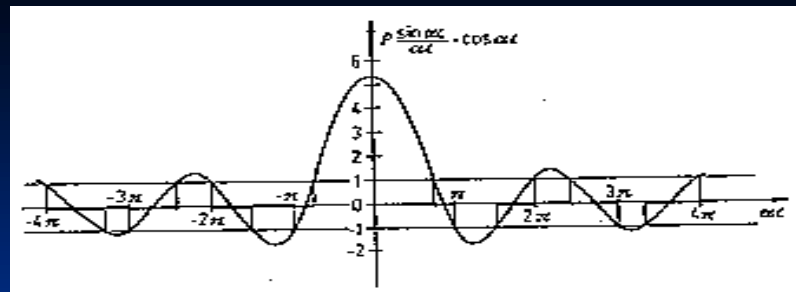
- The failure of free electron theory is because of the over simplified assumption that the electrons move in a region of zero or constant potential in the metals. However the potential experienced by electron is complicated and to reasonable approximation we can assume that electrons move in periodic potential.
- **The Kronig- Penney Model:** Kronig and Penney studied the behavior of electrons in a periodic potential by considering one dimensional model. It is assumed that the potential energy of an electron has the shape of square wells. The period of potential is $(a+b)$, in the region like $0 < x < a$, the potential energy is assumed to be zero and in the region like $-b < x < 0$ the potential energy is V_0 .



- It is assumed that E energy of electron is smaller than V_0 let $2mE/\hbar^2 = \alpha^2$ and $2m(V_0 - E)/\hbar^2 = \beta^2$ where α and β are two real quantities.
- On solving the two Schrodinger wave equations, we get $(\alpha^2 + \beta^2/2\alpha\beta)\sinh\beta b \sin \alpha a + \cosh \beta b \cos \alpha a = \cos k(a + b)$
- In order to make the situation more simple, Kronig and Penney considered the case in which V_0 tends to infinity and b approaches zero but the product bV_0 remain finite and is known as barrier strength so that the potential barrier becomes delta function.

$$(V_0 b m / \alpha \hbar^2) \sin \alpha a + \cos \alpha a = \cos k a$$
 or

$$P \sin \alpha a / \alpha a + \cos \alpha a = \cos k a$$
 where $P = V_0 b m a / \hbar^2$ which is a measure of the area $V_0 b$ of the potential barrier. Large value of P means that electron is more strongly bound to a particular potential well.

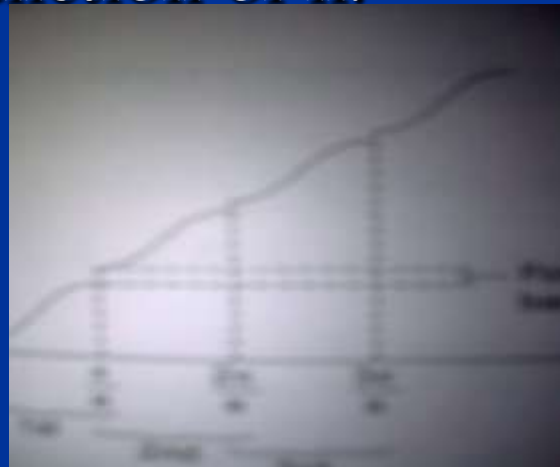


- The value of $\cos \alpha a$ is between +1 and -1 and hence only those value of αa are allowed which make left hand side of the equation lie between +1 and -1. Since α^2 is proportional to energy E hence abscissa gives a measure of energy.
- The energy spectrum of the electrons consists of energy band allowed and forbidden.
- The width of allowed energy region increases with increasing values of αa .
- With increasing P allowed energy band decreases. When $P \rightarrow \infty$, the allowed region becomes infinitely narrow and the energy spectrum becomes line spectrum. $\sin \alpha a = 0$ if $\alpha a = +n\pi$ with $n = 0, 1, 2, 3, \dots$. $E = \alpha^2 \hbar^2 / 2m$ or $E = \hbar^2 \pi^2 n^2 / 2ma^2$ for $P \rightarrow \infty$.
- When $P \rightarrow 0$ $\cos \alpha a = \cos ka$ $\alpha = k$ hence $E = \hbar^2 k^2 / 2m$ this represents energy of a completely free electron.

