

Chapter 8. Semiconductors

I. Maxima and minima of energy band

1. We can always approximate the maxima and minima of an energy band by parabolic surfaces:



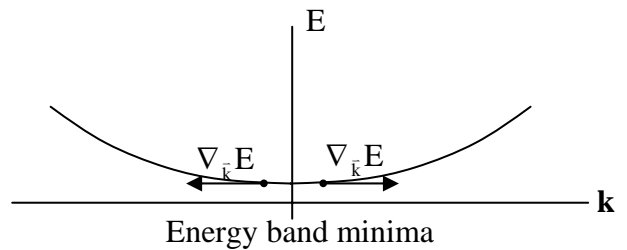
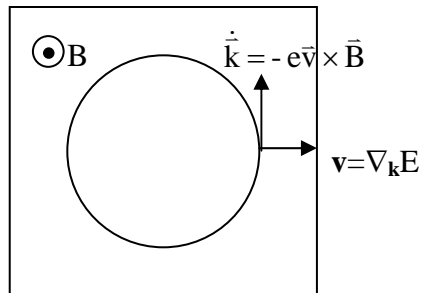
Energy band minima



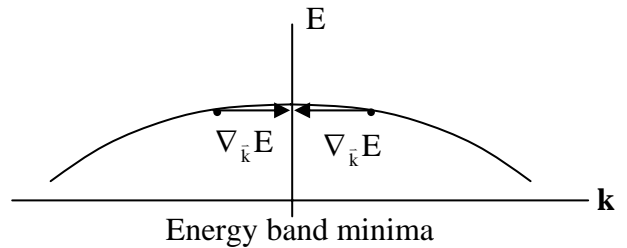
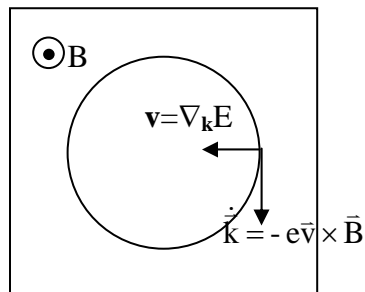
Energy band maxima

2. Electrons behave differently when they are at the energy band maxima and minima:

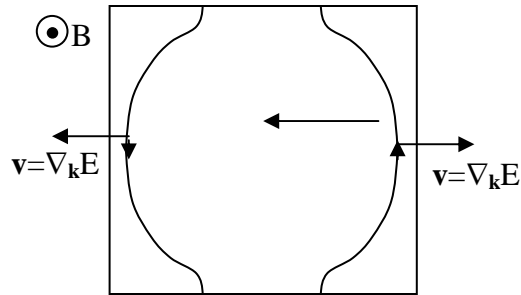
(i) At the band minima
 $\nabla_{\mathbf{k}}E$ points *away* from the minima.
 In k-space



(i) At the band maxima
 $\nabla_{\mathbf{k}}E$ points *towards* the maxima.
 In k-space

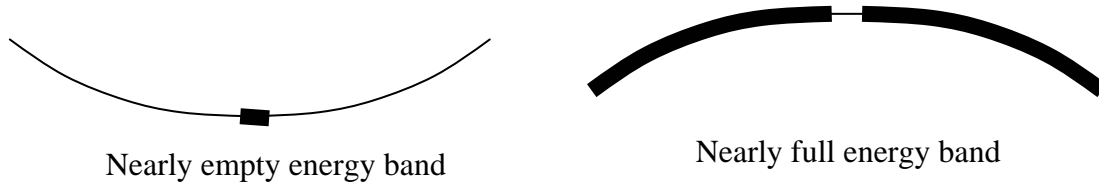


Note that orbit can be open, but the argument is the same.



3. Note that the orbit in *real space* is the same in both cases. The difference is in the sign of $d\mathbf{k}/dt$, or $d\mathbf{v}/dt$ which corresponds to the “centripetal acceleration” in the case of circular orbits.

4. A band is filled from low energy to high energy. In semiconductors, only two cases are important: nearly empty band and nearly full band.



II. Metal, insulator, and semiconductor

1. The argument presented here is based on the inverse symmetry of a crystal:

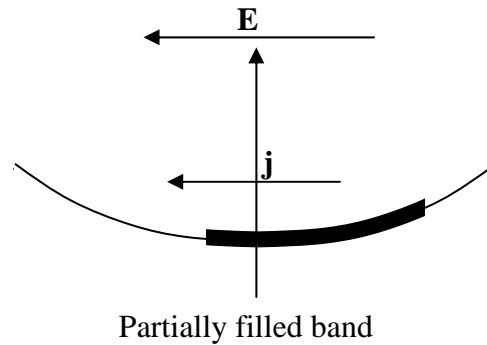
$$\nabla_{\mathbf{k}} E = -\nabla_{-\mathbf{k}} E \Rightarrow \mathbf{v}(\mathbf{k}) = -\mathbf{v}(-\mathbf{k})$$

2. Current due to electron at state \mathbf{k} is canceled by the current due to electron at state $-\mathbf{k}$, $\mathbf{j}(\mathbf{k}) = -\mathbf{j}(-\mathbf{k})$.

3. A full band *cannot* conduct electricity. A full band is always a full band no matter what the external fields are.

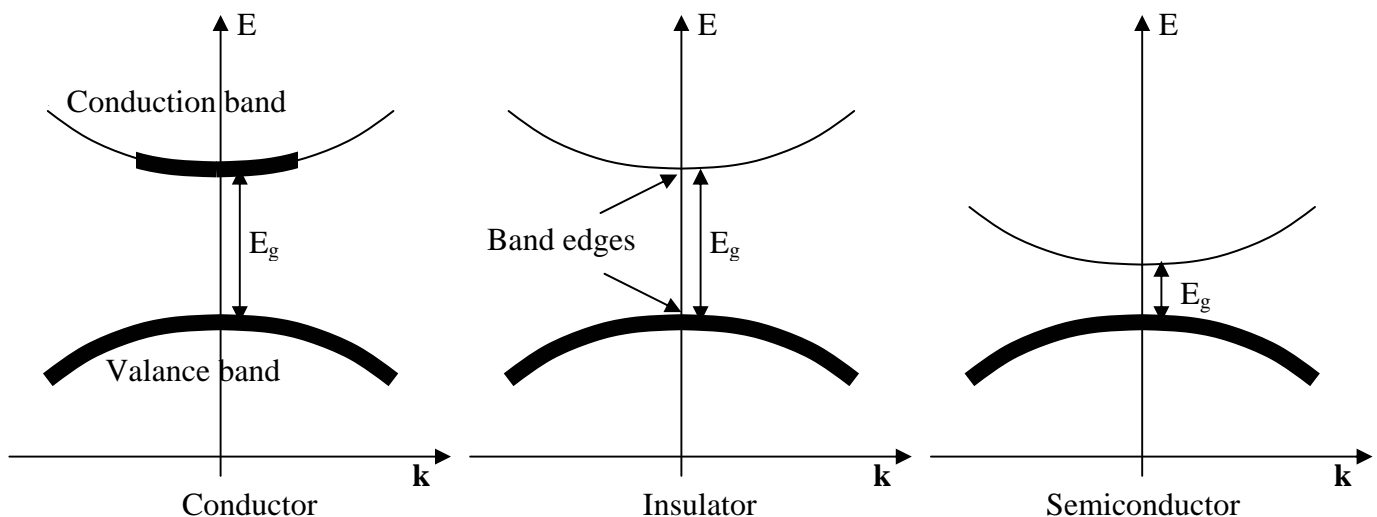
4. An empty band cannot conduct electricity because it does not have charge carrier. An empty band is always an empty band no matter what the external fields are.

5. Only a *partially filled band* can conduct electricity. A partially filled band in an electric field:



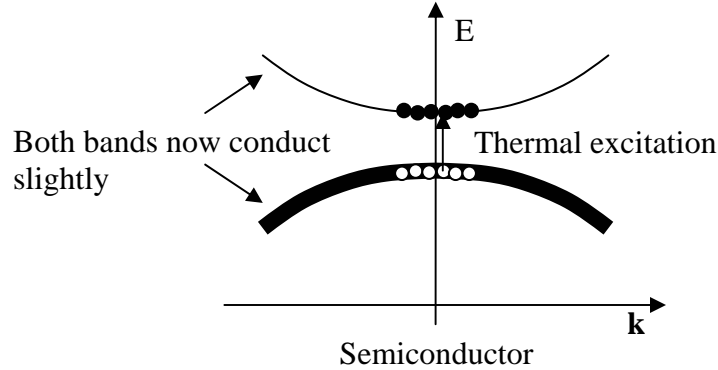
It can be seen that the occupied states are not “balanced” because of the shifting of the Fermi sphere (by an amount of F/τ) under an external field. This unbalance causes the current flow.

6. Now we can define the difference between insulator and conductor:
 All energy bands in an insulator are either *full or empty*.
 A conductor (metal) must have at least one partially filled band.
7. A material with an odd number of valence electrons must be a conductor, because an energy band can hold an even number (spin) of electrons. Note that for an even number of valence electrons, it can be either an insulator or conductor (the electrons can occupy two energy bands instead of one).
8. A partially filled band is called a conduction band. The highest full band is called the valence band.
9. The band gap E_g is the difference in energy between the lowest point of the conduction band and the highest point of the valence band. The lowest point in the conduction band is called the conduction band edge, and the highest point in the valence band is called the valence band edge.
10. A semiconductor is an insulator, but with a small bandgap.



