Lecture 16: Heterojunctions - Electrostatics
Sze And Ng: Chapter 2.7

Announcements
Homework 4/4:

• Online now.
• Due Tuesday 12th March at the start of the lecture (08:30am).
• I will return it on the day of the final (18th March).
• I will post the solutions when I receive the homeworks.
• Homework 4 will consist of content covered in Lectures 12-15.
Announcements

Final Exam

- **Scheduled** for Monday 18th March 2019 at **09:30am**.
- Exam will last 80 minutes.
  - The exam will start exactly at **08:30am**!
- Closed book and closed notes.
- You can, and are expected to, use a calculator.
- Choose 2 out of 3 questions.
  - If you answer 3 I will take best 2 scores.
- It will contribute 30% of overall grade for class.
- The exam will material covered in lectures 9-17 (inclusive).
- There will be 25 marks per question. 50 total.
Lecture 16

• Electrostatics of Anisotype Heterojunction.
• Deriving the Electrostatic Potential.
• Other Parameters.
• Isotype Heterojunctions.

Extra Information

• The below document from Cornell has a good description of what we are talking about today (and Lectures 15 & 17 also):
  • https://courses.cit.cornell.edu/ece533/Lectures/handout2.pdf
• The document goes way beyond the scope of our course.
  • They cover quantized systems as well if you are interested.
Electrostatics of Anisotype Heterojunction

Electrostatics

- Last time we drew the band diagrams of example heterojunctions using thought experiments / intuition.
- Today we are going to derive the electrostatic potential as a function of position.
  - This allows us to derive the band diagram (quantitatively) as a function of position.
  - We can also evaluate parameters such as the width of the depletion width.
Electrostatic Potential

- In order to derive the band-diagram (quantitatively) we need to evaluate the electrostatic potential.
- Energy bands can just then be derived from potential (+ a constant) via:

\[ \phi = - \frac{E_i}{e} \]  

(1)

- Where:
  - \( \phi \) is the electrostatic potential.
  - \( E_i \) is the intrinsic energy.
  - \( e \) is the fundamental unit of charge.
Electrostatic Potential

• We can use Poisson's Equation (in one dimension) to get the electrostatic potential from charge density:

\[ \frac{d^2 \phi}{dx^2} = -\frac{\rho(x)}{\varepsilon_r \varepsilon_0} \] (2)

• Where:
  • \( \phi \) is the electrostatic potential.
  • \( x \) is the direction of interest.
  • \( \rho \) is the charge density.
  • \( \varepsilon_r \) is the relative permittivity.
  • \( \varepsilon_0 \) is the relative permittivity.

Strategy

• Our strategy is very similar to that of a pn-junction.
• We need to solve Poisson's equation, subject to the appropriate boundary condition.
• We will tackle this problem using the depletion approximation, which entails assuming:
  • All of the charge in the SCR is associated with localized ionized impurities.
  • The amount of delocalized charge due to electrons and holes is negligible.
• Note: in the literature sometimes \( n \) and \( p \) subscripts are used rather than 1 and 2 for the semiconductors.
Ideal Band Diagram

- We are going to study the specific example below:

- This is a Type I (Straddling) anisotype heterojunction.

Boundary Conditions

- Let’s start by defining some boundary conditions before we tackle the Poisson Equation.
- Last time we found (technically we enforced) that the potential is continuous across the interface:
Boundary Conditions

- We will label the potential on the left side (p-side in this case) as $\psi_1$.
- We will label the potential on the left side (n-side in this case) as $\psi_2$.
- The use of $\psi$ rather than $\phi$ is simply because we are now running low on variables.
  - For example, we are using $\phi_1$ and $\phi_2$ as work functions now.

We can express the first boundary condition as:

$$\psi_1(x = 0) = \psi_2(x = 0) \equiv \psi(x = 0)$$  \hspace{1cm} (3)

We can also see that as $x \to \infty$ we approach the built-in potential:

$$\psi_2(x \to \infty) = \phi_{bi}$$  \hspace{1cm} (4)
Boundary Conditions

- Additionally, if we assume that there is no interface state charge at the interface, the electrostatic boundary condition states that the \textbf{electric displacement} is continuous across the interface:

\[
\epsilon_1 \frac{d\psi_1(0)}{dx} = \epsilon_2 \frac{d\psi_2(0)}{dx} \quad \text{At } x = 0
\]

• This is our second boundary condition.

