Recitation 1 - Compound Semiconductors; Energy bands and carriers III - Outline

• Announcements
  Postings - Recitation 1 Foils; PS #1 coming later today
  Time change? - Lecture 11 to 1?

• Band-edge plots through homojunction devices
  Thermal equilibrium:
    1. Uniform sample
    2. p-n junction
    3. MOS capacitor
    4. M-S contact
  Non-equilibrium situations; Quasi-Fermi levels:
    1. Definition of quasi-Fermi level
    2. Optical excitation
    3. Applied biases
    4. Significance of quasi-Fermi level gradients

Got this far
Filling states - combining the density of states and Fermi functions

\[ n(E) = \rho(E) \cdot f(E) \]

\[ E_F \text{ s.t. } p_o - n_o + N_d^+ - N_a^- = 0 \]
Effective densities of states:

When the Fermi level is many kT away from either band edge [i.e., \((E_c-E_f) >> kT\) and \((E_f-E_v) >> kT\)], then we can approximate and simplify the two integrals in the expressions for \(n_o\) and \(p_o\). Looking first at \(n_o\):

\[
n_o = \int_{E_c}^{\infty} \rho_c(E) f(E) \, dE = \int_{E_c}^{\infty} \frac{\rho_c(E)}{1 + e^{(E-E_f)/kT}} \, dE \\
= \left[ \int_{E_c}^{\infty} \rho_c(E) e^{-(E-E_c)/kT} \, dE \right] e^{-(E_f-E_c)/kT} = N_c e^{-(E_c-E_f)/kT}
\]

where, \(N_c\), the effective density of states for the conduction band, is

\[
N_c = \int_{E_c}^{\infty} \rho_c(E) e^{-[E-E_c]/kT} \, dE
\]

When the \(E_f\) is close to the band edge, or even in the band, the the full Fermi function must be used. If we can still model the band as parabolic, then in terms of \(N_c\) we find the result is in general:

\[
n_o = \int_{E_c}^{\infty} \rho_c(E) f(E) \, dE = N_c \cdot \mathcal{F}\left(\frac{E_c - E_f}{kT}\right)
\]

The function \(\mathcal{F}[\!(E_c-E_f)/kT]\) is plotted on the next foil. Note that when \((E_c-E_f) > kT\), it reduces to our approximation, \(\exp[-(E_c-E_f)/kT]\).
Effective densities of states, cont:

The next question is, “How far from $E_c$ and $E_v$ must $E_f$ be for this approximation to be valid?” To answer this we can compare the value of exact integral with the approximation. This is done to the right for a parabolic band:

The textbook this is from* says the convention is to say one must be 3 kT away from the band edge, but looking at the curve one could argue that at 2 kT and even at 1 kT the approximation is not bad.

I would argue that it could be used at 0 kT to make a rough estimate.

Effective densities of states, cont:

This modeling shows us that the state density profiles in the bands can be replaced by impulse effective densities of states at the band edges, when the Fermi level is sufficiently far from the band edges.
With these approximate expressions for \( n_o \) and \( p_o \) (which are valid only when the Fermi level is several \( kT \) away from the band edges) the equation for \( E_f \),

\[
p_o - n_o + N_d^+ - N_a^- = 0
\]

becomes:

\[
N_v e^{-(E_f - E_v)/kT} - N_c e^{-(E_c - E_f)/kT} + N_d [1 - f_d (E_d)] - N_a f_a (E_a) = 0
\]

It is still not simple to find \( E_f \), but it is easier. More importantly, we now have a convenient way of knowing when a doping level is large.

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**Note:** If the energy bands are parabolic, i.e., when the density of states depends quadratically on the energy away from the band edge, we find simple expressions for the effective densities of states in terms of the effective masses:

If \( \rho_c (E) = \sqrt{2(m_{ed}^*)^3} \left( E - E_c \right) / \pi^2 \hbar^3 \) then \( N_c = 2 \left[ 2\pi m_{ed}^* \frac{kT}{\hbar^2} \right]^{3/2} \)

and if \( \rho_v (E) = \sqrt{2(m_{hd}^*)^3} \left( E_v - E \right) / \pi^2 \hbar^3 \) then \( N_v = 2 \left[ 2\pi m_{hd}^* \frac{kT}{\hbar^2} \right]^{3/2} \)
**Variation of Fermi level with temperature**