III. Basics of semiconductors

1. For semiconductor, $E_g \leq k_B T_{\text{room}}$. It conducts slightly by thermal excitations. However it will become an insulator at low temperatures.



2. Examples. E_g for Si = 1.11 eV, Ge = 0.66eV, GaAs =1.43eV.

3. Bandgap can be measured by optical absorption method.

For photon,

$$1 \text{ eV} = 2.4 \times 10^{14} \text{ Hz} = 1.25 \text{ } \mu\text{m} \text{ (Infrared region)}$$

wavevector k_{photon} used:

$$k_{\text{photon}} = \frac{2\pi}{\lambda} = \frac{2\pi}{1.25 \times 10^{-6}} \approx 10^6 \text{ m}^{-1}$$

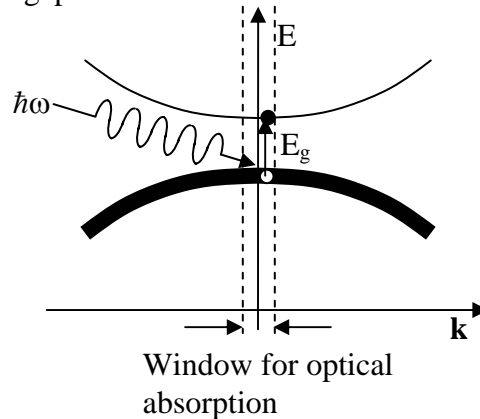
Compare with the zone size,

$$K_{\text{Brillouin}} = \frac{2\pi}{10^{-10}} \approx 10^{10} \text{ m}^{-1}$$

$$\frac{k_{\text{photon}}}{K_{\text{Brillouin}}} \approx \frac{10^6}{10^{10}} = 10^{-4}$$

Photon can detect only a very small region (10^{-4}) near the zone center.

Case 1. Direct gap semiconductor



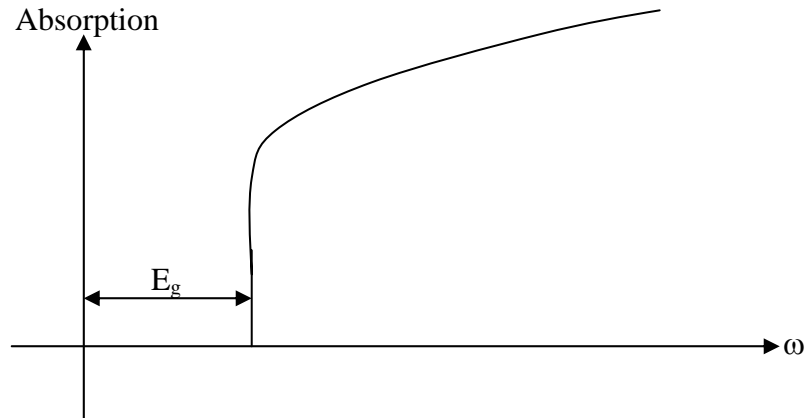
Selection rules:

(i) Conservation of energy

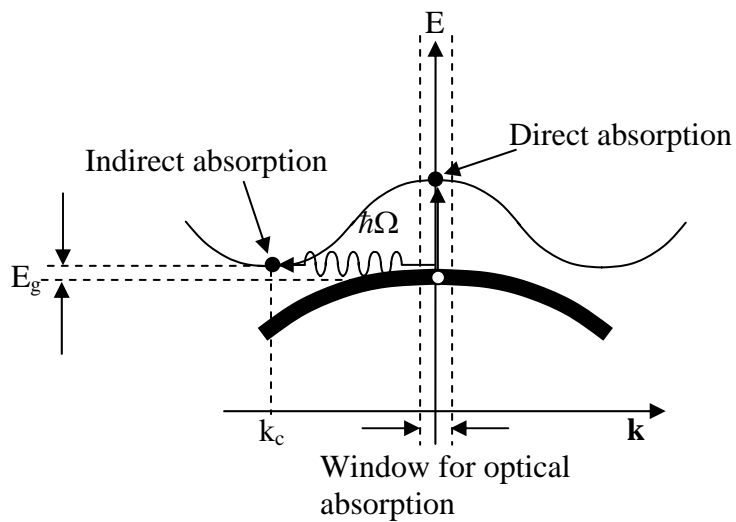
$$E_g = \hbar\omega_{\text{photon}}$$

(ii) \vec{k} selection (conservation of "momentum"):

$$\vec{k}' = \vec{k} + \vec{k}_{\text{photon}} \approx \vec{k}$$



Case 2. Indirect gap semiconductor



Two types of absorption can occur.

(i) Direct absorption, as in the case of direct gap.

(ii) Indirect absorption:

(a) The electron is "pumped up" to an energy near the conduction *band edge* (indirect) by the photon.

(b) It is then transferred to k_c with a low energy *phonon*. In general, energy of phonon is quite small.

$$v \sim 10^3 \text{ m/s} \text{ and } |\mathbf{K}| \sim 2\pi/a \sim 10^{10} \text{ m}^{-1}.$$

- $\therefore \omega_{\text{zone boundary}} \sim 10^{13} \text{ s}^{-1}$.
- $\therefore W \text{ of phonon at zone boundart} \sim 10 \text{ meV}$.

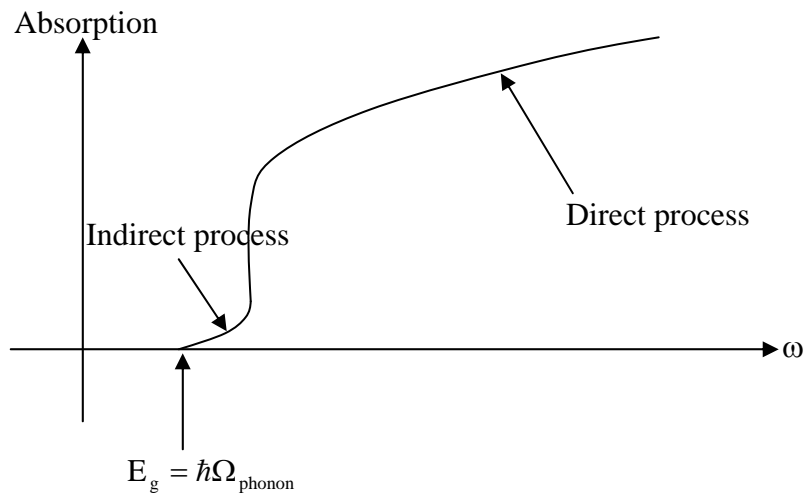
Selection rule for indirect process:

(i) Conservation of energy

$$E_g = \hbar\omega_{\text{photon}} + \hbar\Omega_{\text{phonon}}$$

(ii) \vec{k} selection (conservation of "momentum"):

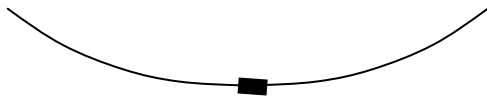
$$\vec{k}_c = \vec{k}_{\text{photon}} + \vec{k}_{\text{phonon}} \Rightarrow \vec{k}_c \approx \vec{k}_{\text{phonon}}$$



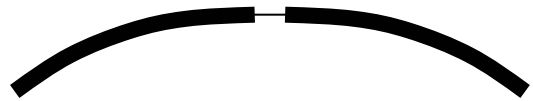
IV. Electrons and holes

1. It is an experimental fact from Hall effect measurement that charge carrier can be either positive or negative. Negative charge carrier is a result of "nearly empty band" and positive carrier is a result of "nearly full band".

2. Nearly empty band :



Nearly full band:

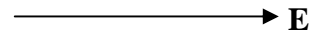


3. These two different bands in an electric field \mathbf{E} :

Nearly empty band :

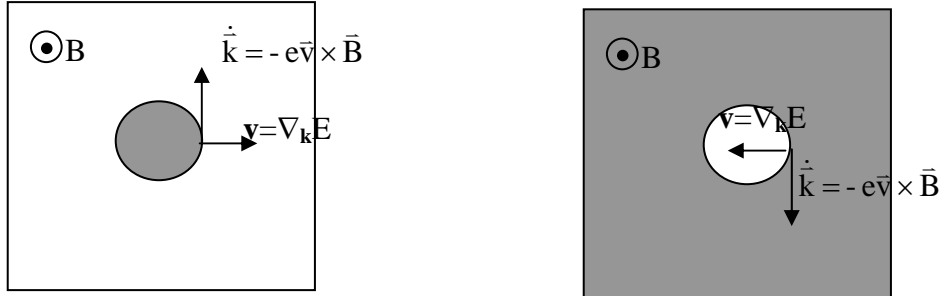


Nearly full band:



Electrons in both cases will shift opposite to \mathbf{E} by an amount of E/τ .

