EE 232 Lightwave Devices
Lecture 3: Basic Semiconductor Physics and Optical Processes

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Optical Properties of Semiconductors

- Optical transitions
  - Absorption: exciting an electron to a higher energy level by absorbing a photon
  - Emission: electron relaxing to a lower energy state by emitting a photon
Band-to-Band Transition

- Since most electrons and holes are near the band-edges, the photon energy of band-to-band (or interband) transition is approximately equal to the bandgap energy:

\[ h\nu = E_g \]

- The optical wavelength of band-to-band transition can be approximated by

\[ \lambda = \frac{c}{\nu} = \frac{hc}{E_g} \approx \frac{1.24}{E_g} \]

\( \lambda \) : wavelength in \( \mu m \)

\( E_g \) : energy bandgap in eV
Energy Band Diagram in Real Space and k-Space

**Real Space**

- Electron energy: $E_e = E_C + \frac{1}{2} m_e v^2$
- Hole energy: $E_h = E_V - \frac{1}{2} m_h v^2$

**K-Space**

- Electron energy: $E_e = E_C + \frac{\hbar^2 k^2}{2m_e}$
- Hole energy: $E_h = E_V - \frac{\hbar^2 k^2}{2m_h}$

Effective Mass Approximation:

- Electron momentum: $\hbar k = m_e v_e$
Bloch Theorem

\[ V(\mathbf{r}) = V(\mathbf{r} + \mathbf{R}) \]

\[ \psi(\mathbf{r}) = u(\mathbf{r}) e^{i k \cdot \mathbf{r}} \quad \text{(Bloch Theorem)} \]
Bloch Theorem (1D proof)

Linear chain of N periodic atoms

\[ |\psi(x + a)|^2 = |\psi(x)|^2 \]

\[ \psi(x + a) = C\psi(x), \quad |C| = 1 \]

Periodic Boundary Condition:

\[ \psi(x + Na) = \psi(x) \]

\[ \psi(x + Na) = C^N \psi(x) = \psi(x) \]

\[ C^N = 1 \quad \Rightarrow \quad C = e^{\frac{i2\pi s}{Na}}, \quad s = 1..N - 1 \]
Bloch Theorem (1D proof)

\[ \psi(x + a) = C \psi(x) = e^{\frac{i2\pi s}{Na}} \psi(x) = e^{ika} \psi(x) \]

where \( k = \frac{2\pi s}{Na} \)

Multiply both sides of the above equation by \( e^{-ik(x+a)} \):

\[ e^{-ik(x+a)} \psi(x + a) = e^{-ik(x+a)} e^{ika} \psi(x) = e^{-ikx} \psi(x) \]

Define \( u(x) \equiv e^{-ikx} \psi(x) \rightarrow u(x + a) = u(x) \)

\[ \Rightarrow \psi(x) = e^{ikx} u(x) \]
Conservation of Energy and Momentum

- Conditions for optical absorption and emission:
  - Conservation of energy
    \[ E_2 - E_1 = h \nu \]
  - Conservation of momentum
    \[ k_2 - k_1 = k_{hv} \]
    \[ k_2, k_1 \sim \frac{2\pi}{a} \]
    \[ k_{hv} \sim \frac{2\pi}{\lambda} \]
    \[ (a \sim 0.5\text{nm}) \ll (\lambda \sim 1\mu\text{m}) \]
    \[ \Rightarrow \quad k_2 = k_1 \]

Optical transitions are "vertical" lines
Direct vs Indirect Bandgaps

- **Direct bandgap materials**
  - CB minimum and VB maximum occur at the same k
  - Examples
    - GaAs, InP, InGaAsP
    - \((\text{Al}_x\text{Ga}_{1-x})\text{As}, x < 0.45\)

- **Indirect bandgap materials**
  - CB minimum and VB maximum occur at different k
  - Example
    - Si, Ge
    - \((\text{Al}_x\text{Ga}_{1-x})\text{As}, x > 0.45\)
    - Not “optically active”
Absorption Coefficient

- Light intensity decays exponentially in semiconductor:
  \[ I(x) = I_0 e^{-\alpha x} \]

- Direct bandgap semiconductor has a sharp absorption edge

- Si absorbs photons with \( h\nu > E_g = 1.1 \text{ eV} \), but the absorption coefficient is small
  - Sufficient for CCD

