Lecture 2: pn Junction Formation
Sze And Ng: Chapter 2

Announcements
Homework 1/4:
• Will be online after the Lecture on Thursday 17th January.
• Total of 25 marks.
• Each homework contributes an equal weight.
  • All homework contributes to 40% of overall grade.
  • Each homework contributes 10% of overall grade.
• Due Thursday 24th January at the start of the lecture (08:30am).
• I will return it one week later (31st January).
• I will post the solutions when I return the homeworks.
• Homework 1 will consist of content covered in Lectures 2 - 4.
Last Time

- Semi-classical Newtonian mechanics may be used to describe the motion of charge carriers in a crystal if $m$ in $F = ma$ is replaced by an effective mass $m^*$.  
  - I.e. This means that $e^-$ and $h^+$ will respond to external fields in a crystal almost as if they were in a vacuum, but with different $m^*$.  

$$m^* = \frac{\hbar}{\frac{\partial^2 E}{\partial k^2}}$$

- Lots of quantum mechanics is buried in the $m^*$ term, which depends on the quantitative characteristics of the band structure.

Lecture 2

- pn-Junction  
- Electrostatics.  
- pn Junction Band Diagrams.
pn-Junctions

pn-Junction Diodes

• While there are various structures that lead to rectification (e.g. Schottky diodes, tunneling diodes), pn-junctions are the most common.

• A pn-junction diode is formed by placing a p-doped semiconductor next to an n-doped semiconductor.
pn-Junction Diodes

- Conceptually this is an easy way to think about pn-junctions.
  - And can actually be achieved with epitaxial growth of one semiconductor on top of another.
- Normally however, a pn-junction would be created by adjusting doping properties of a single semiconductor (e.g. Si).
  - We will not concern ourselves with this detail today.

Doping

- First, let us remind ourselves what we are doing when we dope a semiconductor.
  - N-type:
    - We are **adding** an electron and a proton in a certain position.
  - P-type:
    - We are **removing** an electron and a proton in a certain position.
Doping

• Hence we are not changing the charge on the atom.
  • A doped semiconductor is neutral!

• N-type:
  • Because the valence has changed, the extra electron does not participate in bonding.
  • It is very weakly bound to its host atom, and essentially is free to move around the lattice.

• P-type:
  • Because the valence has changed, there is a broken bond and a missing electron
  • This absence of an electron (hole) can “move” by electrons around it filling its place.
Doped Semiconductors

• What does this look like in a simple band diagram?
• Our intrinsic (undoped) semiconductor can be pictured like this:

\[ E \]
\[ E_C \]
\[ E_V \]

- At room-temperature and in the dark, there should be very few free carriers.
- Intrinsic silicon is highly resistive.

Doped Semiconductors

• Doping the semiconductor will, at room temperature, add electrons to the conduction band (n-type) or add holes to the valence band (p-type):

\[ E \]
\[ E_C \]
\[ E_V \]

- p-type
- n-type
pn-Junctions

- What happens when we bring these two semiconductors into contact?
- Fermi level must be uniform throughout!
  - If not, carriers will move to correct it.

\[ \begin{align*}
\text{p-type} & \quad \text{n-type} \\
\vdots & \quad \vdots \\
& \quad E_F \\
& \quad E_F
\end{align*} \]

- Carriers are now free to diffuse into adjacent semiconductor.
- We now have holes in the n-type semiconductor and electrons in the p-type semiconductor.
pn-Junctions

- This will lead to annihilation.
- The region close to the junction will be devoid of free carriers.
  - This is called the depletion region.

Away from the depletion region there are still free carriers.
- We define the depletion width on the n-side $W_{dn}$ and the depletion width on the p-side $W_{dp}$.

$$\begin{align*}
\text{p-type} & \quad W_{dp} & \quad W_{dn} & \quad \text{n-type}
\end{align*}$$
pn-Junctions

- What about charge neutrality?
- Away from the interface: \( n \approx N_D \) and \( p \approx N_A \).
- Close to the interface however, we are left with ionized dopant atoms.