3. These two different bands in an magnetic field \mathbf{B} :

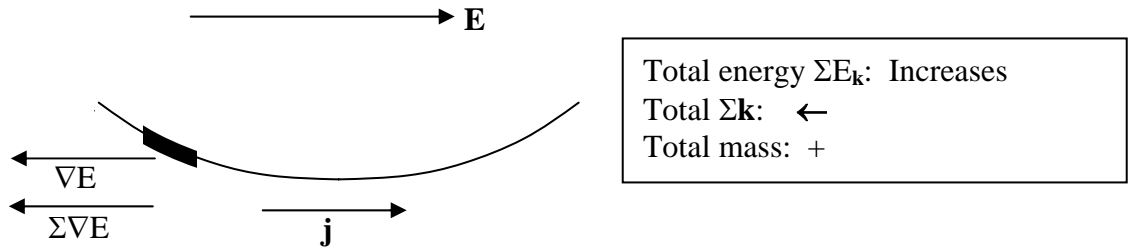


4. Effects on other physical quantities:

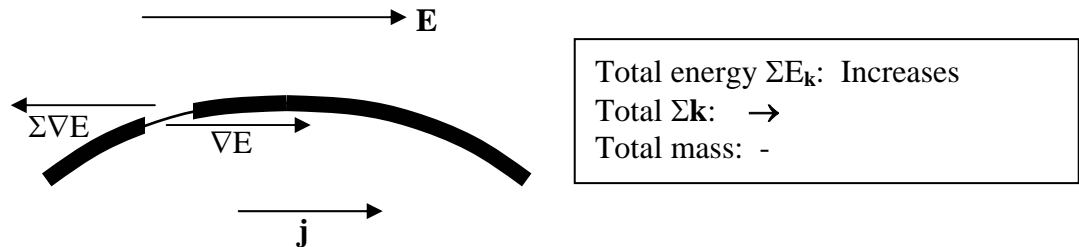
Note that

$$\vec{j} = - \sum ne\vec{v} = - \sum \frac{ne}{\hbar} \nabla_{\mathbf{k}} E$$

Nearly empty band:



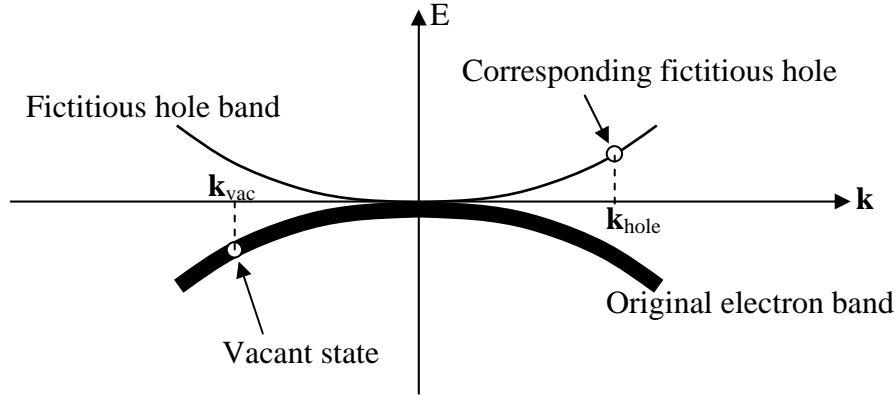
Nearly full band:



5. To establish a consistent picture, invent fictitious particle *hole* and fictitious *hole band*: Each vacant state in the original electron band corresponds to a hole occupying a state in the hole band. A nearly full electron band corresponds to a nearly empty hole band.

6. Let us now consider \mathbf{k} and E . $\Sigma\mathbf{k} = 0$ for a full electron band. If there is a single vacant at \mathbf{k}_{vac} and energy E_{vac} in a full electron band, $\Sigma\mathbf{k}$ for the full band will be $-\mathbf{k}_{\text{vac}}$ and the total energy of the full band will be *decreased* by E_{vac} . increases as holes are

introduced. Therefore the fictitious hole band has to be “turn up side down” as the original nearly full electron band, and $\mathbf{k}_{\text{hole}} = -\mathbf{k}_{\text{vac}}$.



7. Since

$$[m^*(\bar{\mathbf{k}})^{-1}]_{ij} = \frac{1}{\hbar^2} \frac{\partial^2 E(\bar{\mathbf{k}})}{\partial k_i \partial k_j} \quad \therefore [m^*(\bar{\mathbf{k}}_{\text{hole}})]_{ij} = -[m^*(\bar{\mathbf{k}}_{\text{vac}})]_{ij} \text{ because } E_{\text{hole band}}(\bar{\mathbf{k}}) = -E_{\text{real band}}(\bar{\mathbf{k}})$$

or we can simply right $m^*_{\text{hole}} = -m^*_{\text{vac}}$.

8. Since

$$\bar{\mathbf{v}} = \frac{1}{\hbar} \nabla_{\bar{\mathbf{k}}} E \quad \therefore \bar{\mathbf{v}}_{\text{hole}} = \bar{\mathbf{v}}_{\text{vac}} \text{ because } E_{\text{hole band}}(\bar{\mathbf{k}}) = -E_{\text{real band}}(\bar{\mathbf{k}}) \text{ and } \bar{\mathbf{k}}_{\text{hole}} = \bar{\mathbf{k}}_{\text{vac}}$$

9.

$$\hbar \dot{\bar{\mathbf{k}}}_{\text{vac}} = -e(\bar{\mathbf{E}} + \bar{\mathbf{v}}_{\text{vac}} \times \bar{\mathbf{B}})$$

$$\dot{\bar{\mathbf{k}}}_{\text{vac}} = -\dot{\bar{\mathbf{k}}}_{\text{hole}} \text{ and } \bar{\mathbf{v}}_{\text{vac}} = \bar{\mathbf{v}}_{\text{hole}} \text{ and assume } t_{\text{hole}} = t_{\text{vac}} = t$$

$$\therefore -\hbar \dot{\bar{\mathbf{k}}}_{\text{hole}} = -e(\bar{\mathbf{E}} + \bar{\mathbf{v}}_{\text{hole}} \times \bar{\mathbf{B}}) \Rightarrow \hbar \dot{\bar{\mathbf{k}}}_{\text{hole}} = e(\bar{\mathbf{E}} + \bar{\mathbf{v}}_{\text{hole}} \times \bar{\mathbf{B}})$$

$$\therefore Q_{\text{hole}} = -Q_{\text{electron}} = e$$

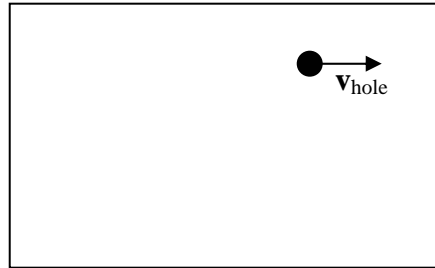
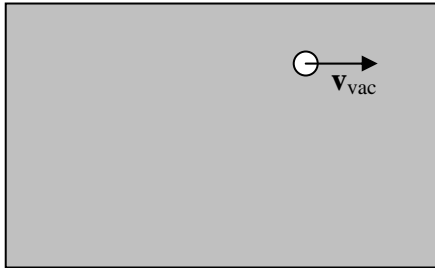
We need to be careful in distinguishing Q_{vac} and Q_{electron} here. Since vacant is the removal of an electron, so $Q_{\text{vac}} = -Q_{\text{electron}} = Q_{\text{hole}}$.

10. The probability for a state to be occupied by an electron (f_e) = 1 – probability for a state to be vacant (f_{vac}), and a vacant state is the same as a hole occupying the corresponding state of the hole band.

$$f_{\text{hole}} = f_{\text{vac}} = 1 - f_e$$

11. Since $\mathbf{j} = -nQ\mathbf{v}$, $\mathbf{j}_{\text{hole}} = \mathbf{j}_{\text{vac}}$.

12. Now we can consider the dynamical variable \mathbf{r} and \mathbf{t} for hole so that we can understand its behavior in *real space*. As indicate previously, we have assumed $t_{\text{hole}} = t_{\text{vac}} = t$. Since $\mathbf{v}_{\text{hole}} = \mathbf{v}_{\text{vac}}$, we have $\mathbf{r}_{\text{hole}} = \mathbf{r}_{\text{vac}}$. Similarly, “acceleration” $\mathbf{a}_{\text{hole}} = \mathbf{a}_{\text{vac}}$. For these reasons, hole and “vacant” in real space are “essentially the same particle”.

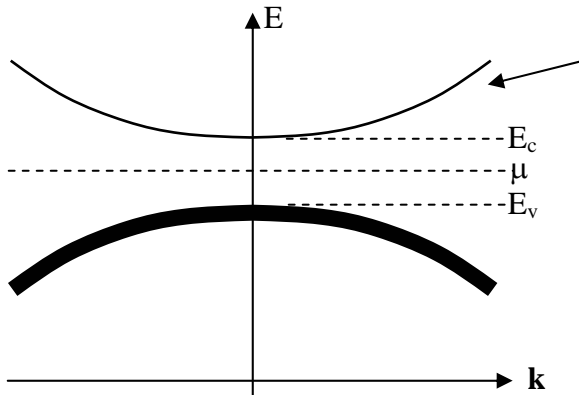


13. In summary:

$$\begin{aligned}
 E_{\text{hole band}} &= -E_{\text{real band}} \\
 E_{\text{hole}} &= -E_{\text{vac}} \\
 \mathbf{k}_{\text{hole}} &= -\mathbf{k}_{\text{vac}} \\
 m^*_{\text{hole}} &= -m^*_{\text{vac}} \\
 \mathbf{v}_{\text{hole}} &= \mathbf{v}_{\text{vac}} \\
 Q_{\text{hole}} &= Q_{\text{vac}} = -Q_{\text{electron}} = e \\
 \mathbf{j}_{\text{hole}} &= \mathbf{j}_{\text{vac}} \\
 f_{\text{hole}} &= f_{\text{vac}} = 1 - f_e
 \end{aligned}$$

V. Intrinsic semiconductor

1. Energy layout



Conduction band.

$$E \approx E_c + \frac{\hbar^2 k^2}{2m_e} \quad m_e = \text{effective mass of electron}$$

in conduction band

Density of states :

$$D(E) = \frac{1}{2\pi^2} \left(\frac{2m_e}{\hbar^2} \right)^{\frac{3}{2}} (E - E_c)^{\frac{1}{2}}$$