• As a temporary aside, consider what this means for the electric field across the interface:

\[
\varepsilon = -\frac{d\psi}{dx}
\]

• Hence if \( \epsilon_1 \neq \epsilon_2 \), this leads to a \textbf{discontinuity} in the electric field across the junction.
Boundary Conditions

- We can also say that the electric field outside of the space charge regions is zero.
- This has not changed re: pn junctions.
- We defining the edge of space charge region using the following notation:
- We can hence express this boundary condition as:

\[
\frac{d\psi_1(-W_{d1})}{dx} = \frac{d\psi_2(W_{d2})}{dx} = 0
\]

- We will call this Boundary Condition 3.

Deriving the Electrostatic Potential
Charge Density

- The approach we follow is similar to what we followed when looking at pn-junctions.
  - The example (anisotype) we are looking at is a pn-junction, just using dissimilar semiconductors.
  - By assuming that each acceptor donates a hole and that each donor donates an electron, we can approximate the free carrier density as follows.
  - Once again, we assume an abrupt interface.

\[ \rho(x) = \begin{cases} 
-eN_A & -W_{d1} < x < 0 \\
+eN_D & 0 < x < W_{d2} \\
0 & \text{elsewhere} 
\end{cases} \]
Electric Field

- We can get the electric field from the first integral of the charge density:
\[
\frac{d\psi}{dx} = -\mathcal{E}(x) = -\int \frac{\rho(x)}{\epsilon_r \epsilon_0} \, dx \tag{9}
\]

- We can show:
\[
\mathcal{E}(x) = \begin{cases} 
- \frac{eN_A}{\epsilon_1 \epsilon_0} (W_{d1} + x) & -W_{d1} < x < 0 \\
- \frac{eN_D}{\epsilon_2 \epsilon_0} (W_{d2} - x) & 0 < x < W_{d2} \\
0 & \text{elsewhere}
\end{cases} \tag{10}
\]

- So this looks pretty similar to a conventional pn junction, except now the relative permittivities are not necessarily equal.

- What about at the interface?
\[
\mathcal{E}_1(0) = -\frac{eN_D}{\epsilon_1 \epsilon_0} W_{d1} \tag{13} \quad \mathcal{E}_2(0) = -\frac{eN_D}{\epsilon_2 \epsilon_0} W_{d2} \tag{14}
\]
**Electric Field**

- I.e. for the heterojunction we observe a discontinuity in the electric field at the interface.
- For example if $\varepsilon_2 > \varepsilon_1$ we would draw the field like this.
- If $\varepsilon_2 = \varepsilon_1$ the field reverts back to the that of a standard pn junction.

**Electrostatic Potential**

- To get the electrostatic potential ($\psi$) we have to integrate again.

$$\frac{d\psi}{dx} = -\varepsilon(x) \quad (9)$$

- We can show that:

$$\psi(x) = \begin{cases} 
0 & x < -W_{d1} \\
\frac{eN_A}{2\varepsilon_1\varepsilon_0} (x + W_{d1})^2 & -W_{d1} < x < 0 \\
\frac{eN_A W_{d1}^2}{\varepsilon_1\varepsilon_0} + \frac{eN_D}{2\varepsilon_2\varepsilon_0} (2W_{d2}x - x^2) & 0 < x < W_{d2} \\
\frac{eN_A W_{d1}^2}{2\varepsilon_1\varepsilon_0} + \frac{eN_D W_{d2}^2}{2\varepsilon_2\varepsilon_0} & x > W_{d2}
\end{cases} \quad (15)$$
Electrostatic Potential

• So is the electrostatic potential continuous?
• Evaluate both sides at $x = 0$:

$$\psi_1(x) = \frac{eN_A}{2\varepsilon_1\varepsilon_0} (x + W_{d1})^2 \quad \psi_1(0) = \frac{eN_A}{2\varepsilon_1\varepsilon_0} W_{d1}^2$$

$$\psi_2(x) = \frac{eN_A W_{d1}^2}{\varepsilon_1\varepsilon_0} + \frac{eN_D}{2\varepsilon_2\varepsilon_0} (2W_{d2}x - x^2) \quad \psi_2(0) = \frac{eN_A W_{d1}^2}{\varepsilon_1\varepsilon_0}$$

• We see that:

$$\psi_1(x = 0) = \psi_2(x = 0) \equiv \psi(x = 0) \quad (3)$$

• Which confirms our first boundary condition.

