Review of Basic Semiconductor Physics

In this lecture you will learn:

• Review of electronic states and energy band in solids
• Structure of semiconductors
• Semiconductor alloys
• Electron and hole statistics in semiconductors
• Doped semiconductors
• Transport in semiconductors and band diagrams in real space
Group IV Cubic Semiconductors

Periodic Table:

Silicon Lattice (Diamond lattice):

Group III-V Cubic Semiconductors

GaAs Lattice (Zinc Blend Lattice):

FCC Lattice Structure
Group III-V Hexagonal Semiconductors

GaN Lattice (Wurtzite Lattice):

Electrons in Solids

Wavefunctions and energies of electrons in solids are obtained by solving the Schrodinger equation:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r)\right] \psi(r) = E \psi(r)$$

Periodic potential of the atoms

Solution can be written in terms of the Bloch functions:

$$\psi(r) = \psi_{n,k}(r) = e^{i k \cdot r} u_{n,k}(r)$$

Bloch functions have the following property:

$$\psi_{n,k}(r + R) = e^{i k \cdot R} \psi_{n,k}(r)$$

$$u_{n,k}(r + R) = u_{n,k}(r)$$

Follow from the periodicity of the atomic potential

Bloch functions satisfy the Schrodinger equation:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r)\right] \psi_{n,k}(r) = E_n(k) \psi_{n,k}(r)$$

Energy of the Bloch functions
Electrons in Solids

The First Brillouin Zone (FBZ):

Two labeling items:
   i) The wavevector \( \mathbf{k} \)
   ii) The band index "n"

The wavevectors are restricted to the first Brillouin zone:

\[ \psi(r) = \psi_{n,k}(r) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{n,k}(r) \]

FBZ of the FCC lattice

Energy Bands:

The band index “n” stands for different energy bands.

Energy Bands in Semiconductors

Parabolic expansion of energy band dispersion:

\[ E_c(\mathbf{k}) = E_c + \frac{\hbar^2}{2m_e} (\mathbf{k} - \mathbf{K}_c) \cdot (\mathbf{k} - \mathbf{K}_c) \]
\[ E_v(\mathbf{k}) = E_v - \frac{\hbar^2}{2m_h} (\mathbf{k} - \mathbf{K}_v) \cdot (\mathbf{k} - \mathbf{K}_v) \]

Germanium, Silicon, GaAs
More generally:

\[ E_c(\hat{k}) = E_c + \frac{\hbar^2}{2}(\hat{k} - \hat{K}_c) \cdot M_{e}^{-1} \cdot (\hat{k} - \hat{K}_c) \]

\[ M_{e} = \begin{bmatrix} m_{xx} & m_{xy} & m_{xz} \\ m_{yx} & m_{yy} & m_{yz} \\ m_{zx} & m_{zy} & m_{zz} \end{bmatrix} \]

Parabolas in 3D can be anisotropic!

\[ E_v(\hat{k}) = E_v - \frac{\hbar^2}{2}(\hat{k} - \hat{K}_v) \cdot M_{h}^{-1} \cdot (\hat{k} - \hat{K}_v) \]

Counting Electronic States in Solids

No two electrons can occupy the same quantum state (Pauli’s exclusion principle)

So how many states are there in the FBZ?

In a solid of volume \( V \), the number of energy levels in one energy band in volume \( d^3\hat{k} \) of the FBZ is:

\[ 2 \times V \cdot \frac{d^3\hat{k}}{(2\pi)^3} \]

Two possible spin states of electrons

Summations over electron state in FBZ can be written as integrals:

\[ \sum_{\hat{k}} V \frac{d^3\hat{k}}{\text{FBZ}(2\pi)^3} \]
Counting Electronic States in Solids

How many electron states per energy band in the entire FBZ?

\[
2 \sum_{k \in FBZ} = 2V \int_{FBZ} \frac{d^3k}{(2\pi)^3} = \frac{2V}{(2\pi)^3} \times \text{volume of FBZ}
\]