2. Concentration of electron in conduction band.

$$\begin{aligned}
 n &= \int_{E_c}^{\infty} D(E)f(E)dE = \int_{E_c}^{\infty} \frac{1}{2\pi^2} \left(\frac{2m_e}{\hbar^2} \right)^{\frac{3}{2}} (E - E_c)^{\frac{1}{2}} \frac{1}{e^{(E-\mu)/k_B T} + 1} dE \\
 &\approx \int_{E_c}^{\infty} \frac{1}{2\pi^2} \left(\frac{2m_e}{\hbar^2} \right)^{\frac{3}{2}} (E - E_c)^{\frac{1}{2}} e^{-(E-\mu)/k_B T} dE \quad (\text{Assume } E - \mu \gg k_B T) \\
 &= \frac{1}{2\pi^2} \left(\frac{2m_e}{\hbar^2} \right)^{\frac{3}{2}} e^{\mu/k_B T} \int_{E_c}^{\infty} (E - E_c)^{\frac{1}{2}} e^{-E/k_B T} dE \\
 &= \frac{1}{2\pi^2} \left(\frac{2m_e}{\hbar^2} \right)^{\frac{3}{2}} e^{\mu/k_B T} \int_0^{\infty} (E)^{\frac{1}{2}} e^{-(E+E_c)/k_B T} dE \quad (E' = E - E_c \rightarrow E) \\
 &= \frac{1}{2\pi^2} \left(\frac{2m_e}{\hbar^2} \right)^{\frac{3}{2}} e^{(\mu-E_c)/k_B T} \int_0^{\infty} (E)^{\frac{1}{2}} e^{-E/k_B T} dE \\
 &= \frac{1}{2\pi^2} \left(\frac{2m_e k_B T}{\hbar^2} \right)^{\frac{3}{2}} e^{(\mu-E_c)/k_B T} \int_0^{\infty} (E)^{\frac{1}{2}} e^{-E} dE \quad (E' = E/k_B T \rightarrow E) \\
 &= \frac{1}{\pi^2} \left(\frac{2m_e k_B T}{\hbar^2} \right)^{\frac{3}{2}} e^{(\mu-E_c)/k_B T} \underbrace{\int_0^{\infty} u^2 e^{-u^2} du}_{\sqrt{\pi}/4} \quad (E = u^2) \\
 &= 2 \underbrace{\left(\frac{m_e k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}}}_{N_c = \text{Effective density of state for the conduction band}} e^{(\mu-E_c)/k_B T}
 \end{aligned}$$

3. Above calculation can be applied to holes in hole band, and this gives the concentration of vacancies in valance band:

$$\begin{aligned}
 p &= \int_{E_{\text{hole}}}^{\infty} D(E)f(E)dE = \int_{E_{\text{hole}}}^{\infty} \frac{1}{2\pi^2} \left(\frac{2m_{\text{hole}}}{\hbar^2} \right)^{\frac{3}{2}} (E - E_{\text{hole}})^{\frac{1}{2}} \frac{1}{e^{(E-\mu)/k_B T} + 1} dE \\
 &= 2 \underbrace{\left(\frac{m_{\text{hole}} k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}}}_{N_v = \text{Effective density of state for the valance band}} e^{(\mu-E_{\text{hole}})/k_B T}
 \end{aligned}$$

But $\mu - E_{\text{hole}} = E_v - \mu$

\therefore concentraion of vacancies in valance band = $p = 2 \underbrace{\left(\frac{m_{\text{hole}} k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}}}_{N_v = \text{Effective density of state for the valance band}} e^{(E_v - \mu)/k_B T}$

4. Law of mass action:

$$\begin{aligned}
 np &= 2 \left(\frac{m_e k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}} e^{(\mu - E_c)/k_B T} \times 2 \left(\frac{m_{\text{hole}} k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}} e^{(E_v - \mu)/k_B T} \\
 &= 4 \left(\frac{k_B T}{2\pi\hbar^2} \right)^3 (m_e m_{\text{hole}})^{\frac{3}{2}} e^{(E_v - E_c)/k_B T} \\
 &= 4 \left(\frac{k_B T}{2\pi\hbar^2} \right)^3 (m_e m_{\text{hole}})^{\frac{3}{2}} e^{-E_g/k_B T}
 \end{aligned}$$

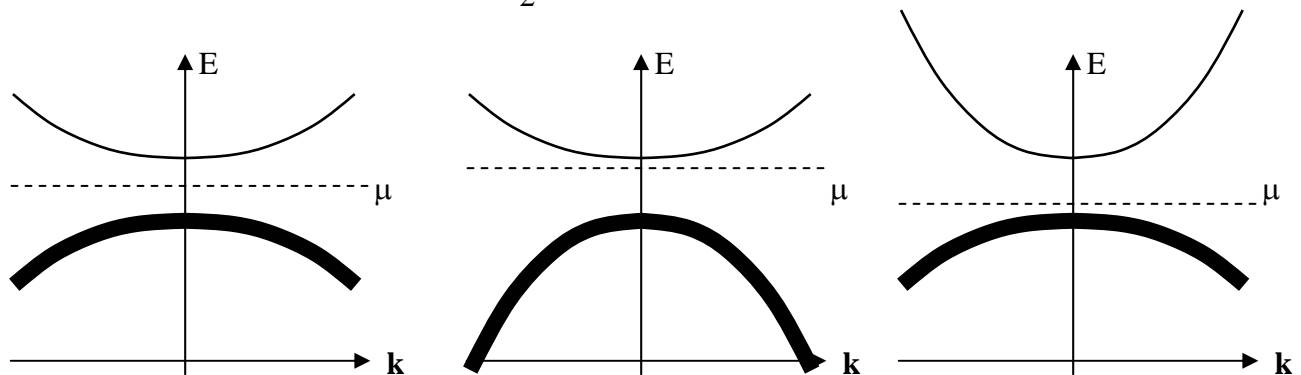
It turns out this relationship is always true, no matter whether the semiconductor is doped or not. For example, if the doped impurities introduce more electrons to the conduction band, n will increase. However, μ will also shift towards the conduction band edge and further away from the valence band edge. This will reduce p and maintain a constant product np .

5. In case of an intrinsic semiconductor, $n=p$

$$\begin{aligned}
 \therefore n = p &\Rightarrow 2 \left(\frac{m_e k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}} e^{(\mu - E_c)/k_B T} = 2 \left(\frac{m_{\text{hole}} k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}} e^{(E_v - \mu)/k_B T} \\
 &\Rightarrow m_e^{\frac{3}{2}} e^{(\mu - E_c)/k_B T} = m_{\text{hole}}^{\frac{3}{2}} e^{(E_v - \mu)/k_B T} \\
 &\Rightarrow e^{(2\mu - E_c - E_v)/k_B T} = \left(\frac{m_{\text{hole}}}{m_e} \right)^{\frac{3}{2}} \\
 &\Rightarrow \mu = E_v + \frac{1}{2} E_g + \frac{3}{2} k_B T \ln \left(\frac{m_{\text{hole}}}{m_e} \right)
 \end{aligned}$$

If $m_{\text{hole}} = m_e$, the Fermi energy is at the mid gap :

$$\mu = E_v + \frac{1}{2} E_g$$



6. Resistivity of semiconductor.

$$\rho = \frac{1}{\sigma} \quad \text{and} \quad \sigma = \frac{ne^2\tau}{m^*}$$

For metal, ρ depends on temperature because τ depends on temperature (according to the phonon concentration).

For semiconductor, n is more sensitive to temperature. Hence,

$$\rho \propto \frac{1}{n} \propto (T)^{-\frac{3}{2}} e^{E_c/2k_B T}$$

This will become dominant at low temperatures.

VI. Doped semiconductors

1. Two types of impurities.

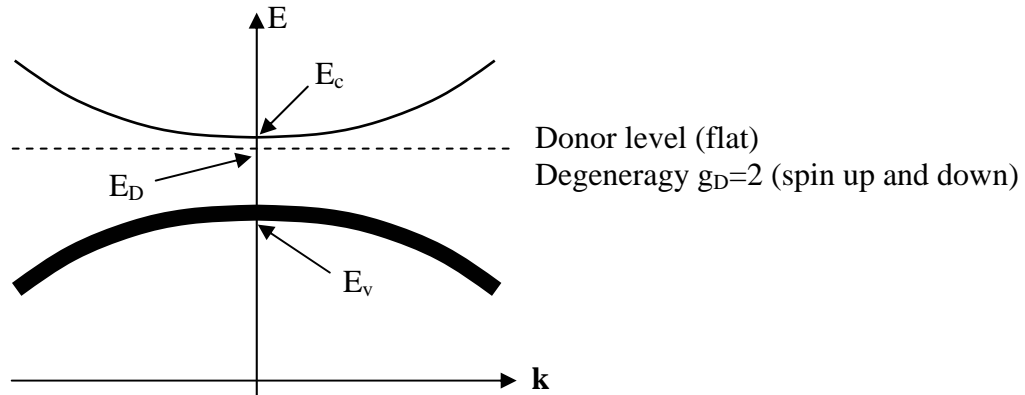
(i) Donor

Add electrons to the conduction band. e.g. P for Si.

No. of impurities per unit volume = N_D .

No. of ionized (i.e. positive ion) impurities per unit volume = N_D^+ .

Donor introduces donor levels just below the conduction band edge.



