6.772 - Compound Semiconductor and Heterostructure Devices

Lecture 3 - Heterostructures I: - Outline

• Energy bands - general, cont.
  Surface States: Fermi level pinning
  Homojunctions using bands one more time: electrostatics + bands
  Biased junctions: energy level occupancy in non-equilibrium situations
  quasi-Fermi levels

• Heterojunction band profiles (the Depletion Approximation extended)
  Abrupt junctions:
    1. Issues new to heterojunctions: $\Delta \chi$, $\Delta E_g$, $\Delta E_c$, $\Delta E_v$
    2. Alignment options/types
    3. Type I heterojunctions:
       a. N-p: i. In equilibrium
          ii. With applied bias
       b. P-n
       c. Iso-type: P-p, N-n
       d. Modulation doping: N-i, concept, significance

Graded compositions:
  1. In bulk regions
  2. At heterojunctions (impact on spikes)
Energy band edge picture - review

• Band edge energies
  The band edge energies relative to the vacuum reference level and to each other are a property of the semiconductor

  Electron affinity, $\chi$:
  Conduction band edge to vacuum ref.

  Energy gap, $E_g$:
  Valence band edge to conduction band edge

• Fermi level
  Depends additionally on the doping level

  \[ n_o = N_c \exp[-q(E_c-E_f)/kT] \quad \text{and thus} \quad E_c - E_f = (kT/q) \ln \left( \frac{N_c}{n_o} \right) \]
  \[ p_o = N_v \exp[-q(E_f-E_v)/kT] \quad \text{and thus} \quad E_f - E_v = (kT/q) \ln \left( \frac{N_v}{p_o} \right) \]

  Work function, $\Phi$:
  Fermi level to vacuum ref.
Surface states - electron states on a surface

• Typical situation

  When the lattice terminates at a surface, additional electron states can appear. The number of states per unit area, $N_{SS}$, can be very large: $10^{12}$ to $10^{13}$ cm$^{-2}$, or more.

  These are typically acceptor-like states that are neutral when unoccupied, and negatively charged when occupied by electrons.

  The states are in a narrow range (± few 100 meV) centered about $E_{ss}$.

  If $E_F \gg E_{ss}$ in be bulk, the surface states will be occupied, and the negative charge in them will lead to depletion of the surface.

  This is shown on the next slide.
**Surface states, cont**

- Integrating $\rho(x)/\varepsilon_{Si}$ twice:

$$\frac{qN_D x_d^2}{2\varepsilon_{Si}} \approx E_c - E_{ss} - kT \ln \left( \frac{N_c}{N_D} \right) \quad \Rightarrow \quad qN_D x_d \approx \sqrt{\frac{2\varepsilon_{Si}}{q^2 N_D} \left[ E_c - E_{ss} - kT \ln \left( \frac{N_c}{N_D} \right) \right]}$$

- If $qN_D x_d < N_{ss}$, this is $x_d$. If not, then $x_d = N_{ss}/N_D$, and $\Delta E = qN_{ss}^2/2\varepsilon_{Si}N_D$
Surface states, cont

What about p-type samples?

We talked about acceptor-like states on n-type samples, states that are neutral when unoccupied ($E_F$ below them), and are negatively charged when occupied ($E_F$ above them).

There are also donor-like states which are neutral when occupied ($E_F$ above them) and positively charged when unoccupied ($E_F$ below them). These states pin the Fermi level near $E_{SS}$ on a p-type sample.

\[
E_F > E_{SS}, \text{ charge } = -q N_{ass} + 0 N_{dss} = -q N_{ass}
\]

\[
E_F < E_{SS}, \text{ charge } = 0 N_{ass} + q N_{dss} = q N_{dss}
\]
Surface states, cont

How many surface states are there? What is $N_{ss}$?

An interesting way to start is to ask how many bonds are broken when a zinc-blend or diamond lattice is cut parallel to a 100 face.

This is a huge number. If each of these bonds formed an acceptor-like surface state, it would take a depletion region 1 mm thick on the surface of an n-type sample ($N_d = 10^{17}$ cm$^{-3}$) to fill them all!

In reality, many of the severed bonds "heal" themselves, and actual surface state densities are typically on the order of $10^{13}$ to $10^{14}$ cm$^{-2}$, but this is still very large.