But:

volume of FBZ = \frac{(2\pi)^3}{\text{volume of the primitive unit cell}}

How many electron states per energy band in the entire FBZ?

\[
\frac{V}{\text{volume of the primitive cell}} = 2 \left\{ \text{number of primitive cells in the crystal} \right\}
\]

Each primitive cell contributes two states or energy levels to each band

---

Case of Silicon:

- Each primitive unit cell contains 2 Si atoms
- Each Si atom contributes 4 electrons to the crystal

Therefore, each primitive cell contributes 8 electrons to the crystal

- Each energy band has twice as many states as the number of primitive cells in the crystals

Therefore, 4 lowest energy bands will be full of electrons and the remaining ones will be empty!
Semiconductor Alloys

Elemental Semiconductors:
Example: Si, Ge, and C

Binary Alloys:
Example: Si_{1-x}Ge_x
Alloy of two elemental semiconductors
Consists of (x) fraction of Ge and (1-x) fraction of Si

Ternary Alloys:
Example: Al_xGa_{1-x}As
Alloy of two compound semiconductors
Consists of (x) fraction of AlAs and (1-x) fraction of GaAs
x AlAs(1-x)GaAs

Quaternary Alloys:
In_{1-x}Ga_xAs_{1-y}P_{1+y} \rightarrow (1-x)y \text{ InAs}(1-x)(1-y)\text{InP} x(1-y)\text{GaP} xy \text{ GaAs}

Semiconductor Alloys: Vegard's Law

Vegard's law says the lattice constant of an alloy is a weighted sum of the lattice constants of each of its constituents, and the weight assigned to each constituent is equal to its fraction in the alloy.

Examples:
\[ a[\text{Si}_x\text{Ge}_{1-x}] = x a[\text{Si}] + (1-x) a[\text{Ge}] \]
\[ a[\text{Al}_x\text{Ga}_{1-x}\text{As}] = x a[\text{AlAs}] + (1-x) a[\text{GaAs}] \]
\[ a[\text{In}_{1-x}\text{Ga}_x\text{As}_{1-y}\text{P}_{1+y}] = (1-x)y a[\text{InAs}] + (1-x)(1-y) a[\text{InP}] + x(1-y) a[\text{GaP}] + xy a[\text{GaAs}] \]
Properties of Semiconductor Alloys

What about other material parameter like dielectric constants, effective masses, band gaps, etc?

If you don’t know any better, the linear rule law can be a good first approximation. But it does not always work very well for quantities other than the lattice constant.

For example, the band gap of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ at the $\Gamma$-point is given more accurately by:

$$E_g(\Gamma)[\text{Al}_x\text{Ga}_{1-x}\text{As}] = a + bx + c x^2$$

$$b = 1.087 \text{ eV}$$
$$c = 0.438 \text{ eV} \{ \text{at 300K} \}$$
$$a = 1.42 \text{ eV}$$

The band gap of $\text{Ga}_x\text{In}_{1-x}\text{As}$ at the $\Gamma$-point is given by:

$$E_g(\Gamma)[\text{Ga}_x\text{In}_{1-x}\text{As}] = a + bx + cx^2$$

$$b = 0.7 \text{ eV}$$
$$c = 0.4 \text{ eV} \{ \text{at 300K} \}$$
$$a = 0.324 \text{ eV}$$

Properties of Semiconductor Alloys

Direct to indirect bandgap transitions in alloys:
Electron Statistics: GaAs Conduction Band

Consider the conduction band of GaAs near the band bottom at the Γ-point:

\[ M^{-1} = \begin{bmatrix} \frac{1}{m_e} & 0 & 0 \\ 0 & \frac{1}{m_e} & 0 \\ 0 & 0 & \frac{1}{m_e} \end{bmatrix} \]

This implies the energy dispersion relation near the band bottom is:

\[ E_c(k) = E_c + \frac{\hbar^2 (k_x^2 + k_y^2 + k_z^2)}{2m_e} = E_c + \frac{\hbar^2 k^2}{2m_e} \]