If we know E_D , we can calculate N_D^+ :

$$N_D^+ = N_D \left[1 - \frac{1}{1 + \frac{1}{g_D} \exp\left(\frac{E_D - \mu}{k_B T}\right)} \right] = N_D \left[\frac{1}{g_D \exp\left(\frac{\mu - E_D}{k_B T}\right) + 1} \right]$$

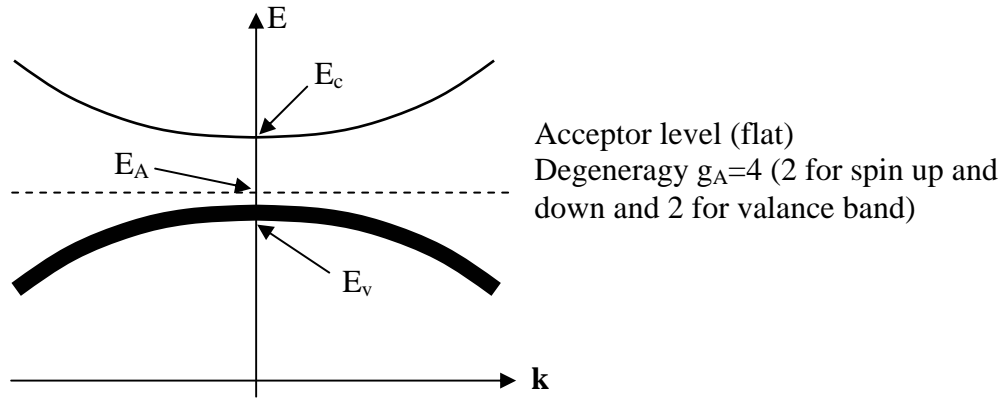
(ii) Acceptor

Take electrons from the valance band. e.g. B for Si.

No. of impurities per unit volume = N_A .

No. of ionized (i.e. negative ion) impurities per unit volume = N_A^- .

Acceptor introduces acceptor levels just above the valance band edge.



If we know E_D , we can calculate N_D^+ :

$$N_A^+ = N_A \left[\frac{1}{g_A \exp\left(\frac{E_A - \mu}{k_B T}\right) + 1} \right]$$

2 Above equations can be derived in this way. Consider a semiconductor is doped with impurities. Some of these impurities will become ions by giving up electrons or absorbing electrons.

If N_D = total number of impurity atoms (before ionization)

and N_D^+ = number of impurity ions

Number of electrons in the donor band is $n_D = N_D - N_D^+$.

Free energy of these electrons are given by:

$$F = n_D E_D - k_B T \log \left[\frac{N_D!}{n_D! (N_D - n_D)!} g_D^{n_D} \right]$$

Number of configurations of n_D electrons distributed over N_D donors

Stirling's formular : $\log n! \approx n \log n - n$

$$\begin{aligned} \therefore F &= n_D E_D - k_B T \left\{ n_D \log g_D + (N_D \log N_D - N_D) - (n_D \log n_D - n_D) \right. \\ &\quad \left. - [(N_D - n_D) \log (N_D - n_D) - (N_D - n_D)] \right\} \\ &= n_D E_D - k_B T \left\{ n_D \log g_D + N_D \log N_D - n_D \log n_D - (N_D - n_D) \log (N_D - n_D) \right\} \\ &= n_D E_D - k_B T \left\{ n_D \log g_D - n_D \log \frac{n_D}{N_D} - (N_D - n_D) \log \frac{(N_D - n_D)}{N_D} \right\} \\ \therefore \mu &= \frac{\partial F}{\partial n_D} = E_D - k_B T \left\{ \log g_D - \log \frac{n_D}{N_D} + \frac{1}{N_D} + \log \frac{(N_D - n_D)}{N_D} - \frac{1}{N_D} \right\} \\ &= E_D - k_B T \left\{ \log g_D - \log \frac{n_D}{N_D - n_D} \right\} \end{aligned}$$

$$\begin{aligned} \therefore \frac{n_D}{N_D - n_D} &= g_D e^{\frac{\mu - E_D}{k_B T}} \Rightarrow \frac{N_D - N_D^+}{N_D^+} = g_D e^{\frac{\mu - E_D}{k_B T}} \\ &\Rightarrow N_D = N_D^+ \left(1 + g_D e^{\frac{\mu - E_D}{k_B T}} \right) \text{ or } N_D^+ = N_D \left(\frac{1}{1 + g_D e^{\frac{\mu - E_D}{k_B T}}} \right) \end{aligned}$$

3 For silicon, it has 4 electrons in p-orbitals that can hold 6 electrons. Therefore we expect these three p-orbitals split into two full valance bands and one empty conduction band. That is the reason why $g_A=4$ and $g_D=2$.

4 Estimation of E_A and E_D :

$E_d = E_C - E_D$ can be consider as the “ionization energy” (or $E_C - E_D$ is the “electron affinity”) of the donor impurity atom in the environment of the semiconductor. Bohr’s equation for ionization energy:

$$E_{\text{ion}} = \frac{Z^2 e^4 m_e}{8\pi^2 \epsilon_0^2 \hbar^2}$$

Obviously, E_d is much smaller than the real ionization atom E_{ion} of the impurity atom in vacuum. There are two major reasons for this:

(i) The mass of the “free electron” should be replaced by the effective mass of the conduction band.

(ii) Potential of the impurity ion should be modified by the surrounding medium. The dielectric constant of the semiconductor has to be taken into account:

Hence the ionization energy should be modified by a factor of (m^*/m_e)

$$\frac{m^*}{m_e} \frac{1}{\epsilon^2} \ll 1$$

$$\text{or } E_D - E_c \approx E_{\text{ion}} \left(\frac{m^*}{m_e} \right) \frac{1}{\epsilon^2}$$

Example: Si doped with P.
 E_{ion} for P = 10.55 eV
 m^* for Si = $0.2m_e$
 ϵ for Si = 11.7

$$\therefore E_D - E_c \approx 10.55 \times (0.2) \frac{1}{(11.7)^2} \approx 20 \text{ meV}$$

This is very small in comparison with E_g ($\sim 1\text{eV}$).

5. Charge neutrality.

A semiconductor can be doped with both donors and acceptors at the same time. Condition of neutrality has to be followed:

$$p + \sum_i Z_i N_i - n = 0$$

Z_i = charge of an impurity type. + for donor, - for acceptor.

N_i = concentration of the impurity type (per volume).

For example, if there are one type of donor and one type of acceptor,

$$p + N_D^+ - N_A^- - n = 0 \Rightarrow p + N_D^+ = n + N_A^-$$

6. For n-type semiconductor:

$$N_D^+ > N_A^-$$

$$\begin{aligned} p + N_D^+ - N_A^- - n = 0 &\Rightarrow n^2 - (N_D^+ - N_A^-)n - np = 0 \\ &\Rightarrow n^2 - (N_D^+ - N_A^-)n - n_i^2 = 0 \\ &\Rightarrow n = \frac{1}{2}[(N_D^+ - N_A^-) + \sqrt{(N_D^+ - N_A^-)^2 + 4n_i^2}] \\ &\quad (n \sim N_D \text{ if } |N_D^+ - N_A^-| \gg n_i) \end{aligned}$$

For $k_B T \ll E_g$,

$$n = N_c e^{\frac{\mu - E_c}{k_B T}} \quad \text{and} \quad p = N_v e^{\frac{E_v - \mu}{k_B T}}$$

$$N_D^+ = N_D \left(\frac{1}{1 + g_D e^{\frac{\mu - E_D}{k_B T}}} \right) \quad \text{and} \quad N_A^- = N_A \left(\frac{1}{1 + g_A e^{\frac{E_A - \mu}{k_B T}}} \right)$$

Assume nearly all donors are ionized, $N_D^+ \sim N_D$.

Also assume that $n, N_D \gg p, N_A$ for the n - type semiconductor.

$$p + N_D^+ - N_A^- - n = 0 \Rightarrow n = N_D^+ = N_D$$

$$\begin{aligned} \therefore N_c e^{\frac{\mu - E_c}{k_B T}} = N_D &\Rightarrow \frac{\mu - E_c}{k_B T} = \ln \frac{N_D}{N_c} \\ &\Rightarrow \mu = E_c - k_B T \ln \frac{N_D}{N_c} \end{aligned}$$

6. For p-type semiconductor:

$$N_D^+ < N_A^-$$

$$\begin{aligned} p + N_D^+ - N_A^- - n = 0 &\Rightarrow p^2 - (N_A^- - N_D^+)p - np = 0 \\ &\Rightarrow p = \frac{1}{2}[(N_A^- - N_D^+) + \sqrt{(N_A^- - N_D^+)^2 + 4p_i^2}] \\ &\quad (p \sim N_A \text{ if } |N_A^- - N_D^+| \gg p_i) \end{aligned}$$

Assume nearly all acceptors are ionized, $N_A^- \sim N_A$.

Also assume that $p, N_A \gg n, N_D$ for the p-type semiconductor.

$$p + N_D^+ - N_A^- - n = 0 \Rightarrow p = N_A^+ = N_A$$

$$\begin{aligned} \therefore N_v e^{\frac{E_v - \mu}{k_B T}} = N_A &\Rightarrow \frac{E_v - \mu}{k_B T} = \ln \frac{N_A}{N_v} \\ &\Rightarrow \mu = E_v + k_B T \ln \frac{N_v}{N_A} \end{aligned}$$

VII. Basic equations use in semiconductors

1. Diffusion equations

In general, conductivity in a semiconductor involves electrons and holes:

$$\vec{j}_n = ne\mu_n \vec{E} + eD_n \nabla n$$

$$\vec{j}_p = pe\mu_p \vec{E} - eD_p \nabla p$$

The second term in the above equation is the diffusion current. It arises from non-uniform carrier density.