- At higher energy (~ 3 eV), absorption coefficient of Si becomes large again, due to direct bandgap transition to higher CB
Band-to-Band Transition

Absorption
Photodetectors; Solar Cells

Spontaneous Emission
LED

Stimulated Emission
Optical Amplifiers; Semiconductor Lasers

$\hbar \nu ~ \sim ~ \sim ~ \sim ~ \sim ~ \sim$

$\hbar \nu$
Density of states in k-space (1D)

Linear chain of N periodic atoms in k-space

Number of states per unit length:

\[ N = \frac{2}{L_x} \sum_{k_x} \rightarrow \frac{2}{L_x} \int \frac{1}{\frac{2\pi}{Na}} dk = \frac{2}{L_x} \int \frac{1}{\frac{2\pi}{L_x}} dk = \frac{2}{L_x} \int \frac{L_x}{2\pi} dk = 2 \int \frac{1}{2\pi} dk \]

(Factor of two from spin degeneracy)
Density of states in k-space (2D and 3D)

Number of states per unit area (2D crystal):

\[ N = \frac{2}{L_x L_y} \sum_{k_x} \sum_{k_y} \rightarrow \frac{2}{L_x L_y} \int \frac{L_x L_y}{(2\pi)^2} d^2k = \int \frac{2}{(2\pi)^2} d^2k \]

Number of states per unit volume (3D crystal):

\[ N = \frac{2}{L_x L_y L_z} \sum_{k_x} \sum_{k_y} \sum_{k_z} \rightarrow \frac{2}{L_x L_y L_z} \int \frac{L_x L_y L_z}{(2\pi)^3} d^3k = \int \frac{2}{(2\pi)^3} d^3k \]
Density of States for CB

- Number of electron states between $E$ and $E + \Delta E$ per unit volume

\[
N = 2 \int \frac{1}{(2\pi)^3} d^3k = 2 \int \frac{4\pi k^2}{(2\pi)^3} dk = \int \frac{k^2}{\pi^2} dk = \int \rho_k(k) dk
\]

\[
\rho_k(k)dk = \frac{k^2}{\pi^2} dk \quad \text{Convert to } \rho_e(E)dE
\]

\[
E = E_C + \frac{\hbar^2 k^2}{2m_e} \Rightarrow dE = \frac{\hbar^2 k}{m_e} dk \quad \text{and} \quad k = \frac{\sqrt{2m_e(E - E_C)}}{\hbar}
\]

\[
\frac{k^2}{\pi^2} dk = \frac{k}{\pi^2} kdk = \frac{k}{\pi^2} \left( \frac{m_e^*}{\hbar^2} dE \right) = \frac{m_e^*}{\hbar^2 \pi^2} \frac{\sqrt{2m_e(E - E_C)}}{\hbar} dE = \rho_e(E)dE
\]

\[
\rho_e(E) = \frac{1}{2\pi^2} \left( \frac{2m_e^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_C}
\]
Density of States for VB

• The density of states for VB can be derived in a similar way

\[ \rho_h(E) = \frac{1}{2\pi^2} \left( \frac{2m^*_h}{\hbar^2} \right)^{3/2} \sqrt{E_V - E} \]
Review of Semiconductor Physics

Electron and hole concentrations:

\[
n = \int_{E_c}^{\infty} f_n(E) \rho_e(E) \, dE
\]

\[
p = \int_{-\infty}^{E_v} f_p(E) \rho_h(E) \, dE
\]

Fermi-Dirac distributions:

\[
f_n(E) = \frac{1}{1 + \exp \left( \frac{E - F_n}{k_B T} \right)}
\]

\[
f_p(E) = \frac{1}{1 + \exp \left( \frac{F_p - E}{k_B T} \right)}
\]

\[F_n : \text{electron quasi-Fermi level}\]

\[F_p : \text{hole quasi-Fermi level}\]
Electron and Hole Concentrations

\[ n = \int_{E_C}^{\infty} f_n(E)\rho_e(E)\,dE = \int_{E_C}^{\infty} \frac{1}{1 + \exp \left( \frac{E - F_n}{k_B T} \right)} \frac{1}{2\pi^2} \left( \frac{2m_e^*}{\hbar} \right)^2 \sqrt{E - E_C} \,dE \]

\[ n = N_C \cdot F_{1/2} \left( \frac{F_n - E_C}{k_B T} \right) \]

\[ N_C = 2 \left( \frac{2\pi m_e^* k_B T}{\hbar^2} \right)^{3/2} \]

\[ p = N_V \cdot F_{1/2} \left( \frac{E_V - F_p}{k_B T} \right) \]

\[ N_V = 2 \left( \frac{2\pi m_h^* k_B T}{\hbar^2} \right)^{3/2} \]