Electrostatic Potential

• Hence we can go ahead and plot our potential as we have previously.
• So the approach we followed in Lecture 2 is almost identical to this.
• However the fact that $\varepsilon_1 \neq \varepsilon_2$ does lead to a discontinuity in the electric field.
Other Parameters

Built-In Potential

- From Equation (15) we can identify the built in potential as:
  \[
  \psi_2(W_{d2}) = \phi_{bi} = \frac{eN_A W_{d1}^2}{2\varepsilon_1 \varepsilon_0} + \frac{eN_D W_{d2}^2}{2\varepsilon_2 \varepsilon_0}
  \] (16)

- We can denote the potential dropped across region 1 and region 2 as follows:
  \[
  \phi_{bi,1} = \psi_1(0) - 0 = \frac{eN_A}{2\varepsilon_1 \varepsilon_0} W_{d1}^2
  \] (17)

  \[
  \phi_{bi,2} = \phi_{bi} - \psi_2(0) = \frac{eN_A W_{d1}^2}{2\varepsilon_1 \varepsilon_0} + \frac{eN_D W_{d2}^2}{2\varepsilon_2 \varepsilon_0} - \frac{eN_A W_{d1}^2}{\varepsilon_1 \varepsilon_0}
  \]

  \[
  \phi_{bi,2} = \frac{eN_D W_{d2}^2}{2\varepsilon_2 \varepsilon_0}
  \] (18)
Built-In Potential

- Identify the built-in potential as the sum of these two variables:

\[ \phi_{bi} = \phi_{bi,1} + \phi_{bi,2} \quad (20) \]

- As usual, we can say that the 2-dimensional charge density either side of the junction is equal:

\[ eN_A W_{d1} = eN_D W_{d2} \quad (21) \]

- Taking the ratio of Equation (17) over Equation (18) and using Equation (21) we find that

\[ \frac{\phi_{bi,1}}{\phi_{bi,2}} = \frac{\epsilon_2 N_D}{\epsilon_1 N_A} \quad (22) \]

This equation shows that \( \phi_{bi} \) is partitioned according to a ratio of the product of the respective dielectric constants and the doping densities.

Since the dielectric constants are not likely to vary too much (~within an order of magnitude) for most semiconductors, \( \phi_{bi} \) partitioning depends primarily on doping (could be many orders of magnitude), similar to a \( pn \) homojunction.
Depletion Width

- Use Equations (17)-(22) we can show:

\[ W_{d1} = \frac{2\varepsilon_0 \varepsilon_1 \varepsilon_2 N_D \phi_{bi}}{eN_A (\varepsilon_1 N_A + \varepsilon_2 N_D)} \]  
(23)

\[ W_{d2} = \frac{2\varepsilon_0 \varepsilon_1 \varepsilon_2 N_A \phi_{bi}}{eN_D (\varepsilon_1 N_A + \varepsilon_2 N_D)} \]  
(24)

- Define the total equilibrium depletion width:

\[ W_0 = W_{d1} + W_{d2} \]  
(25)

\[ W_0 = \frac{2\varepsilon_0 \varepsilon_1 \varepsilon_2 (N_A + N_D)^2 \phi_{bi}}{eN_A N_D (\varepsilon_1 N_A + \varepsilon_2 N_D)} \]  
(26)

Applied Voltage

- This gives us an expression for \( W_0 \) in terms of the semiconductor dielectric constants, doping densities, and \( \phi_{bi} \).

- If we generalize this to account for non-equilibrium conditions in which a voltage \( V \) is applied to the heterojunction we obtain:

\[ W(V) = \frac{2\varepsilon_0 \varepsilon_1 \varepsilon_2 (N_A + N_D)^2 (\phi_{bi} - V)}{eN_A N_D (\varepsilon_1 N_A + \varepsilon_2 N_D)} \]  
(27)
Applied Voltage

\[
W(V) = \sqrt{\frac{2\varepsilon_0 \varepsilon_1 \varepsilon_2 (N_A + N_D)^2 (\phi_{bi} - V)}{eN_A N_D (\varepsilon_1 N_A + \varepsilon_2 N_D)}}
\] (27)

- As usual, \( V \) is positive for forward bias and negative for reverse bias.
- Charge balance allows us to express the depletion layer charge per unit area as:

\[
Q_{depl} = -eN_A W_{d1} = eN_D W_{d2}
\] (28)

\[
Q_{depl} = \sqrt{\frac{2eN_A N_D \varepsilon_0 \varepsilon_1 \varepsilon_2 (\phi_{bi} - V)}{(\varepsilon_1 N_A + \varepsilon_2 N_D)}}
\] (29)