- For $P=0$ the energy spectrum is quasi-continuous and for $P= \infty$ the energy spectrum is line spectrum. For any intermediate value of P , the position and width of allowed and forbidden bands are obtained by drawing a vertical line.



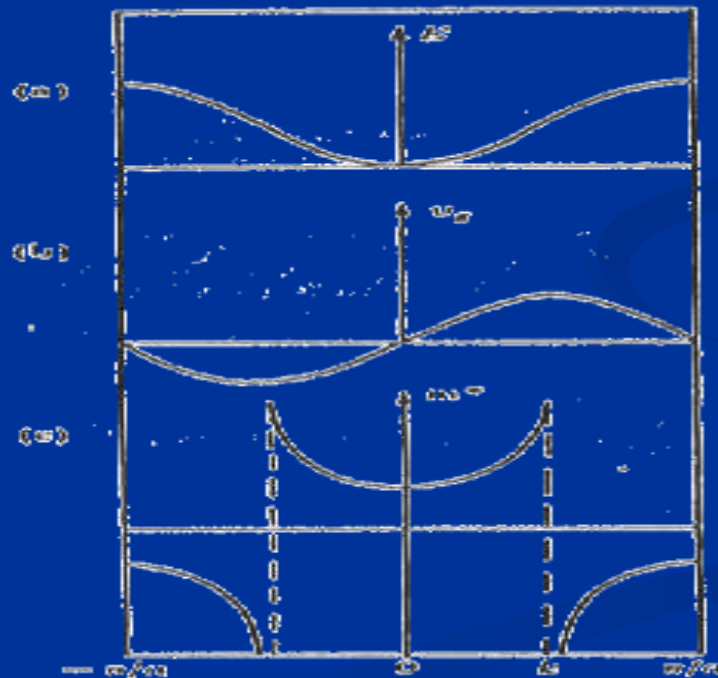
- In E & k graph the curve are
- Horizontal at the top and the bottom.
- Parabolic near the top and the bottom with curvature in opposite direction.
- With in the given energy band, the energy is periodic function of k .



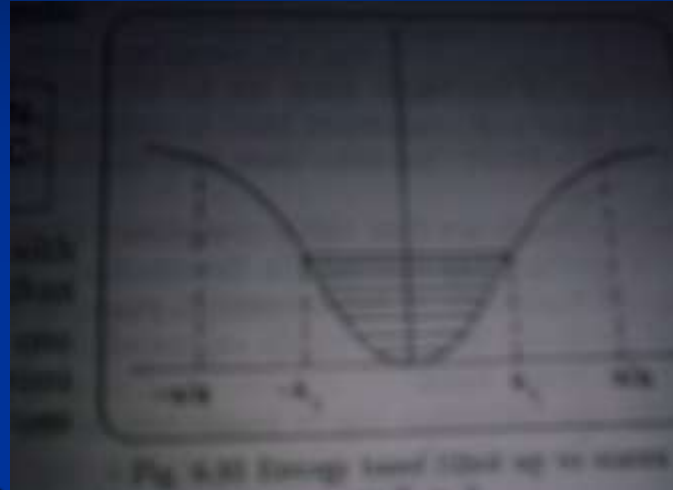
Effective mass of electron

- The electrons in crystal are not completely free but interact with the periodic potential of the crystal. The mass of an electron in a crystal, in general, is different from its free mass which is known as effective mass.
- $m^* = \hbar^2 / (d^2E/dk^2)$
- $f_k = m/m^* = m(d^2E/dk^2) / \hbar^2$ which gives a measure of degree of freedom of an electron.