On silicon we can reduce $N_{SS}$ under $10^{11}$ cm$^{-2}$ by carefully growing a thermal oxide on the surface, and this is small enough that the Fermi level is not longer "pinned" at the surface. With the III-V's this is much more difficult to do (more in Lecture 13).

4 bonds per (5.6 Å x 5.6 Å) 
$\approx 10^{16}$ cut bonds per cm$^2$
Homojunctions - band picture, depletion approximation

- Band picture
  a. Isolated n- and p-type:

  i. Have same vacuum ref.,
  ii. Fermi levels differ
  iii. Both materials neutral
Homojunctions - band picture, depletion approximation

- Band picture, cont.
  
  b. **Electrically connected, and touching:**
  
  i. Charge shifts between sides; now have $\rho(x) \neq 0$
  
  ii. Equilibrium $\rho(x)$ corresponds to a constant Fermi level, $dE_F/dx = 0$
  
  iii. Reference level is now $-q\phi(x)$ where $\phi(x) = (q/\epsilon)\int\int \rho(x) \, dx \, dx$
  
  iv. Depletion approximation is a good estimate of $\rho(x)$
Band-edge profiles - key observations

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

Electrostatics:

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

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 \(\implies\) n large
3. Near VB \(\implies\) 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):

\[ J_e (x) = q n_o (x) \mu_e F (x) + q D_e \frac{d n_o}{dx} \]

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

First we calculate \( d n_o /dx \) and manipulate it a bit to get:

\[
\frac{d n_o}{dx} = n_o \left( - \frac{d E_c}{dx} + \frac{d E_F}{dx} \right) = n_o \left( \frac{n_o}{kT} \right) - qF (x) + \frac{d E_F}{dx} = \frac{\mu_e n_o}{D_e} \left( -F (x) + \frac{1}{q} \frac{d E_F}{dx} \right)
\]

where we have used:

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

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

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

From this result we see clearly that:

\[ J_e (x) = 0 \iff \frac{d E_F (x)}{dx} = 0 \]
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:

\[
\begin{align*}
n(x) &= \int_{E_c}^{\infty} \frac{\rho_{cb}(E)}{1 + e^{[E - E_{Fn}(x)]/kT}} dE \\
p(x) &= \int_{-\infty}^{E_v} \left\{1 - \frac{1}{1 + e^{[E - E_{Fp}(x)]/kT}}\right\} \rho_{vb}(E) dE = \int_{-\infty}^{E_v} \frac{\rho_{vb}(E)}{1 + e^{[E_{Fp}(x) - E]/kT}} dE
\end{align*}
\]
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 $E_{fp}$:

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

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

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* \( E_{Fn} : E_{Fn} (x) \equiv E_c (x) - kT \ln[N_c (x) / n(x)] \)

*We define* \( E_{Fp} \) *similarly:* \( E_{Fp} (x) \equiv E_v (x) + kT \ln[N_v (x) / p(x)] \)
**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

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

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:

\[
\begin{align*}
   n(x) &= n_{op} [ (e^{q v_{ab} / kT} - 1) e^{-x/L_e} + 1 ], \text{where } n_{op} = n_i^2 / N_{Ap} \\
\end{align*}
\]

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

\[
\begin{align*}
   n(x) &= n_{op} [ (e^{q v_{ab} / kT} - 1) e^{-x/L_e} + 1 ] \\&\approx n_{op} e^{q v_{ab} / kT} e^{-x/L_e}
\end{align*}
\]

from which we find:

\[
\begin{align*}
   E_{Fn}(x) = E_c + kT \ln[n(x)/N_c] \\
&\approx E_c + kT \ln[n_o/N_c] + q v_{ab} - kT x/L_e \\
&\approx E_{Fo} + q v_{ab} - kT x/L_e
\end{align*}
\]

We see that \( E_{Fn}(x) \) is \( q v_{AB} \) 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:**
Heterojunctions - band picture, depletion approximation

• Band picture
  a. **Isolated N- and p-type:** (taking an N-p junction as the example)

  ![Band Diagram](image)

  Similar to homojunction except that now the two materials have different electron affinities, energy gaps, dielectric constants, and effective masses.