Fermi-Dirac Integral

\[ F_j(\eta) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{x^j}{1 + e^{x-\eta}} \,dx \]

Gamma Function

\[ \Gamma\left(\frac{3}{2}\right) = \frac{\sqrt{\pi}}{2} \]
Approximation of Electron/Hole Concentration

\[ F_j(\eta) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{x^j}{1 + e^{x - \eta}} dx \approx \begin{cases} e^\eta & \text{when } \eta \ll 1 \\ \frac{4}{3} \left( \frac{\eta^3}{\pi} \right)^{1/2} & \text{when } \eta \gg 1 \end{cases} \]

(1) When \( F_n \ll E_C \) (Boltzmann approximation)

\[ n \approx N_C \cdot e^{-\frac{(E_C - F_n)}{k_BT}} \]

(2) When \( F_n \gg E_C \) (Degenerate)

\[ n \approx N_C \cdot 4 \left( \frac{F_n - E_C}{k_BT} \right)^{3/2} \cdot \frac{3\sqrt{\pi}}{k_BT} \]

\[ \frac{n}{N_C} \]

Boltzmann Approx

Degenerate

Quasi-Fermi Level Cross Band Edge
## Typical Values of Density of States

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>Germanium</th>
<th>Silicon</th>
<th>Gallium Arseneide</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy bandgap at 300 K</td>
<td>$E_g$ (eV)</td>
<td>0.66</td>
<td>1.12</td>
<td>1.424</td>
</tr>
<tr>
<td>Effective mass for density of states calculations</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Electrons</td>
<td>$m^*_{,dos}/m_0$</td>
<td>0.56</td>
<td>1.08</td>
<td>0.067</td>
</tr>
<tr>
<td>Holes</td>
<td>$m^*_{,dos}/m_0$</td>
<td>0.29</td>
<td>0.81</td>
<td>0.47</td>
</tr>
<tr>
<td>Effective density of states in the conduction band at 300 K</td>
<td>$N_C$ (cm$^{-3}$)</td>
<td>$1.05 \times 10^{19}$</td>
<td>$2.82 \times 10^{19}$</td>
<td>$4.37 \times 10^{17}$</td>
</tr>
<tr>
<td>Effective density of states in the valence band at 300 K</td>
<td>$N_V$ (cm$^{-3}$)</td>
<td>$3.92 \times 10^{18}$</td>
<td>$1.83 \times 10^{19}$</td>
<td>$8.68 \times 10^{18}$</td>
</tr>
<tr>
<td>Intrinsic carrier density at 300 K</td>
<td>$n_i$ (cm$^{-3}$)</td>
<td>$1.83 \times 10^{13}$</td>
<td>$8.81 \times 10^9$</td>
<td>$2.03 \times 10^6$</td>
</tr>
<tr>
<td>Effective density of states in the conduction band at 100°C (373.15 K)</td>
<td>$N_C$ (cm$^{-3}$)</td>
<td>$1.46 \times 10^{19}$</td>
<td>$3.91 \times 10^{19}$</td>
<td>$6.04 \times 10^{17}$</td>
</tr>
<tr>
<td>Effective density of states in the valence band at 100°C</td>
<td>$N_V$ (cm$^{-3}$)</td>
<td>$5.44 \times 10^{18}$</td>
<td>$2.54 \times 10^{19}$</td>
<td>$1.12 \times 10^{19}$</td>
</tr>
<tr>
<td>Intrinsic carrier density at 100°C</td>
<td>$n_i$ (cm$^{-3}$)</td>
<td>$3.1 \times 10^{14}$</td>
<td>$8.55 \times 10^{11}$</td>
<td>$6.24 \times 10^8$</td>
</tr>
</tbody>
</table>