In one dimension, for the negative carrier:

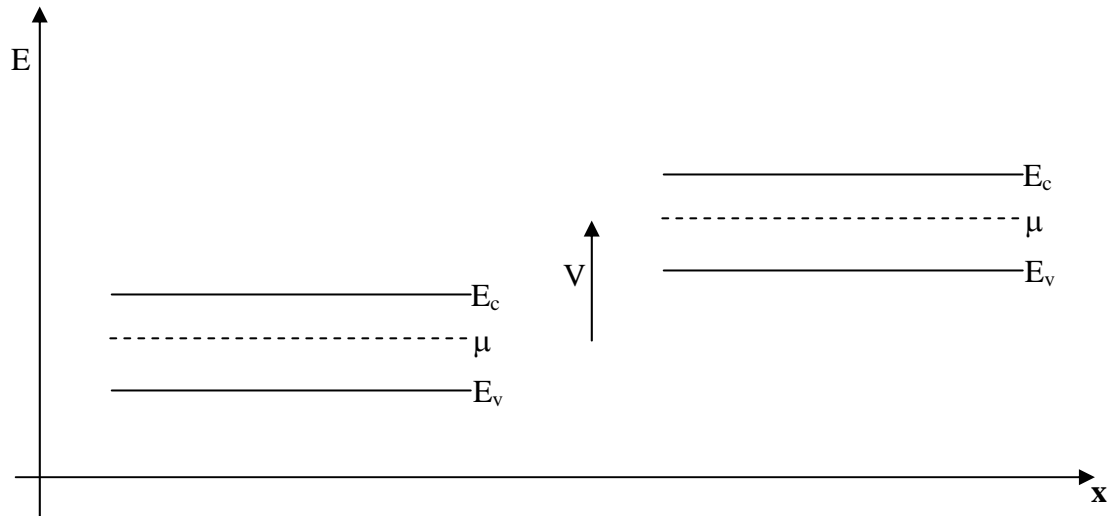
$$j_n = ne\mu_n E + eD_n \frac{\partial n}{\partial x}$$

Consider the case of $j_n=0$

$$\therefore j_n = 0 \Rightarrow 0 = ne\mu_n E + eD_n \frac{\partial n}{\partial x}$$

$$E = -\frac{\partial V}{\partial x} \quad (V = \text{potential})$$

By applying a potential V , all energies will be pushed up by the potential V .



$$\therefore e \frac{\partial V}{\partial x} = - \frac{\partial E_c}{\partial x}$$

$$n \sim N_c e^{\frac{\mu - E_c}{k_B T}}$$

$$\frac{\partial n}{\partial x} = \frac{\partial n}{\partial E_c} \frac{\partial E_c}{\partial x} = - \frac{N_c}{k_B T} e^{\frac{\mu - E_c}{k_B T}} \frac{\partial E_c}{\partial x} = - \frac{n}{k_B T} \frac{\partial E_c}{\partial x} = \frac{en}{k_B T} \frac{\partial V}{\partial x} = - \frac{enE}{k_B T}$$

Substitute this into the diffusion equation,

$$\therefore ne\mu_n E - \frac{e^2 n D_n E}{k_B T} = 0 \Rightarrow D_n = \frac{\mu_n k_B T}{e} \text{ (Einstein relation)}$$

Similarly,

$$D_p = \frac{\mu_p k_B T}{e}$$

2. Maxwell equations

$$\nabla \cdot \vec{D} = \rho_{\text{free}}(x, y, z) \quad (\text{most often used})$$

$$\nabla \cdot \vec{B} = 0$$

$$\nabla \times \vec{E} = - \frac{\partial \vec{B}}{\partial t}$$

$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}_{\text{free}}$$

$$\vec{B} = \mu_0 \vec{H}$$

$$\vec{D} = \epsilon_r \epsilon_0 \vec{E}$$

3. Continuity equations

$$\frac{\partial n}{\partial t} = G_n - U_n + \frac{1}{e} \nabla \cdot \vec{J}_n$$

$$\frac{\partial p}{\partial t} = G_p - U_p - \frac{1}{e} \nabla \cdot \vec{J}_p$$

G_n and G_p are electron and hole generation rate, in $\text{cm}^{-3}\text{s}^{-1}$, caused by external influences such as optical excitations or high electric field.

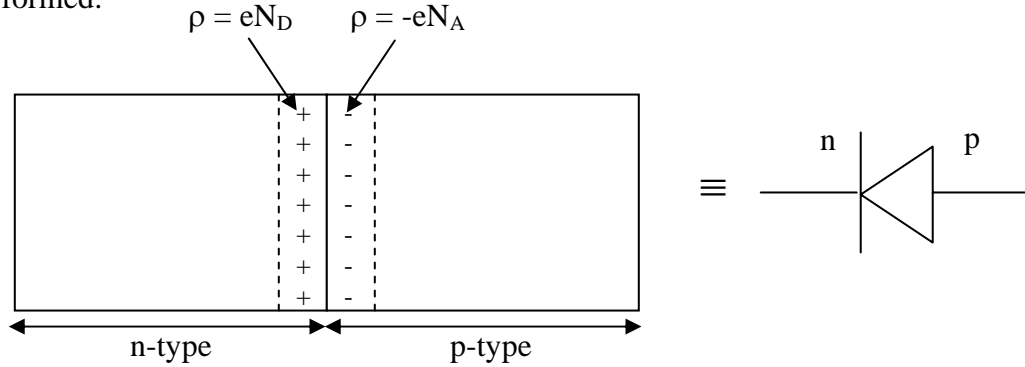
U_n and U_p are the recombination rate. U_n (or U_p correspondingly) can be approximated as

$$U_n \sim \frac{p - p_0}{\tau_p}$$

P is the minority density, p_0 is the thermal equilibrium minority density, and τ_p is the minority lifetime.

VIII. Diode

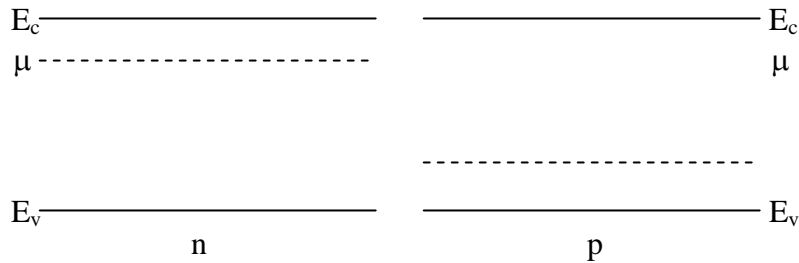
1. When a p-type semiconductor and an n-type semiconductor are joined together, a p-n junction is formed.
2. Charge density near the junction will not be uniform. When the junction is formed, electrons (majority carriers) from the n-side and holes (majority carriers) from the p-side will migrate to the other side through the junction. These migrated particles left the ionized impurities behind and a charged region (+ at the n side and - at the p-side) is formed:



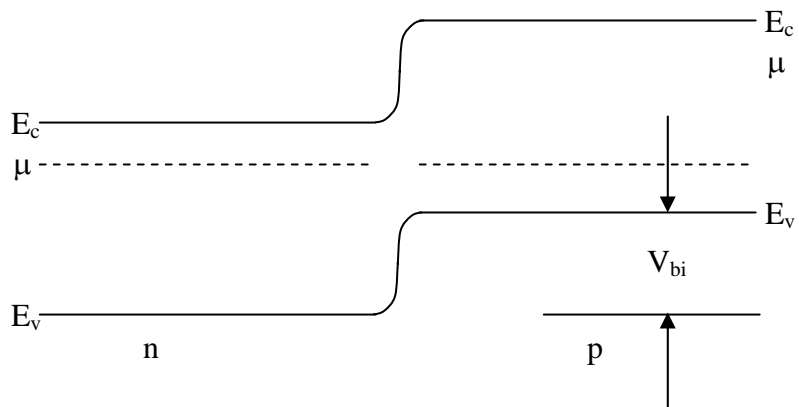
This charge region at the junction area is called the *depletion layer*. The width of the depletion depends on the voltage applied across the diode.

In equilibrium, at zero bias, the chemical potential has to be the same at both sides (because of the charge migration described above). The conduction and valence bands will be bent in real space. The variation will be drastic near the junction area.