Suppose we want to find the total number of electrons in the conduction band:

We can write the following summation:

\[ N = 2 \sum_{k \text{ in FBZ}} f_c(k) \]
The Fermi-Dirac Distribution

A fermion (such as an electron) at temperature $T$ occupies a quantum state with energy $E$ with a probability $f(E - E_f)$ given by the Fermi-Dirac distribution function:

$$f(E - E_f) = \frac{1}{1 + e^{(E - E_f)/kT}}$$

$E_f$ = chemical potential or the Fermi level

$K$ = Boltzmann constant = $1.38 \times 10^{-23}$ Joules/Kelvin

The Fermi level $E_f$ is determined by invoking some physical argument ...(as we shall see)

Electron Statistics: GaAs Conduction Band

$$N = 2 \times \sum_{k \text{ in FBZ}} f_c(k)$$

Where the Fermi-Dirac distribution function is:

$$f_c(k) = \frac{1}{1 + e^{(E_c(k) - E_f)/kT}} = f(E_c(k) - E_f)$$

Another way of writing it

We convert the summation into an integral:

$$N = 2 \times \sum_{k \text{ in FBZ}} f_c(k) = 2 \times V \int_{FBZ} \frac{d^3k}{(2\pi)^3} \frac{1}{1 + e^{(E_c(k) - E_f)/kT}}$$

Then we convert the $k$-space integral into an integral over energy:

$$N = 2 \times V \int \frac{d^3k}{(2\pi)^3} \frac{1}{1 + e^{(E_c(k) - E_f)/kT}}$$

We need to find the density of states function $g_c(E)$ for the conduction band and need to find the limits of integration
Electron Statistics: GaAs Conduction Band

$$N = 2 \times V \int \frac{d^3k}{F B Z (2\pi)^3} \left( \frac{1}{1 + \exp \left( \frac{E_c(k) - E_F}{kT} \right)} \right) = \frac{V}{4} \int dE \ g_c(E) f(E - E_F)$$

Electrons will only be present near the band bottom

Energy dispersion near the band bottom is:

$$E_c(k) = E_c + \frac{\hbar^2 k^2}{2m_e} = E_c + \frac{\hbar^2 k^2}{2m_e}$$

(parabolic and isotropic)

Since the electrons are likely present near the band bottom, we can limit the integral over the entire FBZ to an integral in a spherical region right close to the $\Gamma$-point:

$$N = 2 \times V \int \frac{d^3k}{F B Z (2\pi)^3} f_c(k) = 2 \times V \int \frac{d^3k}{\Gamma$-point (2\pi)^3} f_c(k)$$

$$= 2 \times V \int \frac{4\pi k^2}{8\pi^3} \, dk \, f(E_c(k) - E_F)$$

We know that:

$$E_c(k) = E_c + \frac{\hbar^2 (k_x^2 + k_y^2 + k_z^2)}{2m_e} = E_c + \frac{\hbar^2 k^2}{2m_e}$$

$$\Rightarrow k = \sqrt{\frac{2m_e (E - E_c)}{\hbar^2}}$$

and

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

We have finally:

$$N = 2 \times V \int \frac{4\pi k^2}{8\pi^3} \, dk \, f(E_c(k) - E_F) = \frac{V}{4} \int dE \ g_c(E) f(E - E_F)$$
We have finally:

\[ N = 2 \times V \int_0^\infty \frac{4\pi k^2}{8\pi^3} \, dk \, f(E_c(k) - E_f) = V \int_{E_c}^\infty dE \, g_c(E) \, f(E - E_f) \]

Where the conduction band density of states function is:

\[ g_c(E) = \frac{1}{2\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{3/2} \sqrt{E - E_c} \]

The density of states is the number of states available per unit energy per unit volume of the crystal.

If \( E_c - E_f \gg K T \) then one may approximate the Fermi-Dirac function as an exponential:

\[ f(E - E_f) \approx e^{-\frac{(E - E_f)}{K T}} \]

\[ n = \int_{E_c}^\infty dE \, g_c(E) \, f(E - E_f) = N_c \exp\left(-\frac{(E_c - E_f)}{K T}\right) \]

Where:

\[ N_c = 2 \left[ \frac{m_e}{2\pi \hbar^2} \right]^{3/2} \]
Valence Band in GaAs: Heavy Hole Band and Light Hole Band

- At zero temperature, the valence band is completely filled and the conduction band is completely empty.

- At any finite temperature, some electrons near the top of the valence band will get thermally excited from the valence band and occupy the conduction band and their density will be given by:

  \[ n = N_c \exp\left(\frac{E_c - E_f}{K T}\right) \]

- The question we ask here is how many empty states are left in the valence band as a result of the electrons being thermally excited. The answer is (assuming the heavy-hole valence band):

  \[ P = 2 \times \sum_{\mathbf{k} \text{ in } FBZ} 1 - f(E_{hh}(\mathbf{k}) - E_f) \]

- We call this the number of “holes” left behind in the valence band and the number of these holes is \( P \):

  \[ P = 2 \times \sum_{\mathbf{k} \text{ in } FBZ} 1 - f(E_{hh}(\mathbf{k}) - E_f) = 2 \pi V \int_{FBZ} \frac{d^3 k}{(2\pi)^3} \left[ 1 - f(E_{hh}(\mathbf{k}) - E_f) \right] \]

Valence Band and Holes

- At zero temperature, the valence band is completely filled and the conduction band is completely empty.

- At any finite temperature, some electrons near the top of the valence band will get thermally excited from the valence band and occupy the conduction band and their density will be given by:

  \[ n = N_c \exp\left(\frac{E_c - E_f}{K T}\right) \]

- The question we ask here is how many empty states are left in the valence band as a result of the electrons being thermally excited. The answer is (assuming the heavy-hole valence band):

  \[ P = 2 \times \sum_{\mathbf{k} \text{ in } FBZ} 1 - f(E_{hh}(\mathbf{k}) - E_f) \]

- We call this the number of “holes” left behind in the valence band and the number of these holes is \( P \):
Hole Statistics: GaAs Heavy Hole Band

\[ P = 2 \times V \int_{\text{FBZ}} \frac{d^3 \mathbf{k}}{(2\pi)^3} \left[ 1 - f(E_{hh}(k) - E_f) \right] \]

Holes will only be present near the top of the valence band

Energy dispersion near the top of the valence band is:

\[ E_{hh}(k) = E_v - \frac{\hbar^2}{2m_{hh}} \left( k_x^2 + k_y^2 + k_z^2 \right) = E_v - \frac{\hbar^2 k^2}{2m_{hh}} \]

Since the holes are likely present near the band maximum, we can limit the integral over the entire FBZ to an integral in a spherical region right close to the \( \Gamma \)-point:

\[ P = 2 \times V \int_{\text{Gamma-point}} \frac{d^3 \mathbf{k}}{(2\pi)^3} \left[ 1 - f(E_{hh}(k) - E_f) \right] \]

\[ P = 2 \times V \int_{\Gamma\text{-point}} \frac{4\pi k^2}{8\pi^3} \, dk \left[ 1 - f(E_{hh}(k) - E_f) \right] \]

Since the Fermi-Dirac distribution will be non-zero only for small values of \( k \), one can safely extend the upper limit of the integration to infinity:

\[ P = 2 \times V \int_{0}^{\infty} \frac{4\pi k^2}{8\pi^3} \, dk \left[ 1 - f(E_{hh}(k) - E_f) \right] \]

We know that:

\[ E_{hh}(k) = E_v - \frac{\hbar^2}{2m_{hh}} \left( k_x^2 + k_y^2 + k_z^2 \right) = E_v - \frac{\hbar^2 k^2}{2m_{hh}} \]

\[ \Rightarrow k = \sqrt{\frac{2m_{hh}}{\hbar^2} (E_v - E)} \quad \text{and} \quad \frac{dE}{dk} = \frac{\hbar^2 k}{m_{hh}} \]

We have finally:

\[ P = 2 \times V \int_{0}^{\infty} \frac{4\pi k^2}{8\pi^3} \, dk \left[ 1 - f(E_{hh}(k) - E_f) \right] \]

\[ = V \int_{-\infty}^{\infty} \frac{E_v}{dE} g_{hh}(E) \left[ 1 - f(E - E_f) \right] \]
Hole Statistics: GaAs Heavy Hole Band

We have finally:

\[
P = 2V \int_0^{\frac{4\pi k^2}{8\pi^3}} dk \left[ 1 - f(E_{hh}(k) - E_f) \right]
\]

\[
= V \int_{-\infty}^{E_f} dE \ g_{hh}(E) \left[ 1 - f(E - E_f) \right]
\]

Where the heavy hole band density of states function is:

\[
g_{hh}(E) = \frac{1}{2\pi^2} \left( \frac{2m_{hh}}{\hbar^2} \right)^{3/2} \sqrt{E_v - E}
\]

If \( E_f - E_v >> K\) then one may approximate the Fermi-Dirac function as an exponential:

\[
1 - f(E - E_f) = \frac{1}{1 + \exp \left( \frac{E_f - E}{K} \right)} \approx \exp \left( - \frac{(E_f - E)}{K} \right)
\]

\[
p = \int_{-\infty}^{E_v} dE \ g_{hh}(E) \left[ 1 - f(E - E_f) \right] = N_{hh} \exp \left( - \frac{(E_f - E_v)}{K} \right)
\]

Where:

\[
N_{hh} = 2 \left[ \frac{m_{hh} K T}{2\pi \hbar^2} \right]^{3/2}
\]
**Hole Statistics: GaAs Heavy Hole and Light Hole Bands**

In most semiconductors, the light-hole band is degenerate with the heavy hole band at the $\Gamma$-point. So one always needs to include the holes in the light-hole valence band as well:

$$p = \int_{-\infty}^{E_f} g_{hh}(E) \left[1 - f(E - E_f)\right] + \int_{-\infty}^{E_v} g_{lh}(E) \left[1 - f(E - E_f)\right]$$

$$E_v = \int_{-\infty}^{E_v} \left[g_{hh}(E) + g_{lh}(E)\right] \left[1 - f(E - E_f)\right]$$

$$E_f = \int_{-\infty}^{E_f} g_v(E) \left[1 - f(E - E_f)\right]$$

$$g_v(E) = g_h(E) + g_{hh}(E)$$

$$p = N_v \exp\left(-\frac{(E_f - E_v)}{KT}\right)$$

Where: $N_v = 2\left[\frac{m_h KT^2}{2\pi}\right]^{3/2}$ and $m_h = \left(m_{hh}^2 + m_{lh}^2\right)^{3/2}$

**Example: Electron Statistics in GaAs – Electrons and Holes**

At any temperature, the total number of electrons and holes (including both heavy and light holes) must be equal:

$$\Rightarrow p = n$$

$$\Rightarrow N_v \exp\left(-\frac{(E_f - E_v)}{KT}\right) = N_c \exp\left(-\frac{(E_c - E_f)}{KT}\right)$$

$$\Rightarrow \frac{N_v}{N_c} = \exp\left(\frac{2E_f - E_c - E_v}{KT}\right)$$

$$\Rightarrow E_f = \frac{E_c + E_v}{2} + \frac{KT}{2} \log\left(\frac{N_v}{N_c}\right)$$

Because the effective density of states for electrons and holes are not the same (i.e. $N_v \neq N_c$), the Fermi level at any finite temperature is not right in the middle of the bandgap.

But at zero temperature, the Fermi-level is exactly in the middle of the bandgap.
Example: Electron Statistics in GaAs – Electrons and Holes

At any temperature, the total number of electrons and holes (including both heavy and light holes) must be equal:

\[ p = n = n_i \]

where \( n_i \) is called the intrinsic electron (or hole) density

\[ \implies p = n = n_i \]
\[ \implies p \cdot n = n_i^2 \]
\[ \implies N_v \exp\left(\frac{-\left(E_f - E_v\right)}{KT}\right) N_c \exp\left(\frac{-\left(E_c - E_f\right)}{KT}\right) = n_i^2 \]
\[ \implies N_v N_c \exp\left(\frac{-\left(E_c - E_v\right)}{KT}\right) = n_i^2 \]
\[ \implies n_i = \sqrt{N_v N_c} \exp\left(\frac{-E_g}{2KT}\right) \]

Note that the smaller the bandgap the larger than intrinsic electron (or hole) density

Electron and Hole Pockets in GaAs

- At any non-zero temperature, electrons occupy states in k-space that are located in a spherically symmetric distribution around the \( \Gamma \)-point
- This distribution is referred to as the “electron pocket” at the \( \Gamma \)-point

- At any non-zero temperature, the holes (heavy and light) also occupy states in k-space that are located in a spherically symmetric distribution around the \( \Gamma \)-point
- This distribution is referred to as the “hole pocket” at the \( \Gamma \)-point
Electron and Hole Statistics in Degenerate Semiconductors

\[ n = \int_{E_c}^{\infty} \frac{dE}{E_c} \sigma(E) \ f(E-E_f) \]

\[ p = \int_{-\infty}^{E_f} \frac{dE}{E_f} \ \sigma(E) \ \left[ 1 - f(E-E_f) \right] \]

\[ N_c = 2 \left( \frac{m_e kT}{2\pi \hbar^2} \right)^{3/2} \]

\[ N_v = 2 \left( \frac{m_h kT}{2\pi \hbar^2} \right)^{3/2} \]

Donor Impurities in Semiconductors

Consider a semiconductor (say GaAs) in which one Ga atom site is occupied by a Si atom, as shown:

- Silicon has one more electron in the outermost shell compared to Ga (4 in Si compared to 3 in Ga)
- Since only 3 electrons are needed to form co-valent bonds with the nearby As atoms, the extra electron does not participate in bonding and can drift away leaving behind a positively charged Si atom
Donor Impurities in Semiconductors: N-Type Doping

- At very low temperatures the electron resides in the donor energy level and the donor atom is neutral.
- At room temperature, the electron in the donor energy level can acquire enough energy to jump to the conduction band. When this happens the donor is said to have ionized.
- Once in the conduction band the electron can move around and is no longer localized at the donor atom.
- Donor impurities can therefore be used to dope semiconductors n-type.

Acceptor Impurities in Semiconductors: P-Type Doping

Consider a semiconductor (say GaAs) in which one As atom site is occupied by a carbon atom, as shown:

- C has one less electron in the outermost shell compared to As (4 in C compared to 5 in As).
- Since 4 electrons are needed to form covalent bonds with the nearby Ga atoms, the required electron is taken from the valence band resulting in a negatively charged C atom and a hole in the valence band.
**Acceptor Impurities in Semiconductors: P-Type Doping**

- Acceptor atom gives rise to hydrogenic energy levels near the valence band maximum
- At very low temperatures the hole resides in the acceptor energy level and the acceptor atom location is overall neutral
- At room temperature, the hole in the acceptor energy level can acquire enough energy to jump to the valence band. When this happens the acceptor is said to have ionized.
- Once in the valence band the hole can move around and is no longer localized at the acceptor atom
- Acceptor impurities can therefore be used to dope semiconductors p-type

**Donor Ionization Statistics**

In the grand canonical ensemble the probability of a system to have total particles \( N \) and total energy \( E \) is:

\[
P(N, E) = A e^{-(E-E_f)N/KT}
\]

The donor level can have the following possible states:

1) No electrons present

\[
P(N = 0, E = 0) = A
\]

2) One spin-up electron present

\[
P(N = 1, E = E_d) = A e^{-(E_d-E_f)/KT}
\]