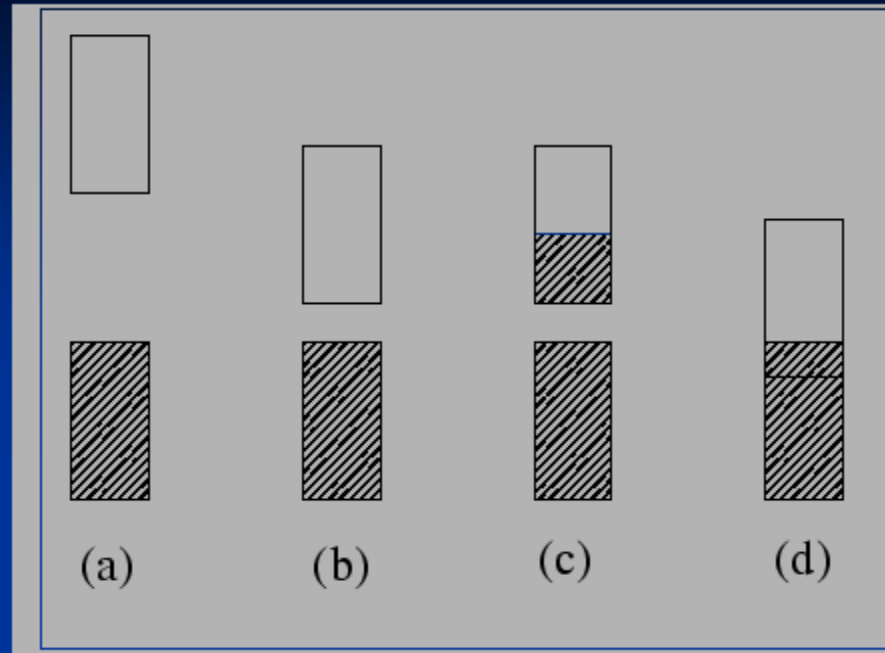
- Graphs between E & k, v & k and m* & k.
- $v = (dE/dk)/\hbar$



Distinction between metal, insulator and semiconductor

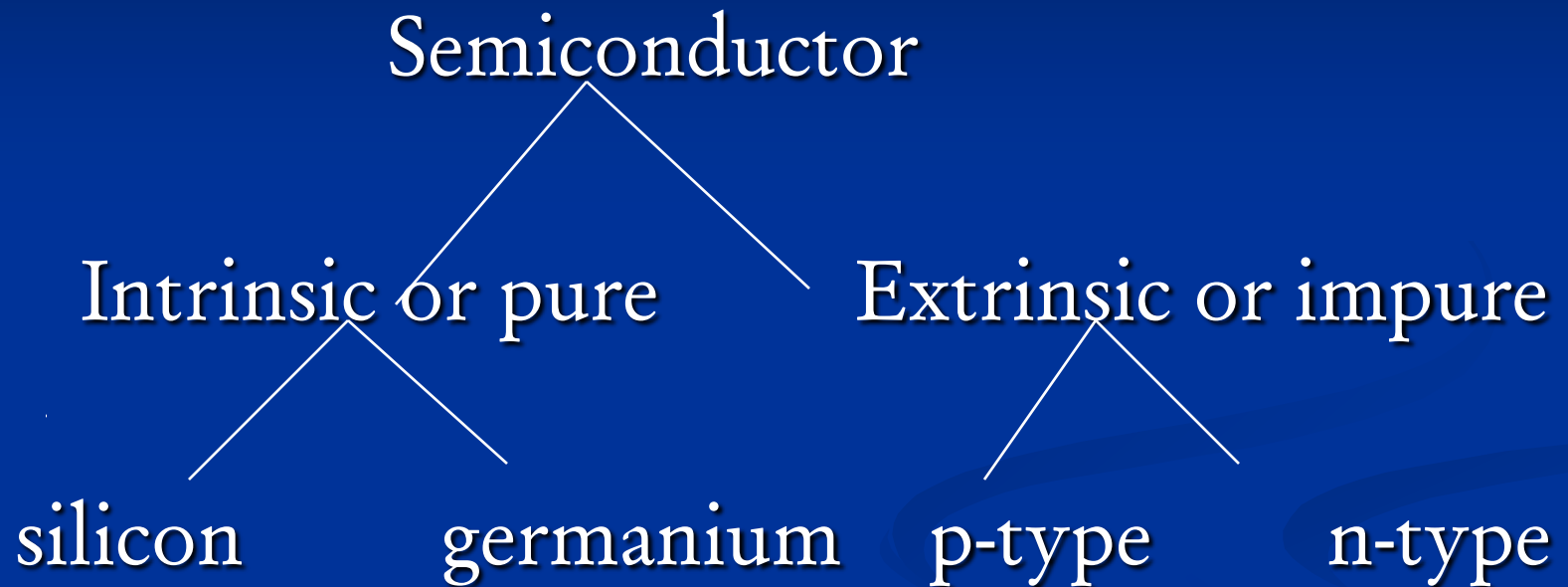


- The effective number of free electrons in shaded region is given by $N_{eff} = 2 \int_{-k_1}^{+k_1} f(k) dk$ at $k = k_1$
- If the band is completely filled, $k = \pm n \pi/a$ where $n = 1, 2, 3, \dots$
 $dE/dk = 0$ and hence $N_{eff} = 0$
- The effective number of free electrons reaches a maximum for a band filled up to $k = k_0$, the point of inflexion.