(Note: for convenience we assume an n-type sample, no acceptors)

- **Around R.T.**
  - Tail of \( f(E) \) extends above \( E_c \)
  - Full ionization
  - Extrinsic doping
  
  \[ E_i < E_f < E_d \]

- **At very low T**
  - \( f(E) \) almost a step function
  - Incomplete ionization
  - Freeze-out of electrons
  
  \[ E_d < E_f < E_c \]

- **At very high T**
  - \( f(E) \) has long tails extending above \( E_c \) and below \( E_v \)
  - Band-to-band thermal excitation of electrons
  - Intrinsic behavior
  
  \[ E_f \approx E_i \]
Definitions: To compare different semiconductor samples, we need to introduce a common reference level, which leads in turn to the introduction of several new quantities, $\chi$ and $\Phi$:

**Vacuum level, 0**
The energy of an electron at rest far removed from the semiconductor. This is taken as the zero reference for energy in this view.

**Electron affinity, $\chi$**
The energy required to take an electron from the bottom of the conduction band and place it at rest far removed from the semiconductor. This is an intrinsic material property.

**Work function, $\Phi$**
The energy required to take an electron from the Fermi level and place it at rest far removed from the semiconductor. This depends on the doping level and temperature, as well as on the material.

**Intrinsic level, $E_i$**
The position of the Fermi level in intrinsic material. This is an intrinsic material property.
**Spatial plots of the important energies**

In device structures in which the compositions and doping levels vary in space it is useful to plot the critical energy levels (band edges, Fermi level, dopant energies, vacuum reference level) spatially. For a uniformly doped n-type Si sample, this would look like the following:

![Diagram of spatial plots of the important energies](image)
Spatial plots for widely separated p- and n-type samples

Samples which are separated and not connected electrically share a common vacuum reference level, and their spatial plots align as shown below:

![Diagram showing electron energy levels for p-type and n-type Si samples](image)

C. G. Fonstad, 2/6/09
Separated, but connected p- and n-type samples

If the samples in the previous foil are now connected electrically, carriers flow from one to the other until the Fermi levels align:
p-n Junctions - progression of the barrier with decreasing separation

C. G. Fonstad, 2/07

Recitation 1 - Slide 5
Unbiased p-n junction

Electrostatic potential:

-\( q \phi(x) \)

Band-edge plot:

Vacuum ref. now -\( q\phi(x) \)

\( E_c(x) \)

\( E_i(x) \)

\( E_f \)

\( E_v(x) \)

Valence band close to \( E_f \) so \( p_o \) is large

Band edges away from \( E_f \) so region is depleted

Conduction band close to \( E_f \) so \( n_o \) is large

C. G. Fonstad, 2/6/09
Semiconductor and metal with an insulator between them

\[ q\Phi_s = q\chi_s + kT \ln \left( \frac{N_C}{N_D} \right) \]
Metal and semiconductor in contact

\[ q\phi_m = q\chi_s \]

\[ q\phi_m = q\Phi_m - q\chi_s \]

Separated metal and semiconductor

\[ q\Phi_m = q\chi_s + kT \ln \left( \frac{N_C}{N_D} \right) \]
Metal-Semiconductor Junctions - progression of the barrier with decreasing separation
Band-edge profiles - key observations

The electrostatics relationships from 6.012 are still useful and provide the basic foundation for profiling:

Electrostatics:
\[
\begin{align*}
\rho(x) &= q \left[ p_o(x) - n_o(x) + N_D^+(x) - N_A^-(x) \right] \\
\phi(x) &= -\int F(x) dx = -\int \frac{\rho(x)}{\varepsilon} dx dx
\end{align*}
\]

The band edges follow the profile of the electrostatic potential energy, \(-q\phi(x)\):

Band edges:
\[
\begin{align*}
E_c(x) &= -q\phi(x) - \chi(x) \\
E_c(x) &= -q\phi(x) - \chi(x) - E_g(x)
\end{align*}
\]

