Chapter 1  Electrons and Holes in Semiconductors

1.1 Silicon Crystal Structure

- **Unit cell** of silicon crystal is cubic.
- **Each Si atom has 4 nearest neighbors.**
Silicon Wafers and Crystal Planes

- The standard notation for crystal planes is based on the cubic unit cell.

- Silicon wafers are usually cut along the (100) plane with a flat or notch to help orient the wafer during IC fabrication.
1.2 Bond Model of Electrons and Holes

- Silicon crystal in a two-dimensional representation.

- When an electron breaks loose and becomes a *conduction electron*, a *hole* is also created.
Dopants in Silicon

- As, a Group V element, introduces conduction electrons and creates **N-type silicon**, and is called a **donor**.
- B, a Group III element, introduces holes and creates **P-type silicon**, and is called an **acceptor**.
- Donors and acceptors are known as dopants. Dopant ionization energy ~50meV (very low).

Hydrogen:  \[ E_{\text{ion}} = \frac{m_0 q^4}{8\varepsilon_0^2 h^2} = 13.6 \text{ eV} \]
• GaAs has the same crystal structure as Si.
• GaAs, GaP, GaN are III-V compound semiconductors, important for optoelectronics.
• Which group of elements are candidates for donors? acceptors?
1.3 Energy Band Model

- Energy states of Si atom (a) expand into energy bands of Si crystal (b).
- The lower bands are filled and higher bands are empty in a semiconductor.
- The highest filled band is the \textit{valence band}.
- The lowest empty band is the \textit{conduction band}.
1.3.1 Energy Band Diagram

- **Energy band diagram** shows the bottom edge of conduction band, $E_c$, and top edge of valence band, $E_v$.
- $E_c$ and $E_v$ are separated by the **band gap energy**, $E_g$. 
Measuring the Band Gap Energy by Light Absorption

- $E_g$ can be determined from the minimum energy ($h \nu$) of photons that are absorbed by the semiconductor.

Bandgap energies of selected semiconductors

<table>
<thead>
<tr>
<th>Semiconductor</th>
<th>InSb</th>
<th>Ge</th>
<th>Si</th>
<th>GaAs</th>
<th>GaP</th>
<th>ZnSe</th>
<th>Diamond</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_g$ (eV)</td>
<td>0.18</td>
<td>0.67</td>
<td>1.12</td>
<td>1.42</td>
<td>2.25</td>
<td>2.7</td>
<td>6</td>
</tr>
</tbody>
</table>
1.3.2 Donor and Acceptor in the Band Model

![Diagram showing the energy band structure with conduction and valence bands, donor and acceptor levels.

Ionization energy of selected donors and acceptors in silicon

<table>
<thead>
<tr>
<th>Dopant</th>
<th>Donors</th>
<th>Acceptors</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Sb</td>
<td>P</td>
</tr>
<tr>
<td>Ionization energy, $E_c - E_d$ or $E_a - E_v$ (meV)</td>
<td>39</td>
<td>44</td>
</tr>
</tbody>
</table>
1.4 Semiconductors, Insulators, and Conductors

- Totally filled bands and totally empty bands do not allow current flow. (Just as there is no motion of liquid in a totally filled or totally empty bottle.)
- Metal conduction band is half-filled.
- Semiconductors have lower $E_g$'s than insulators and can be doped.

\[ E_c - E_g = 1.1 \text{ eV} \]
\[ E_c - E_g = 9 \text{ eV} \]
1.5 Electrons and Holes

- Both electrons and holes tend to seek their lowest energy positions.
- Electrons tend to fall in the energy band diagram.
- Holes float up like bubbles in water.
1.5.1 Effective Mass

The electron wave function is the solution of the three-dimensional Schrödinger wave equation:

\[-\frac{\hbar^2}{2m_0} \nabla^2 \psi + V(r) \psi = \psi\]

The solution is of the form \(\exp(\pm k \cdot r)\)