- In case of insulator there is no free electron. All the bands are completely filled in valance band and conduction band is completely empty and there is large forbidden gap. (fig. a)
- In semiconductor forbidden gap is small. (fig. b)
- In conductor there is extremely small forbidden gap or conduction band overlap with valance band. (fig. c and d)

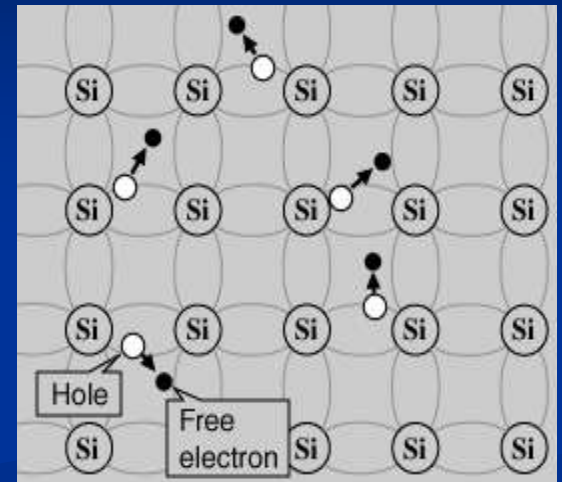
Semiconductors



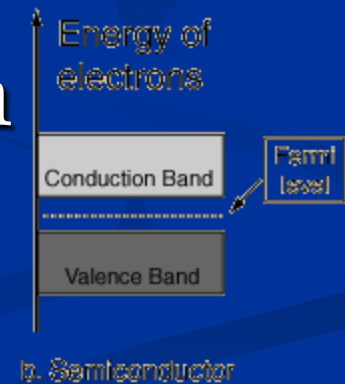
Pure or intrinsic semiconductor

- Silicon(14) and germanium(32) are tetravalent both have four electrons in outermost shell. The valence electrons are held by covalent bonds with the valence electrons of four adjacent atoms. A considerable amount of energy is required to disrupt these bonds. However, with increase in temperature or at room temperature a few covalent bonds are broken due to thermal agitation. The removal of an electron leaves behind a empty space (electron deficiency) known as hole.
- Both free electrons and holes contribute to the current.
- $n_e = n_h$

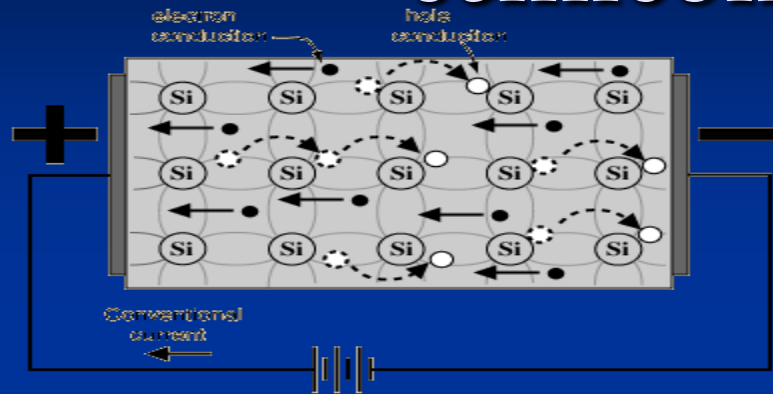
- Structure with electron hole pair



Fermi level is exactly between conduction band and valance band.



Conductivity of intrinsic semiconductor



Let A = area of cross section of sc,

e = charge of electron,

v_e = drift velocity of electrons

v_h = drift velocity of holes

At room temperature due to thermal agitation and lattice vibration, some covalent bond in a semiconductor are broken and some electrons become free. $I = I_e + I_h = n_e e A v_e + n_h e A v_h = A e (n_e v_e + n_h v_h)$

$I = V/R = E l / R = A e (n_e v_e + n_h v_h)$ $V = E l$ where l is length of sc

$l / R A = e (n_e v_e / E + n_h v_h / E) = e (n_e \mu_e + n_h \mu_h)$ where μ_e and μ_h are mobility of electrons and holes.