Rectification

- We will show the Fermi level must be constant.
- This means the absolute values of the bands must be offset relative to each other.
Reverse Bias

- Apply bias from right to left.
- I.e. we are attracting electrons from left to right.

Free carriers will start to move outwards.

Carriers will not be able to continue to flow.
Forward Bias

- Apply bias from left to right.
- i.e. we are attracting electrons from right to left
- As long as we can overcome the barrier potential (e.g. 0.7 eV), carriers can move towards each other.

- Depletion region will shrink.
- Carriers will recombine and can continue to be injected.
Summary of pn Junctions

• At the junction, there is a large gradient of $e^-$ and $h^+$.  
• Diffusion currents flow because of the concentration gradient.  
• As the mobile carriers diffuse across the junction and recombine, they leave behind "uncovered" immobile charge (ionized donors and acceptors).  
• The uncovered ionized dopants give rise to a built in electric field which produces a drift current that opposes and eventually exactly balances (equilibrium) the diffusion of mobile carriers.
Summary of pn Junctions

- This region of uncovered immobile charges near the junction is known as the "space charge" region (SCR). It is also known as the "depletion" region due to the depletion of mobile charge carriers.

Drift Current

- Equilibrium is reached when the overall e\(^-\) and h\(^+\) currents (due to drift and diffusion) are equal to zero.
- Let’s start with holes.
- We describe drift current by:
  \[ J_p = e\mu_p p \varepsilon \]
- \( J_p \) is hole current density.
- \( e \) is the magnitude of the fundamental unit of charge.
- \( \mu_p \) is the mobility of holes.
- \( p \) is the hole number density.
- \( \varepsilon \) is the electric field strength.
**Diffusion Current**

- Equilibrium is reached when the overall $e^-$ and $h^+$ currents (due to drift and diffusion) are equal to zero.
- Let’s start with holes.
- We describe diffusion current by:
  
  $$J_p = eD_p \frac{dp}{dx}$$

- $J_p$ is hole current density.
- $e$ is the magnitude of the fundamental unit of charge.
- $D_p$ is the diffusion coefficient of holes.
- $p$ is the hole number density.
- $x$ is the diffusion direction.

**Boltzmann Distribution**

- We approximate the distribution of carriers by the Boltzmann Distribution:
  
  $$p = p_i \exp\left(\frac{(E_i - E_F)}{k_BT}\right)$$

- $p$ is hole number density.
- $p_i$ is intrinsic hole number density.
- $E_i$ is the energy.
- $E_F$ is the Fermi energy.
- $k_B$ is the Boltzmann Constant.
- $T$ is the temperature.
Boltzmann Distribution

- The Boltzmann Distribution is an approximation of the Fermi Function:

\[ p \approx p_i \exp \left( \frac{E_i - E_F}{k_B T} \right) \]

- Only valid if \( (E_i - E_F) \gtrsim 3k_B T \).

Electrostatic Potential

- Equilibrium is reached when the overall e\(^-\) and h\(^+\) currents (due to drift and diffusion) are equal to zero.

\[ J_p = e \mu_p p \varepsilon - e D_p \frac{dp}{dx} = 0 \] (1)

- Describe carriers by Maxwell-Boltzmann distribution:

\[ p = p_i \exp \left( \frac{E_i - E_F}{k_B T} \right) \] (2)

- We need first derivative with respect to \( x \):

\[ \frac{dp}{dx} = \frac{p}{k_B T} \left[ \frac{dE_i}{dx} - \frac{dE_F}{dx} \right] \] (3)
Electric Field Strength

\[ \frac{dp}{dx} = \frac{p}{k_B T} \left[ \frac{dE_i}{dx} - \frac{dE_F}{dx} \right] \quad (3) \]

- From the definition of voltage \((V)\):
  \[ \mathcal{E} = \frac{dV}{dx} \]