\(k = \) wave vector = \(2\pi/\)electron wavelength

For each \(k\), there is a corresponding \(E\).

\[\text{acceleration} = -\frac{q \varepsilon}{\hbar^2} \frac{d^2E}{dk^2} = \frac{F}{m}\]

\[\text{effective mass} \equiv \frac{\hbar^2}{d^2E / dk^2}\]
1.5.1 Effective Mass

In an electric field, $E$, an electron or a hole accelerates.

$$a = \frac{-qE}{m_n}, \quad \text{electrons}$$

$$a = \frac{qE}{m_p}, \quad \text{holes}$$

Electron and hole effective masses

<table>
<thead>
<tr>
<th></th>
<th>Si</th>
<th>Ge</th>
<th>GaAs</th>
<th>InAs</th>
<th>AlAs</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_n/m_0$</td>
<td>0.26</td>
<td>0.12</td>
<td>0.068</td>
<td>0.023</td>
<td>2</td>
</tr>
<tr>
<td>$m_p/m_0$</td>
<td>0.39</td>
<td>0.3</td>
<td>0.5</td>
<td>0.3</td>
<td>0.3</td>
</tr>
</tbody>
</table>
1.5.2 How to Measure the Effective Mass

Cyclotron Resonance Technique

Centripetal force = Lorentzian force

\[
\frac{m_n v^2}{r} = qvB
\]

\[
v = \frac{qBr}{m_n}
\]

\[
f_{cr} = \frac{v}{2\pi r} = \frac{qB}{2\pi m_n}
\]

- \(f_{cr}\) is the Cyclotron resonance frequency.
- It is independent of \(v\) and \(r\).
- Electrons strongly absorb microwaves of that frequency.
- By measuring \(f_{cr}\), \(m_n\) can be found.
1.6 Density of States

\[ D_c(E) = \frac{\text{number of states in } \Delta E}{\Delta E \cdot \text{volume}} \left( \frac{1}{\text{eV} \cdot \text{cm}^3} \right) \]

\[ D_c(E) = \frac{8\pi m_n \sqrt{2m_n (E - E_c)}}{h^3} \]

\[ D_v(E) = \frac{8\pi m_p \sqrt{2m_p (E_v - E)}}{h^3} \]

Derived in Appendix I
1.7 Thermal Equilibrium and the Fermi Function

1.7.1 An Analogy for Thermal Equilibrium

- There is a certain probability for the electrons in the conduction band to occupy high-energy states under the agitation of thermal energy.
Appendix II. Probability of a State at E being Occupied

• There are $g_1$ states at $E_1$, $g_2$ states at $E_2$… There are $N$ electrons, which constantly shift among all the states but the average electron energy is fixed at $3kT/2$.

• There are many ways to distribute $N$ among $n_1$, $n_2$, $n_3$…. and satisfy the $3kT/2$ condition.

• The equilibrium distribution is the distribution that maximizes the number of combinations of placing $n_1$ in $g_1$ slots, $n_2$ in $g_2$ slots….:

\[
\frac{n_i}{g_i} = \frac{1}{1 + e^{(E - E_F)/kT}}
\]

$E_F$ is a constant determined by the condition $\sum n_i = N$.
1.7.2 Fermi Function–The Probability of an Energy State Being Occupied by an Electron

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

\( E_f \) is called the **Fermi energy** or the **Fermi level**.