  **Note on notation:** Capital letters (N, P, I, NID) are used to denote the doping of the wider bandgap material, and lower case (n, p, i, nid) for the narrower bandgap material.
Heterojunctions - band picture, depletion approximation

- Band picture, cont.
  - Electrically connected:
    i. Charge shifts between sides
    ii. Fermi levels shift until equal
    iii. Vacuum ref. is now $-q\phi(x)$ where $\phi(x) = (q/\varepsilon)\int\int \rho(x) \, dx \, dx$
    iv. $E_c(x)$ is $-q\phi(x) - \chi(x)$ and $E_v(x) = -q\phi(x) - [\chi(x) + E_g(x)]$
    v. Depletion approximation is a good estimate of $\rho(x)$

\[ \Delta E_c = |q(\chi_p - \chi_N)| \]
\[ \Delta E_v = |q(\chi_p - \chi_N) + E_g - E_{gN}| \]
Heterojunctions - band picture, depletion approximation

• Band picture, cont.
  
  c. Useful Observations:

    i. The final electrostatic potential profile, $\phi(x)$, is primarily a consequence of the doping levels.

    ii. The band-edge profiles, $E_c(x)$ and $E_v(x)$, are additionally a consequence of the electron affinity and energy gap profiles, $\chi(x)$ and $E_g(x)$, respectively.

    iii. In an abrupt heterojunction there are frequently discontinuities in the conduction and valence band edges at the junction. The relative sizes of these steps determine the “type” of the HJ.

*********

Type options:

Type I: $\Delta E_c > 0$ and $\Delta E_v < 0$, or vice versa ($\Delta E_c < 0$ and $\Delta E_v > 0$).
Type II: $\Delta E_c$ and $\Delta E_v$ have same sign (both $> 0$, or both $< 0$).
Type III: $\Delta E_c = 0$, $\Delta E_v \neq 0$
Type IV: $\Delta E_c \neq 0$, $\Delta E_v = 0$

(Note: Most heterojunctions by far are Type I. There are a few examples of Type II heterojunctions involving narrow gap arsenides and antimonides, and some Type I heterojunctions approximate Type III and IV heterojunctions.)
Heterojunctions - Types

- Another way of looking at the band line-up options

Focus on undoped structures where $\phi(x) \approx 0$:

**Type I**

$E_c^1 \downarrow \Delta E_{c12} \uparrow E_c^2$

$E_v^1 \downarrow \Delta E_{v12} \uparrow E_v^2$

**Type II**

$E_c^1 \downarrow \Delta E_{c12} \uparrow E_c^2$

$E_v^1 \downarrow \Delta E_{v12} \uparrow E_v^2$

**Type III**

$E_c^1 \downarrow \Delta E_{c12} \uparrow E_c^2$

$E_v^1 \downarrow \Delta E_{v12} \uparrow E_v^2$

**Type IV**

$E_c^1 \downarrow \Delta E_{c12} \uparrow E_c^2$

$E_v^1 \downarrow \Delta E_{v12} \uparrow E_v^2$

**Comments:**

When describing a heterojunction people often list on $E_{g1}$, $E_{g2}$, $\Delta E_c$ and $\Delta E_v$, but not $\chi_1$ and $\chi_2$.

Most heterojunctions are Type I heterojunctions. A few antimonide/arsenide combinations result in Type II heterojunctions. Perfect Type III and IV junctions are rare (if they exist at all), but some Type I heterojunctions are good approximations to them. It is possible to have Type II heterojunctions in which the narrower bandgap material has the smaller electron affinity.
Heterostructures - multiple junction structures

• With multiple junctions we can create potential wells and barriers for electrons and holes
  Again we draw undoped structures where $\phi(x) \approx 0$:

  ![Energy Well](image1) ![Energy Barrier](image2) ![Superlattice](image3)

• Amazingly, this the band-edge profile modeling can be used down to very small dimensions (corresponding to layers a few monolayers thick) even though it is based on modeling perfect lattices infinite in extent.
  This is true as long as we can assume that the lattice is perfect and the periodicity of the atom spacing continues when crossing a heterojunction, even though the identities of the elements occupying the sites may change. This in turn means we have to be careful when choosing the materials for our heterostructures and in producing them.
Modulation doping - separating dopants and carriers

Demonstration structure:

• The objective is to increase the carrier mobility and reduce the noise associated with ionized impurity scattering
Heterostructures - graded structures

- We can also grade the composition over some distance to create structures in which the electron affinity, $\chi$, and energy gap, $E_g$, vary smoothly with position.