Surface States
- In our electrostatic treatment, we assumed that there were no interface states and no interfacial dipole.
- If interface states are present, then the electric displacement is no longer continuous across the interface and the boundary condition would have to be modified as:

\[
\varepsilon_1 \frac{d\psi_1(0)}{dx} \pm eN_{IT} = \varepsilon_2 \frac{d\psi_2(0)}{dx}
\] (30)

- Where \( N_{IT} \) is the number of interface states per unit area and the "+" and "−" signs indicate the polarity of the interface trap charge.
Isotype Heterojunctions

- Up until now we have just looked anisotype heterojunctions.
- While highly technologically relevant, anisotype junctions require only a few generalizations to be made to the theory of pn junctions.
  - This is ideal theory of course.
  - Interface states in heterojunctions are going to be much more prevalent, and influential than pn-junctions.
- We have yet to really discuss isotype junctions.
Isotype Heterojunctions

- Recall from last lecture the distinction is based on the type of semiconductors involved:

  **Isotype**
  - Same conductivity type (n-n or p-p).

  **Anisotype**
  - Opposite conductivity type (p-n, n-p).

Isotype Band Structure

- There are wide range of different isotype junctions we could consider.
- Here let us consider the following nn isotype heterojunction
Isotype Band Structure

• Equilibrate the Fermi energies and include the local vacuum level:

Isotype Band Structure

• Enforce the condition that electron affinity (with respect to $E_{L,VAC}$) is constant up to the interface:
Isotype Band Structure

- Do the same with the ionization potential:

Isotype Band Structure

- So the picture is not dissimilar to what we have seen before:
Built In Potential

- We are going to use the Quasi Fermi-Level model to evaluate some parameters.
- From the previous slide we identify the built-in potential as the difference between the two Fermi levels:
  \[ e\phi_{bi} = E_{F2} - E_{F1} \] (31)
- Recall from Equation (8), Lecture 15, that we can express the Quasi Fermi Energy on an n-type semiconductor by:
  \[ E_{Fn}(x) = E_C(x) - e\phi(x) + k_B T \ln[n(x)] - k_B T \ln[N_C(x)] \] (32)

- Where
  - \( n(x) \) is electron number density at \( x \).
  - \( N_C(x) \) conduction band DOS at \( x \).
  - \( E_{Fn}(x) \) quasi Fermi Level at \( x \).
  - \( \phi(x) \) potential drop at \( x \) due to applied external voltage
- Consider the system with no external applied voltage:
  \[ E_{F0n}(x) = E_C(x) + k_B T \ln[n(x)] - k_B T \ln[N_C(x)] \] (33)
Built In Potential

• Aside from temperature, each of these parameters is going to be distinct for each semiconductor:

\[
E_{F_1}(x) = E_{C_1}(x) + k_B T \ln[n_1(x)] - k_B T \ln[N_{C_1}(x)] \tag{34}
\]

\[
E_{F_2}(x) = E_{C_2}(x) + k_B T \ln[n_2(x)] - k_B T \ln[N_{C_2}(x)] \tag{35}
\]

• When talking about the built-in potential, we are interested in the parameters a long way from the junction.

• We also know that a long way from the interface we can say:

\[
n_1(x \to -\infty) = N_{D_1} \tag{36}
\]

\[
n_2(x \to +\infty) = N_{D_2} \tag{37}
\]

Built In Potential

• A long way from the interface we will also say that the conduction band energies and density of states take their unperturbed values (i.e. their values if isolated):

\[
E_{C_1}(x \to -\infty) \equiv E_{C_1} \tag{38}
\]

\[
E_{C_2}(x \to +\infty) \equiv E_{C_2} \tag{39}
\]

\[
N_{C_1}(x \to -\infty) \equiv N_{C_1} \tag{40}
\]

\[
N_{C_2}(x \to +\infty) \equiv N_{C_2} \tag{41}
\]

• Hence we can say the bulk Fermi Energies are now:

\[
E_{F_1}(x \to -\infty) = E_{C_1} + k_B T \ln[N_{D_1}] - k_B T \ln[N_{C_1}] \tag{42}
\]

\[
E_{F_2}(x \to +\infty) = E_{C_2} + k_B T \ln[N_{D_2}] - k_B T \ln[N_{C_2}] \tag{43}
\]
**Built In Potential**

- Combining Equations (42), (43) and (31) we can say:

\[ e\phi_{bi} = \Delta E_C + k_B T \ln \left( \frac{N_{D2} N_{C1}}{N_{D1} N_{C2}} \right) \]  
(44)

- Where:

\[ \Delta E_C = E_{C2} - E_{C1} \]  
(45)

- So this is the built-in potential, in a reasonably useful form.