Boltzmann approximation:

\[ f(E) \approx e^{-(E-E_f)/kT} \quad E - E_f >> kT \]

\[ f(E) \approx 1 - e^{-(E_f-E)/kT} \quad E - E_f << -kT \]

**Remember:** there is only one Fermi-level in a system at equilibrium.
1.8 Electron and Hole Concentrations

1.8.1 Derivation of $n$ and $p$ from $D(E)$ and $f(E)$

$$n = \int_{E_c}^{\text{top of conduction band}} f(E) D_c(E) dE$$

$$n = \frac{8\pi m_n \sqrt{2m_n}}{h^3} \int_{E_c}^{\infty} \sqrt{E - E_c} e^{-\frac{(E-E_f)}{kT}} dE$$

$$= \frac{8\pi m_n \sqrt{2m_n}}{h^3} e^{-\frac{(E_c-E_f)}{kT}} \int_{0}^{E-E_c} \sqrt{E - E_c} e^{-\frac{(E-E_c)}{kT}} d(E-E_c)$$
Electron and Hole Concentrations

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

\[ N_c \equiv 2 \left[ \frac{2\pi m_n kT}{h^2} \right]^{3/2} \]

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

\[ N_v \equiv 2 \left[ \frac{2\pi m_p kT}{h^2} \right]^{3/2} \]

Remember: the closer \( E_f \) moves up to \( N_c \), the larger \( n \) is; the closer \( E_f \) moves down to \( E_v \), the larger \( p \) is.

For Si, \( N_c = 2.8 \times 10^{19} \text{ cm}^{-3} \) and \( N_v = 1.04 \times 10^{19} \text{ cm}^{-3} \).
1.8.2 The Fermi Level and Carrier Concentrations

Where is $E_f$ for $n = 10^{17}$ cm$^{-3}$? And for $p = 10^{14}$ cm$^{-3}$?

**Solution:**

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

\[ E_c - E_f = kT \ln\left(\frac{N_c}{n}\right) = 0.026 \ln\left(\frac{2.8 \times 10^{19}}{10^{17}}\right) = 0.146 \text{ eV} \]

(b) For $p = 10^{14}$ cm$^{-3}$, from Eq.(1.8.8),

\[ E_f - E_v = kT \ln\left(\frac{N_v}{p}\right) = 0.026 \ln\left(\frac{1.04 \times 10^{19}}{10^{14}}\right) = 0.31 \text{ eV} \]
1.8.2 The Fermi Level and Carrier Concentrations

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

\[ E_f = E_c - kT \ln \left( \frac{N_c}{n} \right) \]

Graph showing the relationship between the Fermi level and carrier concentrations at different temperatures (300K, 400K) for donor-doped and acceptor-doped materials. The graph includes a logarithmic scale for the carrier concentrations.
1.8.3 The *np* Product and the Intrinsic Carrier Concentration

Multiply \( n = N_c e^{-\frac{(E_c - E_f)}{kT}} \) and \( p = N_v e^{-\frac{(E_f - E_v)}{kT}} \)

\[
np = N_c N_v e^{-\frac{(E_c - E_v)}{kT}} = N_c N_v e^{-\frac{E_g}{kT}}
\]

\[
np = n_i^2
\]

\[
n_i = \sqrt{N_c N_v e^{-\frac{E_g}{2kT}}}
\]

- In an intrinsic (undoped) semiconductor, \( n = p = n_i \).
- \( n_i \) is the **intrinsic carrier concentration**, \( \sim 10^{10} \text{ cm}^{-3} \) for Si.
**EXAMPLE: Carrier Concentrations**

**Question:** What is the hole concentration in an N-type semiconductor with $10^{15}$ cm$^{-3}$ of donors?

**Solution:** $n = 10^{15}$ cm$^{-3}$.

$$p = \frac{n_i^2}{n} \approx \frac{10^{20} \text{ cm}^{-3}}{10^{15} \text{ cm}^{-3}} = 10^5 \text{ cm}^{-3}$$

After increasing $T$ by 60 °C, $n$ remains the same at $10^{15}$ cm$^{-3}$ while $p$ increases by about a factor of 2300 because $n_i^2 \propto e^{-E_g/kT}$.

**Question:** What is $n$ if $p = 10^{17}$ cm$^{-3}$ in a P-type silicon wafer?

**Solution:**

$$n = \frac{n_i^2}{p} \approx \frac{10^{20} \text{ cm}^{-3}}{10^{17} \text{ cm}^{-3}} = 10^3 \text{ cm}^{-3}$$
**1.9 General Theory of n and p**

**EXAMPLE: Complete ionization of the dopant atoms**

\( N_d = 10^{17} \text{ cm}^{-3} \). What fraction of the donors are not ionized?

