Band structures of semiconductors

For real solids, the bands are more complicated as illustrated below:

![Graphs of band structures for Silicon, Germanium, Indium Phosphide, and Gallium Arsenide.]

But the basic principles of conduction band on electron & hole are similar.

Electrons & Holes

For a semiconductor, at T = 0
all electrons are in the valence band & there is NO conduction.

At T > 0, if Eg is not too large, some significant number of electrons are excited of the conduction band, giving rise to "free electrons", across Eg.

In the valence band, there are a few missing electrons, having "+" holes.
Fig. 7  Shapes of constant energy surfaces in Ge, Si, and GaAs. For Ge there are eight half-ellipsoids of revolution along the (111) axes, and the Brillouin zone boundaries are at the middle of the ellipsoids. For Si there are six ellipsoids along the (100) axes with the centers of the ellipsoids located at about three-fourths of the distance from the Brillouin zone center. For GaAs the constant energy surface is a sphere at zone center. (After Ziman, Ref. 19.)

See p. 14
Band gap \( (E_g) \)

(a) Insulator \( (Si, O_2 \text{ and many oxides}) \)

\[ E_g > 5 \text{ eV} \quad \\text{and} \quad \kappa T = 25.8 \text{ meV} \]

Energy

\[ \text{Ev} \rightarrow x \rightarrow \text{Ec} \]

(b) Metal \( (Al, Cu, Ag, Au...) \)

\[ \text{Ev} \rightarrow \text{Ec} \]

\[ E_g < 0 \text{ eV} \]

(c) Semiconductor \( (Si, Ge, GaAs) \)

\[ \text{Ev} \rightarrow \text{Ec} \]

\[ E_g \approx 1 \text{ eV} \text{ or a few eV} \]

Here we draw a picture using \( E_c \) (conduction band minimum or \( E_v \) (valence band maximum)) in the real space \( (x) \), not the \( \vec{k} \)-space.

We ignore the dependence of the \( \vec{k} \)-space.
Intrinsic Semiconductor

For a pure (no impurities, no defects), electrons and holes are generated by thermal excitation. We have:

\[ N_i \ (\text{intrinsic electron density}) = P_i \ (\text{intrinsic hole density}) \ (\text{cm}^{-3}) \]

(Not populated by the states)

\[ N_e = \text{effective density of states (cm}^{-3}\text{) of conduction band} \]
\[ N_v = \text{effective density of states of the valence band} \]

Electrons in the conduction band

Electron and hole concentrations, \( N_e, P \) (cm\(^{-3}\))

Effective Density of States (cm\(^{-3}\))
Previously, we showed that the states in the conduction band are arranged in the energy space \((E, k)\) space) according to

\[ E_0 = \frac{\sqrt{2}}{\pi^2} \frac{\hbar^3}{m^*} \sqrt{E - E_c}, \]

where \(E_c\) is introduced to show that in the conduction band, we can refer the energy to the conduction band energy minimum, \(E_c\).

\[ m^*_c = m^*_n = \text{density of state effective mass} \]

Also, we observe that electrons will occupy these states according to the Fermi-Dirac distribution,

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

Now let us assume the \(E_F\) is far from \(E_c\),

\[ (E_c - E_F) \gg \text{a few } kT. \]
Then, we know that the Fermi-Dirac function may be approximated:

\[ f(E) \approx e^{-(E-E_F)/kT} \]  

(nondegenerate case)

"Nondegenerate" means normal as the ideal gas distribution function, Boltzmann distribution was "normal".

Thus, the electron density (cm\(^{-3}\)) is

\[ n = \int_{E_c}^{\infty} \text{density of states} \times \text{distribution function} \ dE \]

\[ = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \int_{E_c}^{\infty} (E - E_c)^{1/2} e^{-\frac{(E - E_c)}{kT}} \ dE \]

\[ = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \left[ \left( \frac{E - E_c}{kT} \right)^{3/2} + \frac{3}{2} (E - E_c) \right] \]

\[ E - E_F = E - E_c - (E_c - E_F) = \frac{3}{2} (E_c - E_F) \frac{kT}{E_c - E_c} \]

\[ n = \frac{2}{\hbar} \left( \frac{2\pi^2 m^* k^2 T}{\hbar^2} \right)^{3/2} e^{-\frac{(E_c - E_F)}{kT}} \]

\[ N_c \]

\[ n = N_c e^{-\frac{(E_c - E_F)}{kT}} \]

\[ N_c = \left( \frac{2m^* k^2 T}{\hbar^2} \right)^{3/2} \]

Generally good for nondegenerate case.

\[ N_c = 2 \left( \frac{2\pi m^* k^2 T}{\hbar^2} \right)^{3/2} \]

Density of states

= effective density of states at \( E_c \) (cm\(^{-3}\))
i.e., to imagine that all the states are at $E_F$; this is possible since most of the electrons occupy near the bottom of the conduction band.