Not functions of \(x\) in homogeneous devices

The Fermi level, \(E_f\): 1. Constant in thermal equilibrium, TE
2. Near CB \(\Rightarrow\) n large
3. Near VB \(\Rightarrow\) p large
The Fermi energy - showing it is constant in TE

In thermal equilibrium the currents are zero. Knowing this we can show that the fermi energy must be a constant in TE. Focus on the electron current (looking at the hole current yields the same result):

\[ J_e(x) = qn_o(x)\mu_e F(x) + qD_e \frac{dn_o}{dx} \]

with \( n_o(x) = N_c e^{(E_c - E_F)/kT} \)

First we calculate \( \frac{dn_o}{dx} \) and manipulate it a bit to get:

\[
\frac{dn_o}{dx} = n_o \left( -\frac{dE_c}{dx} + \frac{dE_F}{dx} \right) = \frac{n_o}{kT} \left( -qF(x) + \frac{dE_F}{dx} \right) = \frac{\mu_e n_o}{D_e} \left( -F(x) + \frac{1}{q} \frac{dE_F}{dx} \right)
\]

where we have used:

\[
\frac{dE_c}{dx} = -q \frac{d\phi}{dx} = qF(x) \quad \text{and} \quad \frac{\mu_e}{D_e} = \frac{q}{kT}
\]

Putting this in \( J_e \) and simplifying the expression yields our final result:

\[ J_e(x) = \mu_e n_o(x) \frac{dE_F(x)}{dx} \]

From this result we see clearly that:

\[ J_e(x) = 0 \iff \frac{dE_F(x)}{dx} = 0 \]
Modeling non-equilibrium populations - quasi-Fermi levels

When we are not in thermal equilibrium, we can expect:

\[ n(x) \neq n_o(x) \quad \text{and} \quad p(x) \neq p_o(x) \]

because the populations are not necessarily in equilibrium with each other. However, it is likely that the electrons are in quasi-equilibrium with the conduction band states, and the holes are similarly in quasi-equilibrium with the valence band states. Thus the energy distribution of the electron population can be described by the Fermi function with the appropriate Fermi energy, now called the “electron quasi-Fermi level”, \( E_{Fn} \); the hole distribution can be similarly described using \( E_{Fp} \).

We find \( E_{Fn} \) and \( E_{Fp} \) knowing \( n \) and \( p \) by solving the following equalities for \( E_{Fn} \) and \( E_{Fp} \), respectively:

\[
n(x) = \int_{E_c}^{\infty} \frac{\rho_{cb}(E)}{1 + e^{\frac{E - E_{Fn}(x)}{E}}} \, dE
\]

\[
p(x) = \int_{-\infty}^{E_v} \frac{\rho_{vb}(E)}{1 + e^{\frac{E - E_{Fp}(x)}{E}}} \, dE
\]
Modeling non-equilibrium populations - quasi-Fermi levels, cont.

When the quasi-Fermi levels are within the band-gap by a few $kT$ we can use the effective density of states concept to find analytical expressions for $E_{fn}$ and $E_{fp}$:

$$n(x) = \int_{E_c}^{\infty} \frac{\rho_{cb}(E)}{1 + e^{E - E_{Fn}(x)}} \, dE \approx N_c e^{[E_c - E_{Fn}(x)]} \quad \Rightarrow \quad E_{Fn}(x) = E_c - kT \ln\left( \frac{n(x)}{N_c} \right)$$

$$p(x) = \int_{-\infty}^{E_v} \frac{\rho_{vb}(E)}{1 + e^{E - E_{Fp}(x)}} \, dE \approx N_v e^{[E_{Fp}(x) - E_v]} \quad \Rightarrow \quad E_{Fp}(x) = E_v + kT \ln\left( \frac{p(x)}{N_v} \right)$$

Returning to our discussion of the electron and hole currents, we find that in non-equilibrium situations, where they are not necessarily zero, they are related to product of the carrier concentration, the mobility, and the gradient of in the quasi-Fermi levels:

$$J_e(x) = \mu_e n(x) \frac{dE_{Fn}(x)}{dx} \quad \text{and} \quad J_h(x) = \mu_h p(x) \frac{dE_{Fp}(x)}{dx}$$