- Voltage and energy are related by:
  \[ E = eV \]

- Hence we can say:
  \[ \frac{dE}{dx} = e\mathcal{E} \quad (4) \]

Electrostatic Potential

- We also need to use the Einstein relationship.
  \[ D_p = \frac{k_B T}{e} \mu_p \quad (5) \]

- Combining (1), (3), (4) and (5), we can show:
  \[ \frac{dE_F}{dx} = 0 \quad (6) \]

- I.e. we have shown that the Fermi Energy must be constant throughout our junction.
pn Junction Band Diagrams

Band Diagram
Electric Field

• The electric field is defined as the force acting on a unit positive charge.

• For electrons:
  \[ \mathbf{E} = \frac{F}{e} \]  
  (7)

• For holes:
  \[ \mathbf{E} = -\frac{F}{e} \]  
  (8)

• For a conservative field.
  \[ F = -\nabla E(r) \]  
  (9)

Since the force is defined with respect to the gradient of the potential energy, we can use the variation \( E_C \), \( E_V \), and \( E_i \) to calculate force.

\[ F = e\mathbf{E} = -\nabla E(r) \]  
(10)

In one dimension this is what we saw:

\[ \frac{dE}{dx} = e\mathbf{E} \]  
(4)

So we can describe the electric field in terms of band curvature:

\[ \mathbf{E} = \frac{1}{e} \frac{dE_C}{dx} \]  
(11)

\[ \mathbf{E} = \frac{1}{e} \frac{dE_V}{dx} \]  
(12)
Electrostatic Potential

• The electric field $\mathcal{E}$ is equal to the negative gradient of the electrostatic potential $\phi$:

$$\mathcal{E} = -\nabla \phi(r)$$  \hspace{1cm} (13)

$$\mathcal{E} = -\frac{d\phi}{dx}$$  \hspace{1cm} (14)

• Substituting Equation (4)

$$\phi = -\frac{E_i}{e}$$  \hspace{1cm} (15)

• This says that $\phi$ is directly related to the intrinsic level ($E_i$) of an energy band diagram. (Just "flip over" $E_i$ (or $E_C$ or $E_V$) to arrive at the electrostatic potential.)

Poisson’s Equation

• To draw the diagrams we want, we need to use Poisson’s Equation:

$$\frac{d^2 \phi}{dx^2} = -\frac{\rho(x)}{\epsilon_r \epsilon_0}$$  \hspace{1cm} (16)

• $\epsilon_r$: relative permittivity

• $\epsilon_0$: vacuum permittivity

• $\rho$ is the charge density at position $x$:

$$\rho(x) = e[p - n + N_D^+ - N_A^-]$$  \hspace{1cm} (17)

• Substitute (15) into (16):

$$\frac{d^2 E_i}{dx^2} = \frac{e \rho(x)}{\epsilon_r \epsilon_0}$$  \hspace{1cm} (18)
Poisson’s Equation

\[
\frac{d^2 E_i}{dx^2} = \frac{e \rho(x)}{\epsilon_r \epsilon_0}
\]  \hspace{1cm} (18)

• Now substitute (4) into (18):

\[
\frac{dE}{dx} = \frac{\rho(x)}{\epsilon_r \epsilon_0}
\]  \hspace{1cm} (19)

• To evaluate electric field, we integrate (19) over \(x\):

\[
E(x) = \frac{1}{\epsilon_r \epsilon_0} \int_{-\infty}^{x} \rho(\bar{x}) d\bar{x}
\]  \hspace{1cm} (20)

• To get potential, we integrate again:

\[
\phi(x) = - \int_{-\infty}^{x} E(\bar{x}) d\bar{x}
\]  \hspace{1cm} (21)

Electrostatic Potential

• If the interface is perfectly abrupt we can picture the system as shown on the right.

• We are considering a situation with zero bias.
**Electrostatic Potential**

- If the interface is perfectly abrupt we can picture the system as shown on the right.