**Solution:** First assume that all the donors are ionized.

\[
n = N_d = 10^{17} \text{ cm}^{-3} \Rightarrow E_f = E_c - 146 \text{ meV}
\]

\[
\text{Probability of not being ionized} \approx \frac{1}{1 + \frac{1}{2} e^{(E_d - E_f)/kT}} = \frac{1}{1 + \frac{1}{2} e^{((146-45)\text{meV})/26\text{meV}}} = 0.04
\]

Therefore, it is reasonable to assume complete ionization, i.e., \( n = N_d \).
1.9 General Theory of n and p

Charge neutrality: \( n + N_a = p + N_d \)

\[
np = n_i^2
\]

\[
p = \frac{N_a - N_d}{2} + \left[ \left( \frac{N_a - N_d}{2} \right)^2 + n_i^2 \right]^{1/2}
\]

\[
n = \frac{N_d - N_a}{2} + \left[ \left( \frac{N_d - N_a}{2} \right)^2 + n_i^2 \right]^{1/2}
\]
1.9 General Theory of on n and p

I. \( N_d - N_a \gg n_i \) (i.e., N-type)
   \[
   \begin{align*}
   n &= N_d - N_a \\
   p &= \frac{n_i^2}{n}
   \end{align*}
   \]

   If \( N_d \gg N_a \), \( n = N_d \) and \( p = \frac{n_i^2}{N_d} \)

II. \( N_a - N_d \gg n_i \) (i.e., P-type)
   \[
   \begin{align*}
   p &= N_a - N_d \\
   n &= \frac{n_i^2}{p}
   \end{align*}
   \]

   If \( N_a \gg N_d \), \( p = N_a \) and \( n = \frac{n_i^2}{N_a} \)
EXAMPLE: Dopant Compensation

What are \( n \) and \( p \) in Si with (a) \( N_d = 6 \times 10^{16} \text{ cm}^{-3} \) and \( N_a = 2 \times 10^{16} \text{ cm}^{-3} \) and (b) additional \( 6 \times 10^{16} \text{ cm}^{-3} \) of \( N_a \)?

(a) \( n = N_d - N_a = 4 \times 10^{16} \text{ cm}^{-3} \)
\[ p = n_i^2 / n = 10^{20} / 4 \times 10^{16} = 2.5 \times 10^3 \text{ cm}^{-3} \]

(b) \( N_a = 2 \times 10^{16} + 6 \times 10^{16} = 8 \times 10^{16} \text{ cm}^{-3} > N_d \)
\[ p = N_a - N_d = 8 \times 10^{16} - 6 \times 10^{16} = 2 \times 10^{16} \text{ cm}^{-3} \]
\[ n = n_i^2 / p = 10^{20} / 2 \times 10^{16} = 5 \times 10^3 \text{ cm}^{-3} \]
1.10 Carrier Concentrations at Extremely High and Low Temperatures

\[ n = N_d \]

\[ n = n_i = \sqrt{N_c N_v} e^{-E_g/2kT} \] (high T)

\[ n = \left( \frac{N_c N_d}{2} \right)^{1/2} e^{-(E_c-E_d)/2kT} \] (low T)
Infrared Detector Based on Freeze-out

• To image the black-body radiation emitted by tumors requires a photodetector that responds to $h\nu$'s around 0.1 eV.

• In doped Si operating in the freeze-out mode, conduction electrons are created when the infrared photons provide the energy to ionize the donor atoms.
1.11 Chapter Summary

Energy band diagram. Acceptor. Donor. $m_n$, $m_p$. 
Fermi function. $E_f$.

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

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

\[ n = N_d - N_a \]

\[ p = N_a - N_d \]

\[ np = n_i^2 \]