PHYS 551 Lecture #23

Title: Semi-Conductors, Band Gaps and the Fermi-level

From the last class, we were able to observe the astounding properties that occurred for “holes” in the valance band.

→ Holes in the VB behave as if they had positive charge and negative mass.

→ Electrons in the CB behave as if they had negative charge and positive mass.

Notice that for a free-electron:

$$\begin{aligned}
E_k &= \frac{\hbar^2 k^2}{2m} \\
\vec{v}_e &= \frac{1}{\hbar}\nabla_k E_k, \quad \vec{v} = \frac{\hbar\vec{k}}{m} \\
\frac{1}{m_e} &= \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k^2} = \frac{1}{m}
\end{aligned}$$

For an electron in a periodic potential

$$E \neq \frac{\hbar^2 k^2}{2m}, \; \vec{v} \neq \frac{\hbar\vec{k}}{m}, \text{ and } \frac{1}{m_e} \neq \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k^2}$$

However, $\vec{v} = \frac{1}{\hbar}\nabla_k E_k$ and the electron (or hole) behaves as if it has mass

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 E(k)}{\partial k_i \partial k_j} \equiv \text{effective mass.}$$

Hence the velocity is given by the gradient of the band and the effective mass is proportional to the curvature.

These properties aside, it was shown that, upon application of an electric field, both holes and electrons contribute to the net current.

$$\begin{aligned}
\vec{j}_T = -ne\,\vec{v}_e + pe\,\vec{v}_h, \quad &\vec{v}_e \quad \text{is opposite to the applied field} \\
&\vec{v}_h \quad \text{is with the applied field}
\end{aligned}$$

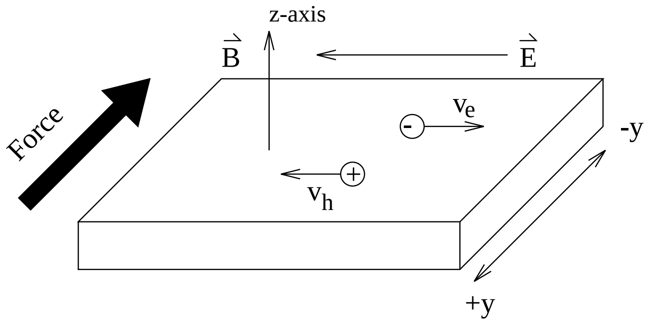
n is the concentration of electrons in the CB

p is the concentration of holes in the VB

In the presence of an $\vec{E}$-field holes tend to sink and electrons tend to rise. If the field is then removed they undergo a reverse process.

Question: How do holes and electrons move in the presence of a magnetic field?

$$\text{Recall} \quad \vec{F} = \frac{d\vec{p}}{dt} = \hbar\frac{d\vec{k}}{dt} = \frac{q}{c}\left(\vec{v} \times \vec{B}\right)$$



Both the electron and the hole experience a force in the <u>same</u> $(-y)$ direction

Thus, they tend to cancel out one another.

A material with only VB holes will have a positive Hall coefficient.

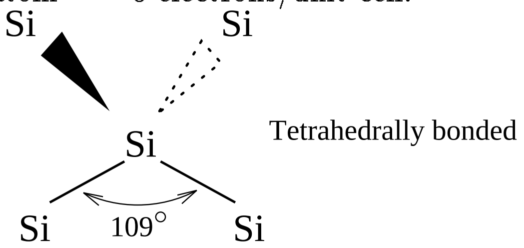
A material with only CB electrons will have a negative Hall coefficient.

Semi-Conductors (in earnest): Now that we have investigated the properties of the VB tops and CB bottoms we will begin to address real elemental semi-conductors.