$1/\rho = e (n_e \mu_e + n_h \mu_h)$ $\sigma = e n_i (\mu_e + \mu_h)$

Conductivity of SC depends on number density and mobility of current carriers.

Fermi level in intrinsic SC

- Density of electrons in conduction band**
 electrons in conduction band have energy lying between E_c to ∞ . the number density of electrons in conduction band is given by

$$n_e = \int_{E_c}^{\infty} Z(E) f(E) dE$$

where $Z(E) = (1/2\pi^2)(2m^*_e/\hbar^2)^{3/2}(E-E_c)^{1/2}$ and Fermi function $f(E) = 1/[1 + \exp(E-E_F)/kT]$ by solving the above integral we get

$$n_e = 2(2\pi m^*_e kT / \hbar^2)^{3/2} \exp(E_F - E_c) / kT$$
- Density of holes in valence band**
 the valence band have energies lying from $-\infty$ to E_v

$$n_h = \int_{-\infty}^{E_v} Z(E) [1-f(E)] dE$$

$$= 2(2\pi m^*_h kT / \hbar^2)^{3/2} \exp(E_v - E_F) / kT$$

- Fermi level we know that for intrinsic SC $n_e = n_h$

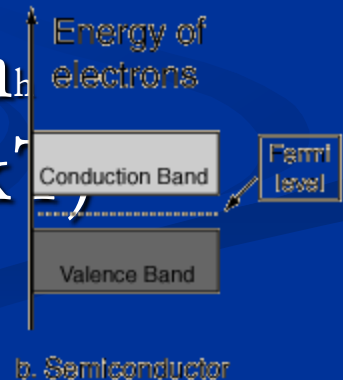
$$m_{*e}^{3/2} \exp(E_F - E_C)/kT = m_{*h}^{3/2} \exp(E_V - E_F)/kT$$

$$\exp(2E_F - E_C - E_V)/kT = (m_{*h} / m_{*e})^{3/2}$$

$$E_F = (E_C + E_V)/2 + (3kT/4) \log(m_{*h} / m_{*e})$$

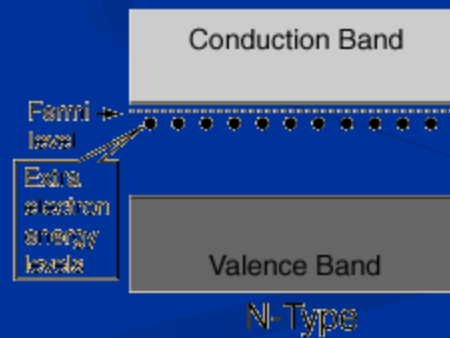
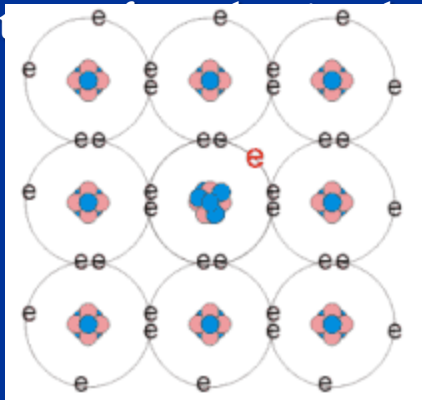
$$\text{if } m_{*h} = m_{*e} \text{ then } E_F = (E_C + E_V)/2$$

- n_e and n_h in terms of band gap $n_e = n_h$
 $= 2(2\pi kT/h^2)^{3/2} (m_{*e} m_{*h})^{3/4} \exp(-E_g/2kT)$



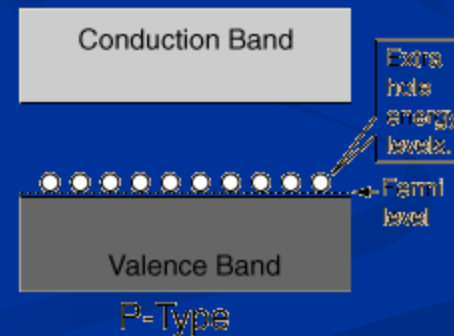
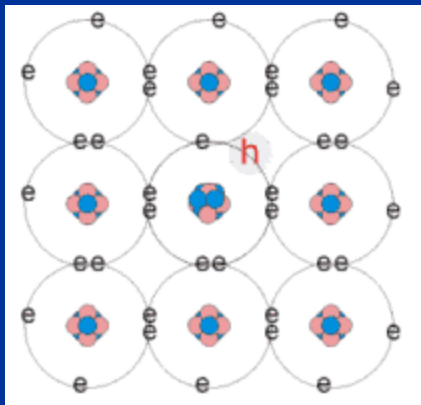
Donor or n-type semiconductor

