Density of States and Band Structure

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Band Structure

In insulators, $E_g > 10eV$, empty conduction band. In metals, conduction bands are partly filled or overlapped with valence bands.

In semiconductors, $E_g$ is smaller than that of metals, so that electrons can possibly jump to conduction band. In doped semiconductors, there is an additional donor level (n doped) near the bottom of conduction band ($E_c$) or an acceptor level (p doped) near the valence band ($E_v$).
Carrier concentration

\[ n = \int_{E_C}^{\infty} g(E) f_F(E) dE \]
\[ g(E) = 4\pi \left( \frac{2m^*_n}{\hbar^2} \right)^{3/2} E^{1/2} \]

\[ p = \int_{-\infty}^{E_V} g(E) f_F(E) dE \]
\[ f_F(E) = \frac{1}{e^{(E-E_F)/kT} + 1} \]

Diagram:
- Plot of \( g(E) \) with \( E_C \) and \( E_V \) labeled.
- Plot of \( f_F(E) \) with \( (E-E_F) \) in eV against \( f_F(E) \) with \( 0.2 \), \( 0.4 \), \( 0.6 \), \( 0.8 \) labels.
- Note: Higher temperature curve.
Density of states

- $g(E)$ is the number of states per volume in a small energy range.

The conduction band is:

$$g_c(E) = 4\pi \left( \frac{2m^*_n}{\hbar^2} \right)^{3/2} (E - E_C)^{1/2} \text{ for } E > E_C$$

The valence band is:

$$g_v(E) = 4\pi \left( \frac{2m^*_p}{\hbar^2} \right)^{3/2} (E_v - E)^{1/2} \text{ for } E < E_v$$
Effective density of states

\[ n = \int_{E_c}^{E_u} g_n(E) f_n(E) \, dE = N_c F_{1/2}(\eta_n) \]

where

\[ N_c = 2 \left( \frac{m_n k_B T}{2 \pi h^2} \right)^{3/2} \]

is called the **effective density of states** for the conduction band.

\[ \eta_n = \frac{E_F - E_c}{k_B T} \]

is the **Fermi integral**. For \( \eta_n > 3 \),

\[ F_{1/2}(\eta_n) \approx \exp(\eta_n) \]

For \( \eta_n < 3 \),

\[ F_{1/2} \approx \frac{4\eta_n^{3/2}}{3\sqrt{\pi}} \]

\[ N_v = 2 \left( \frac{2 \pi m_p^* kT}{h^2} \right)^{3/2} \]

For holes
Fermi Level

• The distribution of electron/holes satisfy Fermi-Dirac distribution

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

• Fermi Level can be defined by the occupation probability of electrons at 0K
Example: Density of states, distribution function and electron density for degenerate and non-degenerate n-type semiconductor.
Basic Properties of Fermi Level

- Fermi Level is an **intrinsic property** of the material, it is sufficient to describe the carrier occupation function by Fermi Level.
- Only the available bands can have electrons/holes even when the occupy function $f(E)$ is not zero.
- Intrinsic carrier density is a strong function of temperature.
Intrinsic semiconductor

Boltzmann approximation:

\[ n_0 = \frac{\pi}{2} \left( \frac{8m_n^*}{\hbar^2} \right)^{3/2} \int_{E_C}^{\infty} (E - E_C)^{1/2} e^{-(E - E_F)/kT} dE = N_C e^{-(E_C - E_F)/kT} \]

\[ p_0 = \frac{\pi}{2} \left( \frac{8m_p^*}{\hbar^2} \right)^{3/2} \int_{-\infty}^{E_v} (E_v - E)^{1/2} e^{-(E_F - E)/kT} dE = N_V e^{-(E_F - E_v)/kT} \]

\[ n_0 p_0 = N_C N_V e^{-(E_C - E_v)/kT} = N_C N_V e^{-E_g/kT} \]

For intrinsic semiconductor: \( n_0 = p_0 = n_i \) where \( n_i \) is the intrinsic carrier density. and

\[ n_0 p_0 = n_i^2 \]