Gradients in the quasi-Fermi levels act like net drift fields pushing the relevant carriers.
Quasi-Fermi levels - looking at this again in a little different way

When a semiconductor is not in thermal equilibrium, it is still very likely that the electron population is at equilibrium within the conduction band energy levels, and the hole population is at equilibrium with the energy levels in the valence band. That is to say, the population on electrons is distributed in the conduction band states with the Boltzmann factor:

\[ e^{-\frac{E - E_{fn}}{kT}} \]

Here \( E_{fn} \) is the effective, or quasi-, Fermi level for electrons. Similarly, there is a quasi-Fermi level for holes, \( E_{fp} \), and the holes are distributed in the valence band states as:

\[ e^{-\frac{E_{fp} - E}{kT}} \]

The quasi-Fermi levels for electrons and holes, \( E_{fn} \) and \( E_{fp} \), are not in general equal. To find them we usually begin with \( n(x) \) and \( p(x) \), and write them in terms of the conduction and valence band densities of states and the quasi-Fermi levels:

For example, we write \( n(x) = N_c(x) e^{-\frac{E_c(x) - E_{fn}(x)}{kT}} \)

This then defines \( E_{fn} : E_{fn}(x) = E_c(x) - kT \ln\left[ \frac{N_c(x)}{n(x)} \right] \)

We define \( E_{fp} \) similarly: \( E_{fp}(x) = E_v(x) + kT \ln\left[ \frac{N_v(x)}{p(x)} \right] \)
**Quasi-Fermi levels** - quasi-Fermi levels in some specific situations

A very important finding involving quasi-Fermi levels is that we can write the electron and hole currents in terms of the gradients of the respective quasi-Fermi levels, at least in the low field limit where drift mobility is a valid concept. We found:

\[ J_n(x) = \mu_e n(x) \frac{\partial E_{fn}(x)}{\partial x} \]

and

\[ J_p(x) = \mu_h p(x) \frac{\partial E_{fp}(x)}{\partial x} \]

**Examples:**

A. **Uniformly doped n-type semiconductor with uniform E-field**

At low to moderate E-fields, the populations are not disturbed from their equilibrium values, and we have

\[ n(x) \approx n_o \approx N_d \quad \text{and} \quad p(x) \approx p_o = n_i^2 / N_d \]

Also, \( E_{fn} \approx E_{fp} \approx E_f - q\phi(x) \), so:

\[ J_e \approx \mu_e n_o (-q \frac{\partial \phi}{\partial x}) = q\mu_e n_o F_x \quad \text{and} \quad J_e \approx q\mu_h p_o F_x \]

As expected, the currents are the respective drift currents.
B. P-side of forward biased n$^+$-p junction, long-base limit:

Diode diffusion theory gives us $n(x)$ on the p-side:\n
$$n(x) = n_{op} \left[ (e^{qv_{ab}/kT} - 1) e^{-x/L_e} + 1 \right]$$

where $n_{op} = n_i^2/N_{Ap}$

When $v_{AB} \gg kT$, and $x$ is not many $L_e$, we can approximate $n(x)$ as:

$$n(x) \approx n_{op} e^{qv_{ab}/kT} e^{-x/L_e}$$

from which we find:

$$E_{fn}(x) = E_c + kT \ln \left[ n(x)/N_c \right]$$

$$\approx E_c + kT \ln \left[ n_o/N_c \right] + qv_{ab} - kT x/L_e$$

$$\approx E_{fo} + qv_{ab} - kT x/L_e$$

We see that $E_{fn}(x)$ is $qv_{AB}$ higher than the equilibrium Fermi level, $E_{fo}$, at the edge of the depletion region on the p-side, and decreases linearly going away from the junction. Farther away from the junction, where $x$ is many $L_e$, $n(x)$ approaches $n_{op}$, and $E_{fn}(x)$ approaches $E_{fo}$.

Finally, notice that for low-level injection, $p(x) \approx p_{po}$, and $E_{fp} \approx E_{fo}$.
Quasi-Fermi levels - Illustrating examples A and B

Figure C-8 from Fonstad, Microelectronic Devices and Circuits with quasi-Fermi levels added:

Example A:

\[ E_{fn} \approx E_{fp} \approx E_{fo} \]

Example B: