EE529 Semiconductor Optoelectronics

Semiconductor Basics

1. Semiconductor materials
2. Electron and hole distribution
3. Electron-hole generation and recombination
4. p-n junction

Reading: Liu, Chapter 12, Sec. 13.1, 13.5
Reference: Bhattacharya, Sec. 2.1-2.2, 2.5-2.6, 4.2
Energy Bands in Semiconductors

Origin: Periodic lattice structure in the crystal.

E-k diagram details the band structure.

**k**: Electron wave vector

\[ k = \frac{2\pi}{\lambda} \]

**Indirect bandgap**

Near the band edge:

\[ E = E_c + \frac{\hbar^2 k^2}{2m^*_e} \]

\[ E = E_v - \frac{\hbar^2 k^2}{2m^*_h} \]

\[ m^*_e, h : \text{Effective masses of electrons/holes} \]
Semiconductor Materials

<table>
<thead>
<tr>
<th>Group II</th>
<th>Group III</th>
<th>Group IV</th>
<th>Group V</th>
<th>Group VI</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>Al</td>
<td>Si</td>
<td>N</td>
<td>O</td>
</tr>
<tr>
<td>Mg</td>
<td>Aluminium</td>
<td>Ge</td>
<td>P</td>
<td>S</td>
</tr>
<tr>
<td>Zn</td>
<td>Ga</td>
<td>As</td>
<td>Te</td>
<td></td>
</tr>
<tr>
<td>Cd</td>
<td>In</td>
<td>Sb</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hg</td>
<td>TI</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Elementary: e.g., Si and Ge

Binary

Ternary

Quaternary

Energy bandgap (eV)

Lattice constant (nm)
III-V Compound Semiconductors

Solid curve: Direct bandgap
Dashed curve: Indirect bandgap

$\text{Al}_x\text{Ga}_{1-x}\text{As}$ closely lattice matched to GaAs

$\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$ lattice matched to InP for $0 \leq y \leq 1$ and $x = 0.47y$

Matching lattice constant is important when depositing one semiconductor on another.
Electron-Hole Generation

How do electrons get to the conduction band (and leave holes in the valence band)?

Free electrons and holes can be generated by:

- Thermal excitation (thermal equilibrium)
- Optical excitation (quasi-equilibrium)
- Current injection (quasi-equilibrium)

It’s important to understand the carrier (electrons and holes) distribution as a function of energy.
Carrier Distribution in the Energy Band

Concentration of electrons (holes) versus energy in the conduction (valence) band =

*Density of states*
(density of allowed energy levels)
Analogy: Density of available office spaces

*Probability of occupancy*
(probability that each of these levels is occupied)
Analogy: People’s desire of occupying these spaces

A skyscraper **without** elevators
Probability of Occupancy

**Fermi-Dirac function**

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

\(f(E)\) = probability of occupancy by an electron

\(1 - f(E)\) = probability of occupancy by a hole (in valence band)

(Electrons like to sink to the bottom, holes like to float to the top.)
Density of States — Bulk Material

\[ \rho(k) = \frac{k^2}{\pi^2} \]

\[ \rho_c(E) = \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} (E - E_c)^{1/2} \]

\[ \rho_v(E) = \frac{(2m_h^*)^{3/2}}{2\pi^2\hbar^3} (E_v - E)^{1/2} \]

---

**Figure 15.1-7**  
(a) Cross section of the \( E-k \) diagram (e.g., in the direction of the \( k_1 \) component with \( k_2 \) and \( k_3 \) fixed). (b) Allowed energy levels (at all \( k \)). (c) Density of states near the edges of the conduction and valence bands. \( \rho_c(E) \) is the number of quantum states of energy between \( E \) and \( E + dE \), per unit volume, in the conduction band. \( \rho_c(E) \) has an analogous interpretation for the valence band.
Density of States — Quantum Wells

Discrete energy levels

\[ E_q = \frac{\hbar^2 (q\pi / d)^2}{2m}, \quad q = 1, 2, \ldots \]

Density of states

\[ \rho_c(E) = \begin{cases} \frac{m_e}{\pi \hbar^2 d_1}, & E > E_C + E_{q_1} \\ 0, & E < E_C + E_{q_1} \end{cases} \]