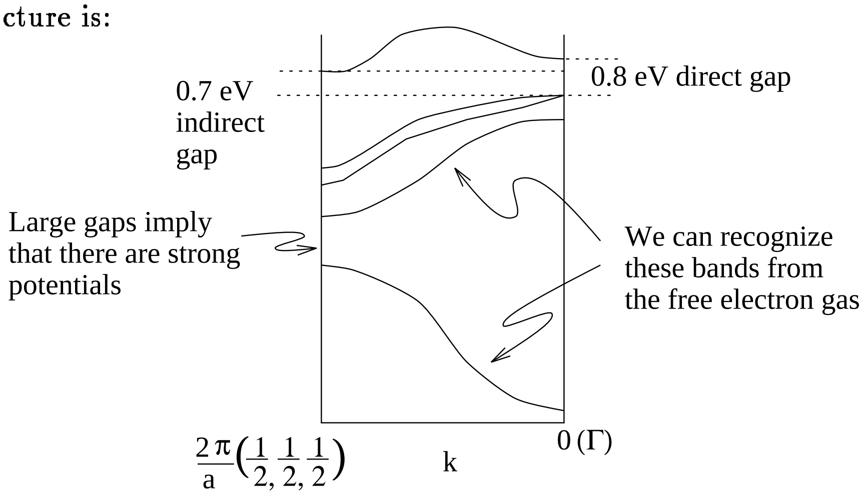
Homogeneous Semi-Conductors are Group IV elements; Si and Ge Heterogeneous Semi-Conductors are $\overset{3}{\mathrm{Ga}}\overset{5}{\mathrm{As}}$, $\overset{4}{\mathrm{Si}}\overset{4}{\mathrm{C}}$, $\overset{2}{\mathrm{Zn}}\overset{6}{\mathrm{Se}}$ and on and on.

Silicon & Germanium:

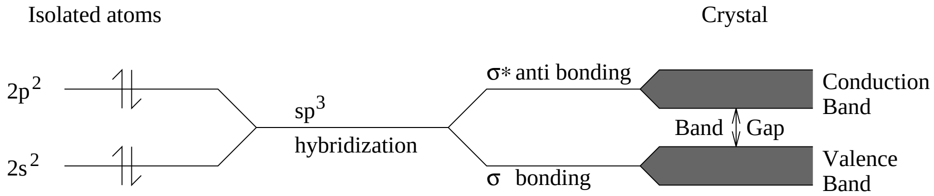
These materials have a diamond lattice $\longrightarrow$ FCC with two atoms per unit cell, 4 valence electrons/atom $\longrightarrow$ 8 electrons/unit cell.



The band structure is:



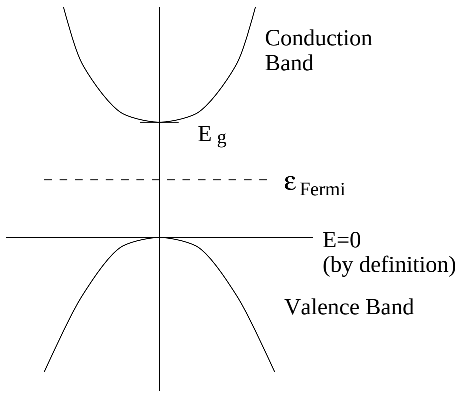
Since the potential is strong we might expect that the FEG model is only a crude estimate. There are other ways to think about the electron configuration:



This approach begins with electrons in atomic orbitals.

For the Direct gap, Indirect gap

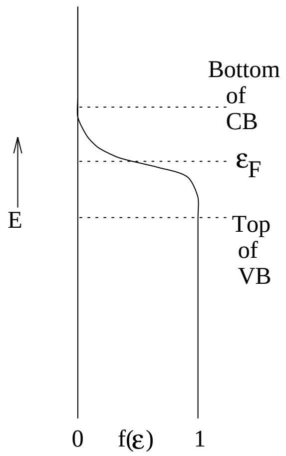
	Direct gap	Indirect gap
C	5.3 eV	-
Si	2.5 eV	1.1 eV
Ge	.8 eV	.7 eV



$$E_e(k) = Eg + \frac{\hbar^2 k^2}{2m_e^*}$$

$$E_h(k) = \frac{\hbar^2 k^2}{2m_h^*}$$

Question: If there is a large gap (with no allowed electron states), how can the Fermi level be determined? The answer to this is important because the location of the Fermi level describes the distribution statistics. At T=0, this is of no consequence since f(ϵ)=1, $\epsilon < \epsilon_f$ and f(ϵ)=0, $\epsilon > \epsilon_f$. In principle, anywhere in the gap would do. However at finite T, a little more work is required.



Recall Fermi-Dirac statistics f(ϵ) $= \frac{1}{\exp((\epsilon-\mu)/k_B T)+1}$

At finite T, there are electrons in the CB and holes in the VB. Since there must be charge neutrality, the number of electrons in the CB must be equal to the number of holes in the VB. On the whole, $\epsilon_F(T)$ must lie near the middle of the gap if f(ϵ) is to be more or less the same at both band edges.