3) One spin-down electron present

\[
P(N = 1, E = E_d) = A e^{-(E_d-E_f)/KT}
\]

4) Two or more electrons present

\[
P(N > 1, E) = 0 \quad \text{Coulomb repulsion does not allow it}
\]

Sum of all probabilities should equal unity:

\[
A \left[1 + 2 e^{-(E_d-E_f)/KT}\right] = 1 \quad \Rightarrow \quad A = \frac{1}{1 + 2 e^{-(E_d-E_f)/KT}}
\]
Donor Ionization Statistics

<table>
<thead>
<tr>
<th>Probability that the</th>
<th>Probability that the</th>
</tr>
</thead>
<tbody>
<tr>
<td>donor level is ionized</td>
<td>donor level has no electrons</td>
</tr>
<tr>
<td>( P(N = 0, E = 0) )</td>
<td>( A )</td>
</tr>
<tr>
<td>( = \frac{1}{1 + 2 e^{-(E_d - E_f)}/kT} )</td>
<td></td>
</tr>
</tbody>
</table>

If the total donor impurity concentration is \( N_d \), then the concentration of ionized donors \( N_d^+ \) is equal to:

\[
N_d^+ = \frac{N_d}{1 + 2 e^{-(E_d - E_f)}/kT}
\]

For acceptors we have a similar relation:

\[
N_a^- = \frac{N_a}{1 + 2 e^{-(E_a - E_f)}/kT}
\]

Carrier Statistics in Doped Semiconductors

Consider a semiconductor that is doped with both donor and acceptor impurity atoms.

• The total charge must be zero:

\[
N_d^+ - N_a^- + p - n = 0
\]

The above equation can be used to find the position of the equilibrium Fermi level since every term depends on the Fermi level position (one equation in one unknown)

\[
N_d^+ = \frac{N_d}{1 + 2 e^{-(E_d - E_f)}/kT}
\]

\[
N_a^- = \frac{N_a}{1 + 2 e^{-(E_a - E_f)}/kT}
\]
Carrier Transport in Semiconductors

Electron current density (units: Amps/cm²) can be written as:
\[ J_e(\vec{r}) = qn(\vec{r})\mu_e E(\vec{r}) + qD_e \nabla n(\vec{r}) \]
- Diffusion component
- Drift component

Einstein relation:
\[ \frac{\mu_e}{D_e} = \frac{q}{kT} \]

Hole current density (units: Amps/cm²) can be written as:
\[ J_h(\vec{r}) = q p(\vec{r})\mu_h E(\vec{r}) - qD_h \nabla p(\vec{r}) \]
- Diffusion component
- Drift component

Einstein relation:
\[ \frac{\mu_h}{D_h} = \frac{q}{kT} \]

Carrier Number Conservation Equations

Electron-hole generation rate
Electron-hole recombination rate
\[ \frac{\partial n(\vec{r})}{\partial t} - \frac{1}{q} \nabla \cdot J_e(\vec{r}) = G_e(\vec{r}) - R_e(\vec{r}) \]
\[ G_h(\vec{r}) = G_e(\vec{r}) \]
\[ R_h(\vec{r}) = R_e(\vec{r}) \]

Electron-hole generation rate
Electron-hole recombination rate
\[ \frac{\partial p(\vec{r})}{\partial t} + \frac{1}{q} \nabla \cdot J_h(\vec{r}) = G_h(\vec{r}) - R_h(\vec{r}) \]
Poisson Equation

\[ \nabla \cdot \varepsilon(r) \mathbf{E}(r) = q \left[ p(r) - n(r) + N_a^+(r) - N_a^-(r) \right] \]