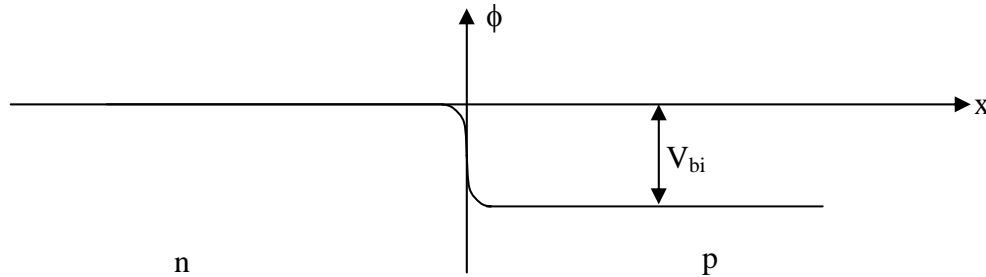
Before junction is formed:



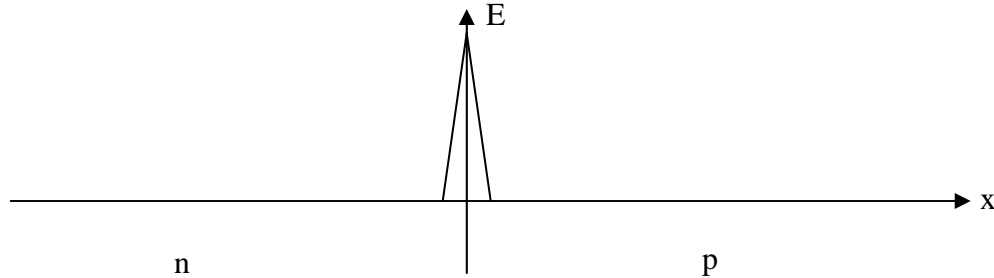
After junction is formed:



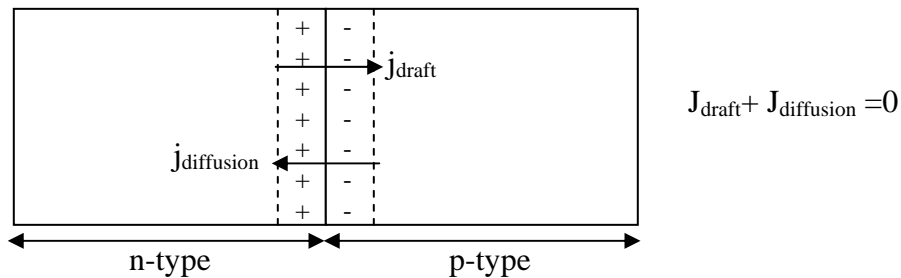
Note that both electrons (n-side) and holes (p-side) have to go to higher energy states (hole band is valance band turn upside down). This prevents further migration. The shift of the band edge energy across the junction is called the built in voltage V_{bi} . The effective electric potential should be higher at the n side and lower at the p side so that the majority carriers will not flow across the junction:



The electric field is given by $E = -\nabla\phi$:



The electric field at the depletion layer is pointing from n to p. This will exert a force acting on the electrons in the n-side in the direction from p to n, and a force on the holes in the p-side in the direction from n to p. Note that this E field is intrinsic to a p-n junction. There are two currents in the junction area. The diffusion current due to the unbalance carrier density, and the drifting current due to the intrinsic electric field. These two currents add up to 0.



- To calculate V_{bi} :
At the n-side:

$$\mu_n = E_{cn} - k_B T \ln \left(\frac{N_c}{N_D} \right)$$

At the p-side:

$$\mu_p = E_{vp} - k_B T \ln\left(\frac{N_v}{N_A}\right) = E_{cp} - E_g + k_B T \ln\left(\frac{N_v}{N_A}\right)$$

$$\mu_n = \mu_p \Rightarrow E_{cn} - k_B T \ln\left(\frac{N_c}{N_D}\right) = E_{cp} - E_g + k_B T \ln\left(\frac{N_v}{N_A}\right)$$

$$\Rightarrow V_{bi} = E_{cp} - E_{cn} = E_g - k_B T \ln\left(\frac{N_c}{N_D}\right) - k_B T \ln\left(\frac{N_v}{N_A}\right)$$

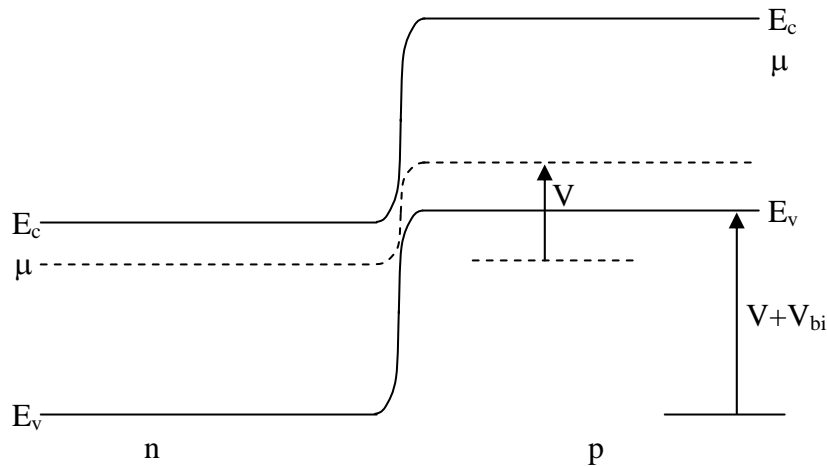
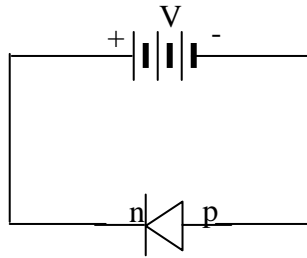
$$= E_g + k_B T \ln\left(\frac{N_A N_D}{N_c N_v}\right)$$

Note that $n_i^2 = N_c N_v e^{-\frac{E_g}{k_B T}}$

$$\therefore V_{bi} = k_B T \ln\left(\frac{N_A N_D}{n_i^2}\right)$$

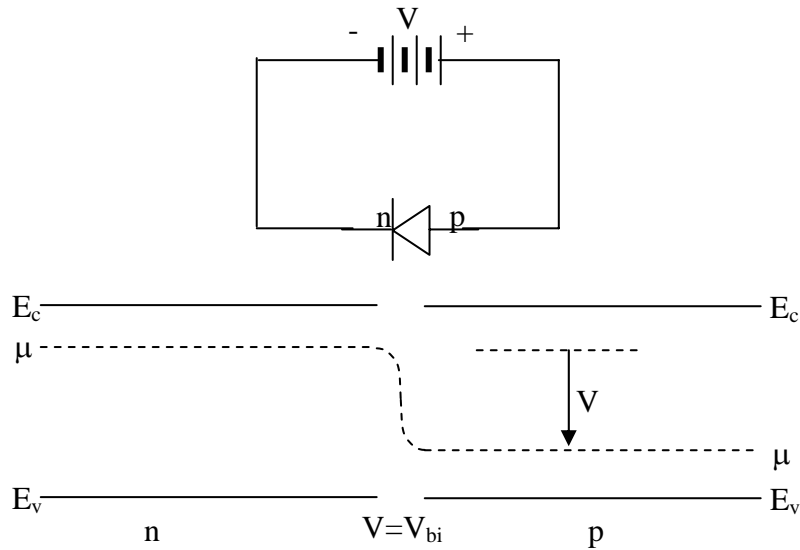
4. Reverse bias

This will draw electrons from the n-side and holes from the p-side. The depletion width will grow and the junction resistance will increase. No further current flow is allowed.

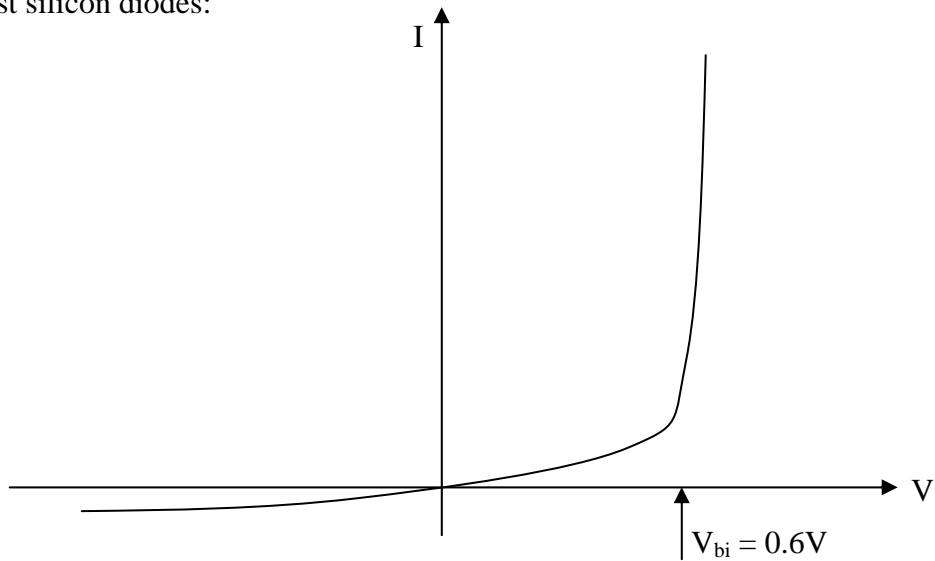


3. Forward bias

This will “push” electrons in the n-side and holes in the p-side towards the junction. The depletion width will become thinner. A current can be established and maintained if the push is large enough.

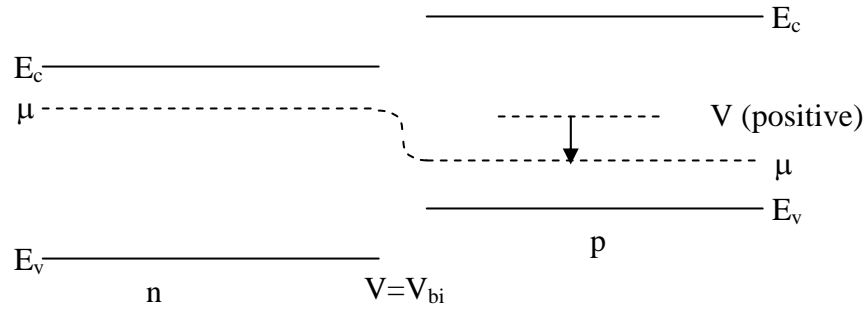


For most silicon diodes:



4. I-V characteristics of a p-n junction

Assume positive V when it is forward bias:



There are two currents from two types of majority carriers, j_n (electrons) and j_p (holes).