Quantum Wires and Quantum Dots

Quantum wires

$$\rho_c(E) = \begin{cases} \frac{(2/d_1 d_2)(\sqrt{m^*_e} / \sqrt{2\pi\hbar})}{(E - E_c - E_{q_1} - E_{q_2})^{1/2}}, & E > E_c + E_{q_1} + E_{q_2} \\ 0, & \text{otherwise} \end{cases}$$

(Gudiksen et al., Nature, 2002)

Quantum dots

$$\rho_c(E) = 2\delta(E - E_c - E_{q_1} - E_{q_2} - E_{q_3}) \frac{1}{d_1 d_2 d_3}$$

3 nm, 5.5 nm, 7.5 nm, 8.3 nm
Thermal-Equilibrium Carrier Concentration

**Bulk Semiconductor**

(a) Energy band diagram. (b) Density of states (number of states per unit energy per unit volume). (c) Fermi-Dirac probability function (probability of occupancy of a state). (d) The product of \( g(E) \) and \( f(E) \) is the energy density of electrons in the CB (number of electrons per unit energy per unit volume). The area under \( n_E(E) \) vs. \( E \) is the electron concentration.

\[
n_0 = \int_{E_c}^{\infty} \rho_c(E) f(E) dE = N_c(T) F_{1/2} \left( \frac{E_F - E_c}{k_B T} \right)
\]

\[
p_0 = \int_{-\infty}^{E_v} \rho_v(E) [1 - f(E)] dE = N_v(T) F_{1/2} \left( \frac{E_v - E_F}{k_B T} \right)
\]

We can simplify this more …
Carrier Concentration and Mass Action Law

For non-degenerate semiconductors, \((E_C - E_F) / k_B T \geq 3.6 \quad (E_F - E_V) / k_B T \geq 3.6\)

\[
n_0 = N_C \exp \left[ -\frac{(E_C - E_F)}{k_B T} \right]
\]

\[
N_C = 2(2\pi m^*_e k_B T / h^2)^{3/2} \quad \text{Effective density of states at the conduction band edge}
\]

\[
p_0 = N_V \exp \left[ -\frac{(E_F - E_V)}{k_B T} \right]
\]

\[
N_V = 2(2\pi m^*_h k_B T / h^2)^{3/2} \quad \text{Effective density of states at the valence band edge}
\]

The location of the Fermi level energy \(E_F\) is the key.

**Mass action law:**

\[
n_0 p_0 = 4 \left( \frac{2\pi k_B T}{h^2} \right)^3 (m_e^* m_h^*)^{3/2} \exp \left( -\frac{E_g}{k_B T} \right) = n_i^2
\]

→ Knowing one carrier concentration, you can determine the other (no matter intrinsic or extrinsic)

<table>
<thead>
<tr>
<th>TABLE 15.1-4</th>
<th>Intrinsic Concentrations in Si and GaAs</th>
<th>at (T = 300) K(^a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(n_i) (cm(^{-3}))</td>
<td>Si</td>
<td>1.5 \times 10^{10}</td>
</tr>
<tr>
<td></td>
<td>GaAs</td>
<td>1.8 \times 10^{6}</td>
</tr>
</tbody>
</table>
Intrinsic and Extrinsic Semiconductor

Intrinsic: \[ E_{Fi} = \frac{E_C + E_V}{2} - \frac{1}{2} k_B T \ln\left(\frac{N_C}{N_V}\right) \]

n-type semiconductor

p-type semiconductor

Electron Energy

\[ E_C \quad E_v \]

\[ \sim 0.05 \text{ eV} \]

B– B– B– B– B–

~0.05 eV

VB

Electron energy

B atom sites every \( 10^6 \) Si atoms

\[ x \quad \text{Distance into crystal} \]
Exercise: Fermi Levels in Semiconductors

a) Where is the Fermi level of intrinsic bulk Si at room temperature?
b) What kind of dopants can make it n-type?
c) If the donor concentration $N_d$ is $10^{16}$ cm$^{-3}$, where will the Fermi level be?
d) If the wafer is compensation-doped with boron ($N_a = 2 \times 10^{17}$ cm$^{-3}$), where will the Fermi level be?