The Five Shockley Equations

\[ \begin{align*}
J_e(r) &= q n(r) \mu_e \mathbf{E}(r) + q D_e \nabla n(r) \\
J_h(r) &= q p(r) \mu_h \mathbf{E}(r) - q D_h \nabla p(r) \\
\frac{\partial n(r)}{\partial t} - \frac{1}{q} \nabla \cdot J_e(r) &= G_e(r) - R_e(r) \\
\frac{\partial p(r)}{\partial t} + \frac{1}{q} \nabla \cdot J_h(r) &= G_h(r) - R_h(r) \\
\nabla \cdot \varepsilon(r) \mathbf{E}(r) &= q \left[ p(r) - n(r) + N_a^+(r) - N_a^-(r) \right] 
\end{align*} \]

Minority Carriers and Recombination Rates

In a p-type semiconductor, electrons are the minority carriers and holes are the majority carriers: \( n \ll p \)

In a n-type semiconductor, holes are the minority carriers and electrons are the majority carriers: \( p \ll n \)

We consider a non-equilibrium situation in a p-type semiconductor in which the electron and hole concentrations are slightly perturbed from their equilibrium values

Equilibrium values: \( p_0, n_0 \)

Net recombination rate: \( R_e - G_e = \frac{n - n_0}{\tau_e} \) \hspace{1cm} \text{Minority carrier lifetime} \]

We consider a non-equilibrium situation in a n-type semiconductor in which the electron and hole concentrations are slightly perturbed from their equilibrium values

Equilibrium values: \( p_0, n_0 \)

Net recombination rate: \( R_h - G_h = \frac{p - p_0}{\tau_h} \) \hspace{1cm} \text{Minority carrier lifetime} \]
Band Diagrams in Real Space - I

For devices, it is useful to draw the conduction and valence band edges in real space:

\[ E_c \quad \quad \quad E_v \]

\[ E_F \quad \quad \quad k \]

N-type semiconductor

\[ n = N_c e^{-(E_c - E_F)/kT} \]

P-type semiconductor

\[ p = N_v e^{-(E_F - E_v)/kT} \]

Band Diagrams in Real Space - II

Electrostatic potential and electric field:

An electrostatic potential (and an electric field) can be present in a crystal:

\[ \phi(\vec{r}) \quad \text{and} \quad \vec{E}(\vec{r}) = -\nabla \phi(\vec{r}) \]

The total energy of an electron in a crystal is then given not just by the energy band dispersion \( E_n(k) \) but also includes the potential energy coming from the potential:

\[ E_n(k) \rightarrow E_n(k) - e\phi(\vec{r}) \]

Therefore, the conduction and valence band edges also become position dependent:

\[ E_c \rightarrow E_c - e\phi(\vec{r}) \]

\[ E_v \rightarrow E_v - e\phi(\vec{r}) \]

Example: Uniform \( x \)-directed electric field

\[ \vec{E}(\vec{r}) = E_x \hat{x} \]

\[ \phi(\vec{r}) = \phi(x = 0) - E_x x \]

\[ E_c(x) = E_c(x = 0) + eE_x x \]
Non-Equilibrium Situations and Current Flow

\[ J_e(\vec{r}) = qn(\vec{r})\mu_e \nabla \vec{E}(\vec{r}) + q D_e \nabla n(\vec{r}) \]

\[
\begin{align*}
n(\vec{r}) &= N_e e^{-(E_c(\vec{r}) - E_f(\vec{r})) / kT} \\
\Rightarrow \nabla n(\vec{r}) &= -\frac{n(\vec{r})}{kT} \nabla [E_c(\vec{r}) - E_f(\vec{r})] \\
\vec{E}(\vec{r}) &= \frac{1}{q} \nabla E_c(\vec{r})
\end{align*}
\]

\[ J_e(\vec{r}) = n(\vec{r})\mu_e \nabla E_c(\vec{r}) - q D_e \frac{n(\vec{r})}{kT} \nabla [E_c(\vec{r}) - E_f(\vec{r})] \]

Non-uniform Fermi level implies current flow

Similarly:

\[ J_h(\vec{r}) = p(\vec{r})\mu_h \nabla E_v(\vec{r}) - q D_e \frac{p(\vec{r})}{kT} \nabla [E_v(\vec{r}) - E_f(\vec{r})] \]

Non-uniform Fermi level implies current flow