Nearly all electric field (and hence potential) are used to “push” carriers through the depletion layer. In other words, $E \sim 0$ at area outside the depletion layer \Rightarrow mostly diffusion current outside the depletion layer.

Diffusion current needs inhomogeneity in carrier density. This is indeed the case, because of *recombination*. Recombination is the combination of electrons in the conduction band and holes in the valance band. i.e.

$$\delta p_n = \delta n_n \Rightarrow \frac{\partial p_n}{\partial x} = \frac{\partial n_n}{\partial x} \quad (\text{subscript n indicates n - side})$$

Similarly, we have

$$\frac{\partial p_p}{\partial x} = \frac{\partial n_p}{\partial x} \quad (\text{subscript p indicates p - side})$$

To calculate the current in the diode, we need only to consider one side, say, the n-side. The current at the p-side should be similar to the n-side. Define V to be positive when the bias is forward and negative when the bias is reverse, as shown in the above figure. Current equation in neutral region (i.e. away from the depletion layer) is given by the continuity equation:

$$\begin{aligned} \frac{\partial n}{\partial t} &= G_n - U_n + \frac{1}{e} \nabla \cdot \bar{J}_n \\ \frac{\partial p}{\partial t} &= G_p - U_p - \frac{1}{e} \nabla \cdot \bar{J}_p \end{aligned} \quad \text{Depletion layer}$$

For steady case,

$$\begin{aligned} \frac{\partial n}{\partial t} = \frac{\partial p}{\partial t} &= 0 \Rightarrow \\ 0 &= G_n - U_n + \frac{1}{e} \frac{\partial J_n}{\partial x} \\ 0 &= G_p - U_p - \frac{1}{e} \frac{\partial J_p}{\partial x} \end{aligned}$$

Current equations:

$$j_n = ne\mu_n \bar{E} + eD_n \nabla n$$

$$j_p = pe\mu_p \bar{E} - eD_p \nabla p$$

Since $E \approx 0$ in this region,

$$\therefore j_n = eD_n \frac{\partial}{\partial x} n$$

$$j_p = -eD_p \frac{\partial}{\partial x} p$$

Combine these with the continuity equation:

$$D_n \frac{\partial^2}{\partial x^2} n_n + G_n - U_n = 0$$

$$D_p \frac{\partial^2}{\partial x^2} p_n + G_p - U_p = 0$$

It is suffice to solve for only one equation since

$$\frac{\partial n}{\partial x} = \frac{\partial p}{\partial x} \Rightarrow \frac{j_n}{j_p} = -\frac{D_n}{D_p}$$

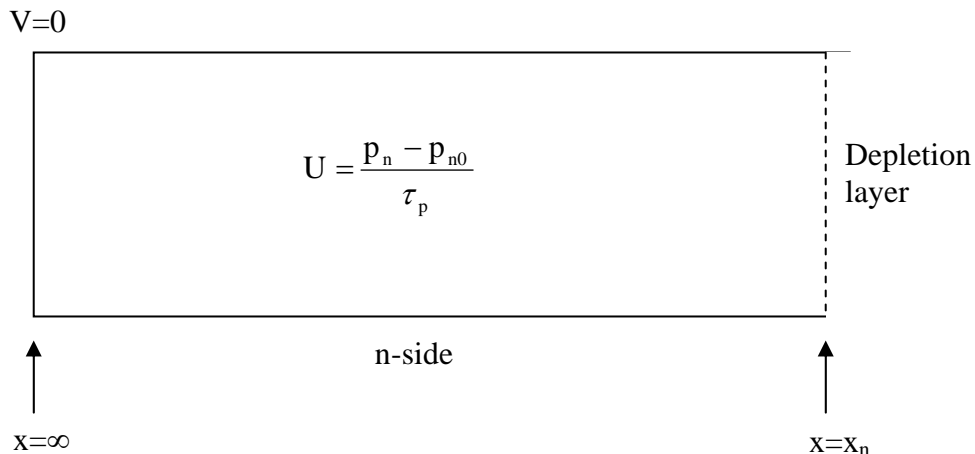
Assume there is no external excitation, i.e., $G=0$. The second equation becomes

$$D_p \frac{\partial^2}{\partial x^2} p_n - U = 0 \quad (U = U_n)$$

and approximate the recombination rate of the majority electrons (depends on the minority hole density) as

$$U = \frac{p_n - p_{n0}}{\tau_p}$$

τ_p is the hole relaxation time. p_{n0} is the hole density of the n-side at thermal equilibrium with $V=0$. For a long diode, p_{n0} is the hole density at the very end of the n-side.



$$D_p \frac{\partial^2}{\partial x^2} p_n - U = 0 \Rightarrow D_p \frac{\partial^2}{\partial x^2} p_n - \frac{p_n - p_{n0}}{\tau_p} = 0$$

General solution:

$$p_n = \underbrace{A e^{\frac{x}{\sqrt{D_p \tau_p}}} + B e^{-\frac{x}{\sqrt{D_p \tau_p}}}}_{\text{Solution for homogeneous equation}} + \underbrace{p_{n0}}_{\text{Inhomogeneous part}}$$

\Now consider the boundary condition in solving this equation. In the depletion layer,

$$\text{At n side : } n = N_c e^{(\mu_n - E_c)/k_B T}$$

$$\text{At p side : } p = N_v e^{(E_v - \mu_p)/k_B T}$$

$$\therefore np = N_c N_v e^{(\mu_n - \mu_p - E_g)/k_B T}$$

$$= n_i^2 e^{(\mu_n - \mu_p)/k_B T} \quad (n_i^2 = N_c N_v e^{-\frac{E_g}{k_B T}})$$

$$= n_i^2 e^{eV/k_B T}$$

At the n - side, $n \sim N_D$

$$\therefore p_n = \frac{n_i^2}{N_D} e^{eV/k_B T} = p_{n0} e^{eV/k_B T} \quad (p_n = p_{n0} \text{ when } V = 0)$$

\therefore For the n - side :

$$p_n(x = x_n) = p_{n0} e^{eV/k_B T}$$

$$p_n(x = \infty) = p_{n0}$$

$$P_n(x=\infty) = P_{n0} \Rightarrow A = 0$$

$$p_n = + B e^{-\frac{x}{\sqrt{D_p \tau_p}}} + p_{n0}$$

$$p_n(x = x_n) = p_{n0} e^{eV/k_B T}$$

$$\Rightarrow p_{n0} e^{eV/k_B T} = B e^{-\frac{x_n}{\sqrt{D_p \tau_p}}} + p_{n0}$$

$$\Rightarrow B = e^{\frac{x_n}{\sqrt{D_p \tau_p}}} [e^{eV/k_B T} - 1] p_{n0}$$

$$\therefore p_n = \left(e^{\frac{x_n}{\sqrt{D_p \tau_p}}} [e^{eV/k_B T} - 1] p_{n0} \right) e^{-\frac{x}{\sqrt{D_p \tau_p}}} + p_{n0}$$

$$= e^{\frac{x_n - x}{\sqrt{D_p \tau_p}}} [e^{eV/k_B T} - 1] p_{n0} + p_{n0}$$

$$\therefore p_n - p_{n0} = e^{\frac{x_n - x}{L_p}} [e^{eV/k_B T} - 1] p_{n0}$$

where $L_p = \sqrt{D_p \tau_p}$ is the hole diffusion length.

$$j_p = -eD_p \frac{\partial p}{\partial x}$$

$$= \frac{eD_p p_{n0}}{L_p} \left[e^{eV/k_B T} - 1 \right] e^{-\frac{x-x_n}{L_p}}$$

As shown earlier before.

$$\frac{j_n}{j_p} = -\frac{D_n}{D_p}$$

$$\therefore j_n = -\frac{eD_n p_{n0}}{L_p} \left[e^{eV/k_B T} - 1 \right] e^{-\frac{x-x_n}{L_p}}$$

\therefore The total current is

$$j = j_p + j_n = \frac{e(D_p - D_n)p_{n0}}{L_p} \left[e^{eV/k_B T} - 1 \right] e^{-\frac{x-x_n}{L_p}}$$

This current depends on x because of the recombination process. The current through the diode depends on the geometry (e.g. length) of the diode. For simplicity, we can define the current to be the current at the depletion layer ($x=x_n$) because the depletion layer is thin and there is not too many recombination in this region, i.e. $L_p \gg x_n + x_p$, and similarly $L_n \gg x_n + x_p$.

Current at the depletion layer boundary in the n - side :

$$j|_{x=x_n} = \frac{e(D_p - D_n)p_{n0}}{L_p} \left[e^{eV/k_B T} - 1 \right]$$

If we carry our similar calculation for the current at the depletion layer boundary in the p - side :

$$j|_{x=x_p} = \frac{e(D_n - D_p)n_{p0}}{L_p} \left[e^{eV/k_B T} - 1 \right]$$

$$\therefore \boxed{j = j_s \left[e^{eV/k_B T} - 1 \right]}$$

where

$$j_s = \frac{e(D_p - D_n)p_{n0}}{L_p} + \frac{e(D_n - D_p)n_{p0}}{L_p} = \left(\frac{ep_{n0}}{L_p} - \frac{en_{p0}}{L_p} \right) (D_p - D_n)$$