Properties of Selected Semiconductors at 300 K

$\varepsilon_r(0)$ and $\varepsilon_r(\infty)$ represent the relative permittivity at dc (low frequency) and at optical (high) frequencies. $\varepsilon_r(\infty)$ excludes ionic polarization but includes electronic polarization. Effective mass related to conductivity ($a$) is different than that related to the density of states ($b$).

<table>
<thead>
<tr>
<th>Property</th>
<th>Ge</th>
<th>Si</th>
<th>GaAs</th>
<th>In$<em>{0.53}$Ga$</em>{0.47}$As</th>
<th>InP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density g cm$^{-3}$</td>
<td>5.33</td>
<td>2.33</td>
<td>5.32</td>
<td>6.15</td>
<td>4.81</td>
</tr>
<tr>
<td>$E_g$ (eV)</td>
<td>0.66</td>
<td>1.12</td>
<td>1.42</td>
<td>0.75</td>
<td>1.35</td>
</tr>
<tr>
<td>$n_e$ (cm$^{-3}$)</td>
<td>$2.4 \times 10^{13}$</td>
<td>$1.45 \times 10^{16}$</td>
<td>$1.8 \times 10^{6}$</td>
<td>$1.2 \times 10^7$</td>
<td></td>
</tr>
<tr>
<td>$N_e$ (cm$^{-3}$)</td>
<td>$1.04 \times 10^{19}$</td>
<td>$2.8 \times 10^{19}$</td>
<td>$4.7 \times 10^{17}$</td>
<td>$5.4 \times 10^{17}$</td>
<td></td>
</tr>
<tr>
<td>$N_d$ (cm$^{-3}$)</td>
<td>$6 \times 10^{16}$</td>
<td>$1.02 \times 10^{19}$</td>
<td>$7 \times 10^{18}$</td>
<td>$1.2 \times 10^{19}$</td>
<td></td>
</tr>
<tr>
<td>$\varepsilon_r(0)$</td>
<td>16</td>
<td>11.9</td>
<td>13.1; 10.6</td>
<td>12.5; 9.3</td>
<td></td>
</tr>
<tr>
<td>$\varepsilon_r(\infty)$</td>
<td>0.07$a,b$</td>
<td>0.07$a,b$</td>
<td>0.07$a,b$</td>
<td>0.07$a,b$</td>
<td></td>
</tr>
<tr>
<td>$m_e^*/m_e$</td>
<td>0.12$a$</td>
<td>0.26$a$</td>
<td>0.40$a$</td>
<td>0.40$a$</td>
<td></td>
</tr>
<tr>
<td>$m_h^*/m_e$</td>
<td>0.56$b$</td>
<td>1.08$b$</td>
<td>0.56$b$</td>
<td>0.56$b$</td>
<td></td>
</tr>
<tr>
<td>$\mu_e$ (cm$^2$ V$^{-1}$ s$^{-1}$)</td>
<td>3900</td>
<td>1350</td>
<td>8500</td>
<td>13800</td>
<td></td>
</tr>
<tr>
<td>$\mu_h$ (cm$^2$ V$^{-1}$ s$^{-1}$)</td>
<td>1900</td>
<td>450</td>
<td>400</td>
<td>400</td>
<td></td>
</tr>
</tbody>
</table>

**TABLE 15.1-2** A Section of the Periodic Table

<table>
<thead>
<tr>
<th>II</th>
<th>III</th>
<th>IV</th>
<th>V</th>
<th>VI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zinc (Zn)</td>
<td>Aluminum (Al)</td>
<td>Silicon (Si)</td>
<td>Phosphorus (P)</td>
<td>Sulfur (S)</td>
</tr>
<tr>
<td>Cadmium (Cd)</td>
<td>Gallium (Ga)</td>
<td>Germanium (Ge)</td>
<td>Arsenic (As)</td>
<td>Selenium (Se)</td>
</tr>
<tr>
<td>Mercury (Hg)</td>
<td>Indium (In)</td>
<td>Antimony (Sb)</td>
<td>Tellurium (Te)</td>
<td></td>
</tr>
</tbody>
</table>
Quasi Equilibrium

— What happens to the Fermi levels during photon absorption

Probability of occupancy for electrons:

\[
f_c(E) = \frac{1}{\exp\left(\frac{E - E_{F_c}}{k_B T}\right) + 1}
\]

Probability of occupancy for holes:

\[
f_v(E) = \frac{1}{\exp\left(\frac{E_{F_v} - E}{k_B T}\right) + 1}
\]

How to calculate the quasi Fermi levels?
Quasi-Fermi Levels

The figure below shows positions of quasi-Fermi levels as a function of photo-generated electron-hole pair density. The semiconductor is n-type GaAs with $N_D = 10^{15}$ cm$^{-3}$.