This is usually done for one of two reasons:

1. Grading to remove band-edge discontinuities and eliminate spikes

2. Grading to create built-in fields to drift minority carriers

Graded composition, p-type (linear grading shown)

Graded interface (linear grading shown)
Heterojunctions

- Grading out a spike
  N-p heterojunction

Top right: abrupt HJ
Lower right: interface graded over 0.2 µm
Key below
Graded composition p-type heterostructure with uniform low level electron injection.

Assume the grading is from $E_{g1}$, $\chi_1$ @ $x = 0$, and $E_{g2}$, $\chi_2$ @ $x = L$.

$$E_g(x) = E_{g1} + x(E_{g2} - E_{g1})/L; \quad \chi(x) = \chi_1 + x(\chi_2 - \chi_1)/L$$

In thermal equilibrium the Fermi level, $E_{fo}$, is flat, and the valence band edge is flat:

$$E_v = E_{fo} - kT \ln(N_v/N_{Ap})$$

whereas the conduction band edge slopes:

$$E_c(x) = E_v - E_g(x)$$

With low-level electron injection, $n(x) \approx n' (\gg n_{po})$:

Hole population is changed insignificantly, and $E_{fp}(x) \approx E_{fo}$

Electron population is now $n'$, and so

$$E_{fn}(x) = E_c + kT \ln[n'/N_c] \approx E_v + E_g(x) + kT \ln[n'/N_c]$$

Using this to get $J_e(x)$, we find

$$J_e(x) \approx \mu_e n' \frac{\partial E_g(x)}{\partial x} = q \mu_e n' F_{e,eff}, \text{ where } F_{e,eff} = q^{-1} \frac{\partial E_g(x)}{\partial x}$$

From this we see that the band gap grading acts like an effective electric field acting on the electrons (but not on the holes)!
**Quasi-Fermi levels** - Illustrating example C

**Example C:**

\[ F_{e,\text{eff}} \equiv q^{-1} \partial E_c(x)/\partial x = -(E_{g1} - E_{g2})/qL \]
D. General meaning of band-edge gradings

In general we can write the electron quasi-Fermi level as:

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

and thus in general we can write the electron current as:

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

\[ = \mu_e n(x) \frac{\partial E_c(x)}{\partial x} + \mu_e kT \frac{\partial n(x)}{\partial x} + \mu_e kT \frac{n(x)}{N_c(x)} \frac{\partial N_c(x)}{\partial x} \]

\[ = \sigma_e \frac{q^{-1} \partial E_c(x)}{\partial x} + D_e \left( \frac{\partial n(x)}{\partial x} + \frac{n(x)}{N_c(x)} \frac{\partial N_c(x)}{\partial x} \right) \]

Drift Term

Diffusion Term

typically small

Note: In getting this we have used the Einstein relation and definition of conductivity:

\[ \mu_e kT = q D_e, \quad \text{and} \quad \sigma_e = q \mu_e n(x) \]

From our final result we see that the gradient in the conduction band edge is the force leading to electron drift, while the gradient in the carrier and density of states concentrations are the diffusion force.

Discussion continued for holes on next foil.
We obtain the corresponding result for holes if we similarly substitute valence band quantities for conduction band quantities. Begin with:

\[ E_{fp}(x) = E_v(x) + kT \ln[p(x)/N_v(x)] \]

and thus

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

\[ J_h(x) = \mu_h p(x) \frac{\partial E_v(x)}{\partial x} + \mu_h kT \frac{\partial p(x)}{\partial x} + \mu_h kT \frac{p(x)}{N_v(x)} \frac{\partial N_v(x)}{\partial x} \]

Now we see that the gradient in the valence band edge is the force leading to hole drift, while the gradient in the carrier and density of states concentrations are the diffusion force.

Summarizing, the conduction and valence band-edge gradients can be viewed as effective electric fields for electrons and holes, respectively:

\[ F_{e,\text{eff}} = q^{-1} \frac{\partial E_c(x)}{\partial x} \]  
\[ \text{and} \]  
\[ F_{h,\text{eff}} = q^{-1} \frac{\partial E_v(x)}{\partial x} \]