$\mu \equiv \epsilon_F(T)$

If $k_B T$ is small and $\varepsilon > \varepsilon_F$ (CB)

$f(\varepsilon) \approx e^{-(\varepsilon-\varepsilon_F)/k_B T}$ since $e^{(\varepsilon-\varepsilon_F)/k_B T} >> 1$

Recall $\mathcal{D}_{3D}(\epsilon) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\epsilon}$ for a FEG
Letting $m \longrightarrow m_e^*$ and $\epsilon \longrightarrow (E - Eg)^{1/2}$ gives (which is exactly true if the curvature of the CB is constant)

$$\mathcal{D}(\epsilon) = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}(E - Eg)^{1/2} \qquad E > Eg$$

Since f(ϵ) is an exponential falling function with increasing ϵ, only the shape at the bottom of the CB matters at all for the following calculation.

$$\text{Thus} \qquad N \equiv \#\text{ of electrons in the CB } = \int_{E_G}^{\infty}\mathcal{D}(\epsilon)f(\epsilon)d\epsilon$$

becomes

$$N \approx \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2} e^{E_F(T)/k_BT}\int_{E_G}^{\infty}(\epsilon - Eg)^{1/2}e^{-\epsilon/k_BT}d\epsilon$$

let

$$\begin{aligned}
x &= (\epsilon - Eg)/k_BT \\
N &= \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2} e^{-(E_G-\epsilon_F(T))/k_BT}(k_BT)^{3/2}\underbrace{\int_0^{\infty}x^{1/2}e^{-x}dx}_{\sqrt{\pi}/2} \\
N &= 2\left[\frac{m_e^*k_BT}{2\pi\hbar^2}\right]^{3/2} e^{-(Eg-\epsilon_F(T))/k_BT}
\end{aligned}$$

This gives the number of electrons in the CB in terms of $\epsilon_F(T)$. We still need to solve for the number of holes.

$$\begin{aligned}
f_h(\epsilon) &= 1 - f(\epsilon) \text{ for } \epsilon < \epsilon_F \\
f_h(\epsilon) &= 1 - \frac{1}{\exp[(\epsilon - E_F(T))/k_BT] + 1} = \frac{1}{\exp[(E_F(T) - \epsilon)/k_BT] + 1}
\end{aligned}$$

$$\text{Now} \quad E_F(T) - \epsilon >> k_BT \text{ for holes in the VB}$$

$$\text{So } f_h(\epsilon) \approx \exp[-(E_F(T) - \epsilon)/k_BT]$$

$$\mathcal{D}_h(\epsilon) = \frac{1}{2\pi^2}\left(\frac{2m_h^*}{\hbar^2}\right)^{3/2}(-\epsilon)^{1/2} \quad (\epsilon = 0 \text{ at VB edge})$$

Thus

$$p = \# \text{ of holes in VB} = \int_{-\infty}^{0} e^{-(E_F(T)-\epsilon)/k_BT} \frac{1}{2\pi^2} \left(\frac{2m_h^*}{\hbar^2}\right)^{3/2} (-\epsilon)^{1/2} d\epsilon$$

$$p = 2\left(\frac{m_h^* k_B T}{2\pi\hbar^2}\right)^{3/2} e^{-E_F(T)/k_BT}$$

Notice the product of np is *independent* of $E_F(T)$

$$np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 (m_e^* m_h^*)^{3/2} e^{-E_G/k_BT}$$

This is just an expression of a "law of mass action". If we were able to increase the number of electrons in the CB, the number of holes would have to decrease.

But for pure Si, $n = p$, since the electrons in the CB must orginate from the valance band so

$$n = p = \sqrt{np} = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} (m_e^* m_h^*)^{3/4} e^{-E_G/2k_BT}$$

and

$$p = 2\left(\frac{m_h^* k_B T}{2\pi\hbar^2}\right)^{3/2} e^{-E_F(T)/k_BT}$$

Equating and solving for E_F gives

$$e^{-E_F(T)/k_BT} = \left(\frac{m_e^*}{m_h^*}\right)^{3/4} e^{-E_G/2k_BT}$$

or

$$E_F = \frac{E_G}{2} - \frac{3}{4} k_B T \, \ell n \left(\frac{m_e^*}{m_h^*}\right)$$

Thus E_F lies in the middle of the gap at T=0 and moves toward the lower density of states with increasing T.