Q: Why does $\varepsilon_{fp}$ decrease gradually with increasing density while $\varepsilon_{fn}$ shows a sudden increase?
A n-type \((n_0 = 5 \times 10^{18} \text{ m}^{-3})\) GaAs is under optical excitation generating excess carrier concentration \(N = n - n_0 = p - p_0\). It has the following recombination coefficients: \(A = 5 \times 10^5 \text{ s}^{-1}\), \(B = 8 \times 10^{-17} \text{ m}^3\text{s}^{-1}\), and \(C = C_e + C_h = 5 \times 10^{-42} \text{ m}^6\text{s}^{-1}\). Assume that \(C_e = C_h = C/2\). (1) Find the range of \(N\) where each of the three different recombination processes (Shockley-Read, bimolecular, Auger) dominates. (2) Plot the spontaneous carrier lifetime \(\tau_s\) as a function of \(N\) for \(10^{18} \leq N \leq 10^{26} \text{ m}^{-3}\). (3) Assume only the bimolecular recombination process is radiative, plot the internal quantum efficiency vs \(N\).
Bimolecular Recombination and Steady-State Concentration

Rate of recombination

\[ R = Bnp \quad \left( \frac{1}{\text{cm}^3 \cdot \text{sec}} \right) \]

In thermal equilibrium, generation = recombination

\[ G_0 = Bn_0p_0 \quad \left( \frac{1}{\text{cm}^3 \cdot \text{sec}} \right) \]

With electron-hole injection (by external current or photon)

Net radiative recombination rate

\[ R = Bnp - G_0 = \frac{N}{\tau_{rad}} \]

\[ \tau_{rad} = \frac{1}{B(N + n_0 + p_0)} \]

In steady state:

\[ \frac{dN}{dt} = G - \frac{N}{\tau_{rad}} = 0 \]

→ Determines \( N \) if \( G \) is known, and therefore the quasi-Fermi levels.
Exercise: Carrier Injection at Steady State

Electron-hole pairs are injected into n-type GaAs at a rate $G = 10^{23}/\text{cm}^3\text{s}$. At room temperature GaAs has the following parameters: $E_g = 1.42 \text{ eV}$, $n_i = 2.33 \times 10^6 \text{ cm}^{-3}$, $N_c = 4.35 \times 10^{17} \text{ cm}^{-3}$, and $N_v = 9.41 \times 10^{18} \text{ cm}^{-3}$. The thermal equilibrium concentration of electrons is $n_0 = 10^{16} \text{ cm}^{-3}$. Assume bimolecular recombination process dominates and the coefficient for bimolecular recombination $B = 8 \times 10^{-11} \text{ cm}^3\text{s}^{-1}$. Determine:

(a) The thermal equilibrium concentration of holes $p_0$.

(b) The steady-state excess carrier concentration $N$.

(c) The recombination lifetime $\tau_{\text{rad}}$.

(d) The separation between the quasi-Fermi levels $E_{Fc} - E_{Fp}$. 
The p-n Junction

**Build-in field**

\[ E_0 = -\frac{eN_d W_n}{\varepsilon} = -\frac{eN_a W_p}{\varepsilon} \]

**Built-in potential**

\[ V_0 = -\frac{1}{2} E_0 (W_n + W_p) \]

\[ = k_B T \frac{e}{\ln \left( \frac{N_a N_d}{n_i^2} \right)} \]