- But how do we evaluate electric field?
- First we need to consider what charges there are (if any).

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**Electric Field**

- Let’s return to our diagram:

- Do we have a depletion region in such a heterojunction? It is not immediately obvious.
Charge Density

- Let’s start by thinking about semiconductor 1.
- What gives rise to a charge density in pn junctions?
  - Ionized impurity atoms. I.e. dopants that do not have their respective hole / electron.
  - In an n-type semiconductor we can say that the charge density at position $x$ is due to the dopant density minus the mobile charge density.
  - I.e. in semiconductor 1 we can say:
    $$\rho_1(x) = e[N_{D1} - n(x)]$$  \hspace{1cm} (46)
- We have seen similar expressions in terms of non-abrupt pn-junctions.

Charge Density

- From our Quasi-Fermi Level Theory, we have an expression for the carrier density in an n-type semiconductor:
  $$n(x) = N_C(x) \exp \left[ \frac{E_{F_n}(x) - E_C(x) + e\phi(x)}{k_B T} \right]$$  \hspace{1cm} (47)
- We are not going to worry about applied biases for now:
  $$n(x) = N_{C1}(x) \exp \left[ \frac{E_{F1}(x) - E_{C1}(x)}{k_B T} \right]$$  \hspace{1cm} (48)
- How do we get this into a useable form?
Electric Field

- Let’s put electrostatic potential into our diagram:

![Diagram of Electric Field](image)

- We see here that at \( x \to -\infty, \psi_1 = 0 \).

Charge Density

- From our diagram we also see that the conduction band at \( x \) can be re-written as:

\[
E_{C1}(x) = E_{C1}(-\infty) - e\psi_1(x)
\]  
(49)

- (Follow the conduction band if you are not sure why this is the case).

- Put (49) into (48):

\[
n(x) = N_{C1}(x) \exp \left[ \frac{E_{F1}(x) - E_{C1}(-\infty) + e\psi_1(x)}{k_B T} \right]
\]  
(50)

\[
n(x) = N_{C1}(x) \exp \left[ \frac{E_{F1}(x) - E_{C1}(-\infty)}{k_B T} \right] \exp \left[ \frac{-e\psi_1(x)}{k_B T} \right]
\]  
(51)
Charge Density

• We identify the density of donor states:

\[ N_{D1} = N_{C1} \exp \left[ \frac{E_{F1} - E_{C1}(\infty)}{k_B T} \right] \quad (52) \]

• Hence we can say:

\[ n(x) = N_{D1} \exp \left[ \frac{e \psi_1(x)}{k_B T} \right] \quad (53) \]

• Putting this back into (46):

\[ \rho_1(x) = e \left[ N_{D1} - N_D \exp \left[ \frac{e \psi_1(x)}{k_B T} \right] \right] \quad (54) \]

\[ \rho_1(x) = eN_{D1} \left[ 1 - \exp \left[ \frac{e \psi_1(x)}{k_B T} \right] \right] \quad (55) \]

Electric Field

• Putting (55) into Poisson’s Equation gives you:

\[ \frac{d^2 \psi_1}{dx^2} = -\frac{eN_{D1}}{\epsilon_1 \epsilon_0} \left[ 1 - \exp \left[ \frac{e \psi_1(x)}{k_B T} \right] \right] \quad (56) \]

• We are not going to solve the equation, just quote the result at \( x = 0 \).

\[ \mathcal{E}_1(x = 0) = \sqrt{\frac{2N_{D1} k_B T}{\epsilon_1 \epsilon_0}} \left[ \exp \left[ \frac{e \psi_1(0)}{k_B T} \right] - 1 - \frac{e \psi_1(0)}{k_B T} \right] \quad (57) \]

• On the other side we find:

\[ \mathcal{E}_2(x = 0) = \sqrt{\frac{2N_{D2} \psi_2(0)}{\epsilon_2 \epsilon_0}} \quad (58) \]
Summary

- We derived the electrostatic potential of an anisotype junction.
- We looked at an example of an isotype junction and were able to evaluate the electric field at the interface.

Next Time…

- Current voltage characteristics
- And Final Exam details / course summary.