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
  \[ E_e = E_C + \frac{1}{2} m^*_e v_e^2 \]
  \[ E_h = E_V - \frac{1}{2} m^*_h v_h^2 \]

- K-Space
  \[ E_e = E_C + \frac{\hbar^2 k^2}{2m^*_e} \]
  \[ E_h = E_V - \frac{\hbar^2 k^2}{2m^*_h} \]

Effective Mass Approximation
Band-to-Band Transition

Absorption

Spontaneous Emission

Stimulated Emission

Photodetectors; Solar Cells

LED

Optical Amplifiers; Semiconductor Lasers

Conservation of Energy and Momentum

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

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"

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**Absorption Coefficient**

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

- Direct bandgap semiconductor has a sharp absorption edge

- Si absorbs photons with \(h\nu > E_g = 1.1\) 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
Review of Semiconductor Physics

Electron and hole concentrations:
\[ n = \int \rho_e(E) f_n(E) dE \]
\[ p = \int \rho_h(E) f_p(E) dE \]

Fermi-Dirac distributions:
\[ f_n(E) = \frac{1}{1 + \exp \left( \frac{E - E_F}{kT} \right)} \]
\[ f_p(E) = \frac{1}{1 + \exp \left( \frac{E_p - E}{kT} \right)} \]

\( E_F \) : electron quasi-Fermi level
\( E_p \) : hole quasi-Fermi level

Electron/Hole Density of States (1)

- Electron wave with wavevector \( k \)
  \[ e^{i\vec{k} \cdot \vec{r}} \]

- Periodic boundary conditions
  \[ e^{i\vec{k} \cdot \vec{r}} = e^{i\vec{k} \cdot (\vec{r} + \vec{L}_x \cdot \hat{x})} = e^{i\vec{k} \cdot (\vec{r} + \vec{L}_y \cdot \hat{y})} = e^{i\vec{k} \cdot (\vec{r} + \vec{L}_z \cdot \hat{z})} \]

- An electron state is defined by
  \[ (k_x, k_y, k_z) \uparrow \downarrow = \left( \frac{2\pi}{L_x} m, \frac{2\pi}{L_y} n, \frac{2\pi}{L_z} l \right) \uparrow \downarrow \]

- Number of electron states between \( k \) and \( k + \Delta k \) in k-space per unit volume
  \[ \frac{2}{V} \frac{4\pi k^2 dk}{2\pi 2\pi 2\pi} = \frac{k^2}{\pi^2} dk = \rho_e(k) dk \]
Electron/Hole Density of States (2)

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

$$E = E_c + \frac{\hbar^2 k^2}{2m_e} \Rightarrow dE = \frac{\hbar^2}{m_e} dk$$

$$\frac{k^2}{\pi^2} dk = \frac{m_e^*}{\hbar^2 \pi^2} \sqrt{\frac{2m_e^*}{\hbar}} (E - E_c) \frac{dE}{\hbar} = \rho_e(E) dE$$

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

- Likewise, hole density of states

$$\rho_h(E) = \frac{1}{2\pi^2} \left( \frac{2m_h^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_v}$$

Electron and Hole Concentrations

$$n = \int_{E_c}^{\infty} f_e(E) \rho_e(E) dE = \int_{E_c}^{\infty} \frac{1}{1 + \exp \left( \frac{E - F_n}{k_B T} \right)} \cdot \frac{1}{2\pi^2} \left( \frac{2m_e^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_c} dE$$

$$n = N_c \cdot F_{1/2} \left( \frac{E - E_c}{k_B T} \right)$$

$$N_c = 2 \left( \frac{\pi m_e^* k_B T}{2 \pi^2 \hbar^2} \right)^{3/2}$$

$$p = N_v \cdot F_{1/2} \left( \frac{E_v - F_p}{k_B T} \right)$$

$$N_v = 2 \left( \frac{\pi m_h^* k_B T}{2 \pi^2 \hbar^2} \right)^{3/2}$$

Fermi-Dirac Integral

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

Gamma Function

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

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

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

\[ n \approx N_C \cdot \exp\left(\frac{E_n - E_C}{k_BT}\right) \]

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

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

Where \( n \approx N_C \cdot \exp\left(\frac{E_n - E_C}{k_BT}\right) \) for Boltzmann approximation

\[ \frac{n}{N_C} \approx 10^9 \] for Degenerate

\[ 10^{10} \] for Quasi-Fermi Level Cross Band Edge

\[ 10^{11} \] for Boltzmann Approx

\[ 10^{12} \] for Degenerate

\[ 10^{13} \] for Quasi-Fermi Level Cross Band Edge

\[ F_n = E_C \frac{N_C}{k_BT} \]