Intrinsic Fermi level:

\[ E_F = \frac{E_C + E_v}{2} - \frac{3}{4} kT \ln \left( \frac{m_n^*}{m_p^*} \right) = E_{F_i} \]
The non-Boltzmann approx. hole Concentration

\[ p_0 = \frac{4\pi}{h^3} \left(2m_p^*\right)^{3/2} \int_{-\infty}^{E_v} \frac{(E_v - E)^{1/2} dE}{1 + \exp\left(\frac{(E_F - E)}{kT}\right)} \]

Let: \( \eta = \frac{E_v - E}{kT} \) and \( \eta_F = \frac{E_v - E_F}{kT} \)

\[ p_0 = 4\pi \left(\frac{2m_p^* kT}{h^2}\right)^{3/2} \int_0^{\infty} \frac{\eta^{1/2} d\eta}{1 + \exp(\eta - \eta_F)} \]

Define: \( F_{1/2}(\eta_F) = \int_0^{\infty} \frac{\eta^{1/2} d\eta}{1 + \exp(\eta - \eta_F)} \)

We have: \[ p_0 = \frac{2}{\sqrt{\pi}} N_v F_{1/2}(\eta_F) \]
Why do we need non-Boltzmann model

- The available situation for Boltzmann approximation if that the Fermi level is far from band edges.
- When highly doped, Fermi Levels are very near band edges.
- Most laser devices are highly doped.
- The 3-D integration is a hard work. That is the challenge of using Fermi-Dirac Model.
Doping

- **N-type**

- **P-type**

\[ E_D \leftrightarrow E_C \]

\[ E_V \leftrightarrow E_A \]
Doped semiconductor (extrinsic)

Introducing dopant will shift the Fermi level but the Fermi-Dirac distribution function remains the same. This is the characteristics of thermal equilibrium.

\[ n_0 p_0 = n_i^2 \]

Still hold.
where \( n_0 \) and \( p_0 \) denote the electron and hole density at thermal equilibrium.

When we introduce dopant, the neutral dopant atom does not change the overall neutrality of the semiconductor.

Assuming 100% ionization of dopants, charge neutrality requires that:

\[ n_0 + N_A^- = p_0 + N_D^+ \]

where \( N_A^- \) and \( N_D^+ \) are ionized acceptor and donor concentrations, respectively.

\[ n_0 + N_A^- = \frac{n_i^2}{n_0} + N_D^+ \]
Temperature dependence

http://touch.caltech.edu/courses/EE40%20Web%20Files/Thermoelectric%20Notes.pdf
Steady state vs. Equilibrium State

- Equilibrium refers to a condition of no external excitation except for temperature, and no net motion of charge.
- Steady state refers to a nonequilibrium condition in which all processes are constant and are balanced by opposing process.
Quasi-Fermi level

For convenient, we introduce the concept of quasi-Fermi levels $E_{Fn}, E_{Fp}$ such that:

\[
\begin{align*}
    n &= n_0 + \Delta n = n_i \exp \left( \frac{E_{Fn} - E_{Fi}}{kT} \right) \\
p &= p_0 + \Delta p = n_i \exp \left( \frac{E_{Fi} - E_{Fp}}{kT} \right)
\end{align*}
\]

Since

\[
\begin{align*}
    n_0 &= n_i \exp \left( \frac{E_F - E_{Fi}}{kT} \right) \\
p_0 &= n_i \exp \left( \frac{E_{Fi} - E_F}{kT} \right)
\end{align*}
\]

Obviously, when the excess carrier concentration is small compare to the equilibrium carrier concentration, the quasi-Fermi level must be very close to the Fermi level. Otherwise it will be far from Fermi Level.

For device operation, we often use a low-level injection condition, meaning that while the minority carrier concentration is changed, the majority carrier concentration remain un-affected. Thus the quasi-Fermi level of the majority carrier is the same as the Fermi level.
References

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