Is the assumption good? Recall that $E = E_F$, $f = \frac{1}{2}$ for intrinsic semiconductors, since $n = p$, $E_F$ is between $E+Ev$.

Likewise, for holes in the valence band,

$$f_p = 1 - f = \frac{1}{1 + e^{(E-E_F)/k_BT}} = \frac{1}{1 + e^{(E-E_F)/k_BT}}$$

$$\rho = N_v e^{-\frac{(E-E_F)}{k_BT}}$$

$$N_v = 2 \left( \frac{2\pi m^* k_B T}{h^2} \right)^{3/2} \text{ (cm}^{-3}\text{)}$$

= effective density of states at $E_F$, only all the valence band states were at the valence band maximum!

**Intrinsic carrier density: $N_i$ (cm$^{-3}$)**

For intrinsic (pure & perfect) semiconductors

$$n = p = N_i$$

$$E_F \equiv E_i \text{ (intrinsic Fermi level)}$$

$$N_i = N_e e^{-\frac{(E_c - E_F)}{k_BT}} = N_v e^{-\frac{(E_v - E_F)}{k_BT}}$$

(For Si at 300K, $N_i(E_i) = 1.45 \times 10^{10} \text{ cm}^{-3}$ at 300K)
\[
\begin{align*}
N_i^2 &= N_c N_r e^{-\frac{(E_i - E_r)^2}{k_B T}} = N_c N_r e^{-\frac{E_i}{k_B T}} \\
N_i &= \sqrt{N_c N_r} e^{-\frac{E_i}{k_B T}} \\
\text{Law of mass action.}
\end{align*}
\]

\[
\frac{N_c}{N_r} = \exp\left(\frac{E_c - E_r - (E_i - E_V)}{k_B T}\right)
\]

\[
2E_i = (E_c + E_V) - k_B T \ln \frac{N_c}{N_r}
\]

\[
E_i = \frac{E_c + E_V}{2} - \frac{k_B T}{2} \ln \frac{N_c}{N_r}
\]

\[
E_i = \frac{E_c + E_V}{2} + \frac{3}{2} k_B T \ln \left(\frac{M_{el}}{M_{et}}\right)
\]

\[-0.013 \text{ ev}\]

\[
\begin{align*}
E_i &= E_c \\
E_i &= \frac{E_c + E_V}{2} \\
E_i &= E_V
\end{align*}
\]
Example (1)

\[
N_c = 2 \left( \frac{2\pi \cdot 9.1 \times 10^{-31} \cdot 7.38 \times 10^{-23}}{6.628 \times 10^{-34}} \right)^{3/2}
\]

= \(2.51 \times 10^9\) cm\(^{-3}\)

Example (2) calculate effective density of states

\[
\text{Si, Ge, As at 30K:}
\]

\[
\text{GaAs: } \quad M_n^+ = 0.067 M_0
\]

\[
N_c = 2 \left( \frac{2\pi \cdot 3 \times 10^{-31} \cdot 0.067 \cdot 1.38 \times 10^{-23}}{6.628 \times 10^{-34}} \right)^{3/2}
\]

= \(4.15 \times 10^{17}\) cm\(^{-3}\)

\[
S_i: \quad M_n^+ = 0.19 M_0 \), but there are 6 ellipsoids
\]

\[
M_n^+ = 6 \left( 0.98 \cdot 0.19 \cdot 0.19 \right)^{3/2} M_0
\]

= \(1.08 M_0\)

\[
N_c = 2 \left( \frac{2\pi \cdot 1.08 \times 9.1 \times 10^{-31} \cdot 1.38 \times 10^{-23}}{6.628 \times 10^{-34}} \right)^{3/2}
\]

= \(2.78 \times 10^9\) cm\(^{-3}\)

For the valence bands,

\[
N_v = 2 \left( M_n^+ + M_h^+ \right) \left( \frac{2\pi \cdot k_B T}{\hbar^2} \right)^{3/2}
\]
\( \text{GaAs} \)

\[ N_{i,f} = 0.45 \, n_0, \quad N_{i,h} = 0.08 \, n_0 \]

\[ N_{i}(\text{GaAs}) = 7.72 \times 10^{18} \, \text{cm}^{-3} \]

\( \text{Si} \)

\[ N_{i} = \begin{cases} 0.5 \, n_0, & \mu_{ih} = 0.15 \, n_0 \end{cases} \]

\[ N_{i}(\text{Si}) = 9.84 \times 10^{18} \, \text{cm}^{-3} \]