- The electrical properties of pure semiconductor are drastically modified by addition of a small amount of suitable impurity (doping).
- When small amount of impurity (pentavalent like arsenic or antimony) is added to Si or Ge, one valence electron is left over after the four covalent bonds that bind the impurity atom to its four nearest neighbors. Donor impurities contribute conduction electron to SC without contributing holes. Hence the concentration of electrons in conduction band is increased and exceeds the concentration of holes in valence band. Thus Fermi level shifts upwards towards the bottom of the conduction band.



Acceptor or p-type semiconductor

- In acceptor or p-type semiconductor extremely small amount of trivalent impurity (say boron, gallium) is added to Si or Ge, there is a strong tendency of a SC crystal to form is more covalent bonds, attract one electron from a nearby covalent bond, consequently a new hole is created at originally occupied place of electron. The concentration of holes in valence band is more than the concentration of electrons in conduction band, Fermi level shifts nearer valence band.



Carrier concentration, Fermi level of extrinsic semiconductor

- In n-type semiconductor: $n_e = N_{d+} + h$ where N_{d+} is concentration of ionized donor and h is concentration of thermally generated holes

$$n_e = N_{d+}$$

we know $n_e = 2(2\pi m^* kT / h^2)^{3/2} \exp(E_F - E_c) / kT$ and $N_{d+} = N_d [1 - F(E_d)]$ by solving above equation we get

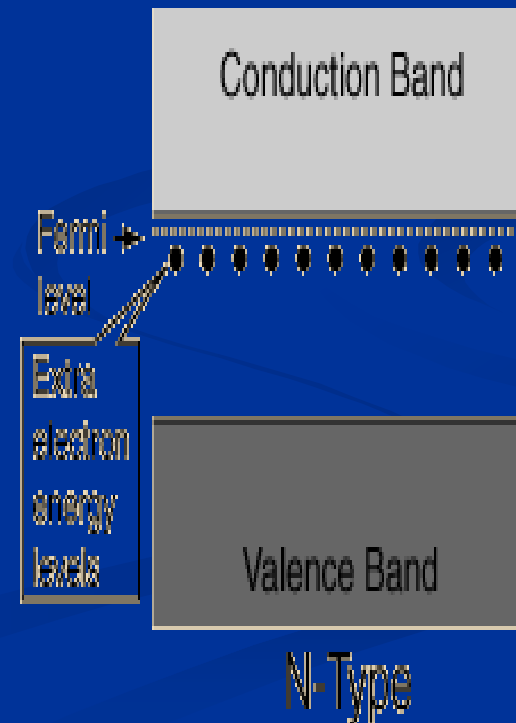
$$E_F = \{ (E_d +$$

$E_c) / 2 \} + (kT / 2) \log(N_d / N_c)$ where

$$N_c = 2(2\pi m^* kT / h^2)^{3/2}$$

At $T = 0K$ $E_F = (E_d + E_c) / 2$

- Fermi level lies exactly half way between donor level and the bottom of the conduction band.



- In p-type semiconductor: $n_h = N_{a^-} + n$ where n_h is hole concentration in valence band, n is electron concentration in conduction band and N_{a^-} is concentration of ionized acceptors. In p-type SC $n_h = N_{a^-}$ we know $n_h = 2(2\pi m^*_{*h} kT / h^2)^{3/2} \exp(E_V - E_F) / kT$ and $N_{a^-} = N_a F(E_a)$ by solving above equation we get $E_F = \{(E_a + E_V) / 2\} - (kT / 2) \log(N_a / N_V)$ where $N_V = 2(2\pi m^*_{*h} kT / h^2)^{3/2}$
 At $T = 0K$, $E_F = (E_a + E_V) / 2$

- Fermi level lies exactly half way between the acceptor level and top of the valence band.