**Depletion widths**

\[ W_n = \sqrt{\frac{2e N_a}{e N_d \left( \frac{1}{N_d + N_a} \right)} V_0} \]

\[ W_p = \sqrt{\frac{2e N_d}{e N_a \left( \frac{1}{N_d + N_a} \right)} V_0} \]

\[ W_0 = W_n + W_p \]

\[ = \sqrt{\frac{2e N_a + N_d}{e N_a N_d} V_0} \]
Figure 12.9  Spatial distributions of the p and n regions, the energy bands, and the electrostatic potential of an abrupt p–n homojunction (a) in thermal equilibrium, (b) under forward bias, and (c) under reverse bias.
**p-n Junction Under Forward Bias**

**Law of the junction**

\[ p_n(0) = p_{n0} \exp\left(\frac{eV}{k_B T}\right) \]

\[ n_p(0) = n_{p0} \exp\left(\frac{eV}{k_B T}\right) \]

**Excess minority carrier concentration**

\[ \Delta p_n(x') = \Delta p_n(0) \exp\left(-\frac{x'}{L_h}\right) \]

\[ \Delta n_p(x'') = \Delta n_p(0) \exp\left(\frac{x''}{L_e}\right) \]

**Diffusion length**

\[ L_{h,e} = \sqrt{D_{h,e} \tau_{h,e}} \]

- \( D_{h,e} \): Diffusion coefficient
- \( \tau_{h,e} \): Minority carrier lifetime
Current in Forward-biased p-n Junction

The total current anywhere in the device is constant. Just outside the depletion region it is due to the diffusion of minority carriers.

Diffusion current

\[
J_{D,\text{hole}} = \left( \frac{eD_h n_i^2}{L_h N_d} \right) \exp \left( \frac{eV}{k_B T} \right) - 1
\]

\[
J_{D,\text{elec}} = \left( \frac{eD_e n_i^2}{L_e N_a} \right) \exp \left( \frac{eV}{k_B T} \right) - 1
\]

\[
J_{\text{diff}} = J_{D,\text{hole}} + J_{D,\text{elec}}
= \left( \frac{eD_h}{L_h N_d} + \frac{eD_e}{L_e N_a} \right) n_i^2 \exp \left( \frac{eV}{k_B T} \right) - 1
\]

Recombination current

A more accurate result:

\[
J_{\text{recom}} = J_{r0} \left[ \exp \left( \frac{eV}{2k_B T} \right) - 1 \right]
\]
I-V Characteristics of a p-n Junction

Reverse I-V characteristics of a pn junction (the positive and negative current axes have different scales)

\[ I = I_0 \left[ \exp \left( \frac{eV}{\eta k_B T} \right) - 1 \right] \]

η: Diode ideality factor
η = 1: Diffusion controlled
η = 2: SCL recombination controlled

Shockley equation
Space charge layer generation.
p-n Junction under Reverse Bias

Current due to thermally generated EHP:

\[
J_{gen} = \frac{eWn_i}{\tau_g}
\]

\(\tau_g\) : Mean thermal generation time

Total reverse current

\[
J_{rev} \approx J_s + J_{gen}
\]

\[
= \left( \frac{eD_h}{L_h N_d} + \frac{eD_e}{L_e N_a} \right) n_i^2 + \frac{eWn_i}{\tau_g}
\]

Minority Carrier Concentration

Hole PE(x)

Electrons → Holes

Diffusion → Drift

\(n_{po}\)

\(\rho_{no}\)

\(+\)

\(-\)

\(V_r\)

Thermally generated EHP

Neutral \(p\)-region

Neutral \(n\)-region

\(E_o + E\)

\(W\)

\(W_o\)

\(W(V = -V_r)\)
Exercise: GaAs p-n Junction

• Device parameters:
  – Cross sectional area $A = 1 \text{ mm}^2$.
  – $N_a$ (p-side doping) = $N_d$ (n-side doping) = $10^{23} \text{ m}^{-3}$.
  – Coefficient of recombination $B = 7.21 \times 10^{-16} \text{ m}^3\text{s}^{-1}$
  – $n_i = 1.8 \times 10^{12} \text{ m}^{-3}$
  – $\varepsilon_r = 13.2$
  – $\mu_h$ (in the n-side) = 250 cm$^2$V$^{-1}$s$^{-1}$, $\mu_e$ (in the p-side) = 5000 cm$^2$V$^{-1}$s$^{-1}$
  – Carrier recombination time in the depletion region = 10 ns

• What is the I-V characteristics? Calculate the diffusion current and the recombination current under 1V bias.