Example 5. Calculate \( N_i \) at 300 K and 600 K

\[ E_g(\text{InAs}) = 0.35 \, \text{eV} \]

\[ m_i = 0.027 \, m_0, \quad m_r^* = 0.4 \, m_0 \]

\[ n_i = \frac{2}{3} \left( \frac{2 \pi k_B T}{h^2} \right)^{3/2} \left( n_e m_r^* \right)^{3/4} e^{-\frac{E_g}{k_B T}} \]

\[ = 2 \left( \frac{2 \pi \times 0.026 \times 1.6 \times 10^{-19}}{6.626} \right)^{3/2} \left( 0.027 \times 0.4 \times (9.1 \times 10^{-31})^2 \right)^{3/4} e^{-\frac{0.35}{0.052}} \]

\[ = 1.028 \times 10^{15} \, \text{cm}^{-3} \]

\[ N_i(600 \, \text{K}) = 2.87 \times 10^{15} \, \text{cm}^{-3} \]
<table>
<thead>
<tr>
<th>Property</th>
<th>Symbol</th>
<th>Units</th>
<th>Si</th>
<th>Ge</th>
<th>GaAs</th>
<th>GaP</th>
<th>SiO₂</th>
<th>Si₃N₄</th>
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<td>Diamond</td>
<td>Diamond</td>
<td>Zincblende</td>
<td>Zincblende</td>
<td>Amorphous</td>
<td>for most IC applications</td>
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<td>8</td>
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<td>31/33</td>
<td>31/15</td>
<td>14/8</td>
<td>14/7</td>
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<td>g/g-mole</td>
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<td>2.47 × 10²²</td>
<td>2.20 × 10²²</td>
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<td>eV</td>
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<td>eV</td>
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<td>Temperature dependence</td>
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<td>eV K⁻¹</td>
<td>-2.7 × 10⁻⁴</td>
<td>-3.7 × 10⁻⁴</td>
<td>-5.0 × 10⁻⁴</td>
<td>-5.4 × 10⁻⁴</td>
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<tr>
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<td>10.2</td>
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<td>°C</td>
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<td>1467</td>
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<td>-1900</td>
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<td>Vapor pressure</td>
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<td>Torr (mm Hg)</td>
<td>10⁻¹ (1050)</td>
<td>10⁻¹ (750)</td>
<td>1 (1050)</td>
<td>10⁻⁶ (770)</td>
<td></td>
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</tr>
<tr>
<td>(at °C)</td>
<td></td>
<td>(at °C)</td>
<td>10⁻¹ (1250)</td>
<td>10⁻¹ (880)</td>
<td>10⁻¹ (1220)</td>
<td>10⁻¹ (920)</td>
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<tr>
<td>Specific heat</td>
<td>C_p</td>
<td>J (g K)⁻¹</td>
<td>0.70</td>
<td>0.32</td>
<td>0.35</td>
<td>0.4</td>
<td>1.4</td>
<td>0.17</td>
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<td>α</td>
<td>W(cm K)⁻¹</td>
<td>1.412</td>
<td>0.66</td>
<td>0.456</td>
<td>0.97</td>
<td>0.014</td>
<td>0.185(?)</td>
</tr>
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<td>Dₐ</td>
<td>cm² s⁻¹</td>
<td>0.87</td>
<td>0.36</td>
<td>0.44</td>
<td>0.004</td>
<td>0.32(?)</td>
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<td>Coefficient of linear thermal</td>
<td>αₜ</td>
<td>K⁻¹</td>
<td>2.5 × 10⁶</td>
<td>5.7 × 10⁶</td>
<td>5.9 × 10⁶</td>
<td>5.3 × 10⁶</td>
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<td>expansion</td>
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<tr>
<td>Intrinsic carrier concentration*</td>
<td>nᵯ</td>
<td>cm⁻³</td>
<td>1.45 × 10¹⁹</td>
<td>2.4 × 10¹⁴</td>
<td>9.6 × 10⁹</td>
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<tr>
<td>Electron</td>
<td>μₑ</td>
<td>cm²(V s)⁻¹</td>
<td>1417</td>
<td>3900</td>
<td>8800</td>
<td>300</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>Hole</td>
<td>μₜ</td>
<td>cm²(V s)⁻¹</td>
<td>471</td>
<td>1900</td>
<td>400</td>
<td>100</td>
<td>-10⁻⁴</td>
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</table>

Effective density of states

*Calculated from the energy band gap and the density of states at the Fermi level.
<table>
<thead>
<tr>
<th>Source</th>
<th>Effect</th>
<th>Effect</th>
<th>Effective mass</th>
<th>Effective density of states</th>
<th>Effective field attenuation</th>
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</thead>
<tbody>
<tr>
<td>6.9 × 10⁻⁵</td>
<td>1.0 × 10⁻⁴</td>
<td>3.5 × 10⁻⁵</td>
<td>0.3 × 10⁻¹</td>
<td>0.062 × 10⁻¹</td>
<td>0.017 × 10⁻¹</td>
</tr>
<tr>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
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