- If the free carrier concentrations decrease very (infinitely) rapidly at the edge of the depletion region, we can describe the concentrations as shown.

Assume every dopant atom provides one electron / hole.

- $N_A$: acceptor density.
- $N_D$: donor density.

**Electrostatic Potential**

- We know the depletion region will be charged.

- What will the charge density ($\rho$) look like as a function of position?

- We can just count charges on ionized dopant atoms:

\[
\rho = \begin{cases} 
-eN_A & -W_{dp} < x < 0 \\
+eN_D & 0 < x < W_{dn} \\
0 & \text{elsewhere}
\end{cases}
\]
Electrostatic Potential

- The electrostatic potential ($\phi$) is related to charge density by Poisson’s Equation:
  \[
  \frac{d^2 \phi}{dx^2} = -\frac{\rho(x)}{\varepsilon_r \varepsilon_0}
  \]
  - $\varepsilon_r$: relative permittivity
  - $\varepsilon_0$: vacuum permittivity
  - The first integral of which gives electric field:
    \[
    \frac{d\phi}{dx} = -\mathcal{E}(x) = -\int \frac{\rho(x)}{\varepsilon_r \varepsilon_0} dx
    \]

Electrostatic Potential

- Carrying-out the integration for our junction gives:
  - For $-W_{dp} < x < 0$:
    \[
    \mathcal{E} = -\frac{e N_A}{\varepsilon_r \varepsilon_0} (x + W_{dp})
    \]
  - For $0 < x < W_{dn}$:
    \[
    \mathcal{E} = \frac{e N_D}{\varepsilon_r \varepsilon_0} (x - W_{dn})
    \]
  - By requiring $\mathcal{E}$ is continuous at $x = 0$ we also find:
    \[
    N_A W_{dp} = N_D W_{dn}
    \]
Electrostatic Potential

• Finally, we can get the electrostatic potential by integrating the electric field with respect to position:
  • For \(-W_{dp} < x < 0:\)
    \[
    \phi(x) = \frac{eN_A}{2\varepsilon_r \varepsilon_0} (x + W_{dp})^2
    \]
  • For \(0 < x < W_{dn}:\)
    \[
    \phi(x) = \Delta \phi_0 - \frac{eN_D}{2\varepsilon_r \varepsilon_0} (x - W_{dn})^2
    \]
• Where:
  \[
  \Delta \phi_0 = \frac{e}{2\varepsilon_r \varepsilon_0} \left( N_A W_{dp}^2 + N_D W_{pn}^2 \right)
  \]

Electrostatic Potential

• Plotting \(\phi(x):\)
  • So notice now there is a very large potential for electrons from left to right (reverse bias).
  • However it is very easy for electrons to flow from right to left (forward bias).
  • This is why rectification takes place.
Band Energies

- To get the energy band diagram from the electrostatic potential, we just use Equation (15):
  \[ \phi = -\frac{E_i}{e} \]

- I.e. we can just flip over the electrostatic potential to get the band structure.

- \( E_i \) is the intrinsic energy, to get \( E_C \) and \( E_V \) we add a constant. See Figure 1 Chapter 2.

Band Energies

- Figure 1, Chapter 2 from Sze and Ng illustrates this as well.
- They use a few different notations:
  - \( \phi \rightarrow \psi \).
  - \( e \rightarrow q \).
  - \( \psi_{bi} \): Built in potential.
- Electrostatic potential difference between p and n sides of junction.
Maximum Electric Field

• We can now calculate several important properties of abrupt pn junctions.
• The first is the maximum electric field strength in the junction.
• Recall the charge density looked something like:
• We evaluate $E_{\text{max}}$ by integrating one (any) side of the junction:

$$E(x) = \int \frac{\rho(x)}{\varepsilon_r \varepsilon_0} dx \quad \Rightarrow \quad E_{\text{max}} = \frac{e}{\varepsilon_r \varepsilon_0} \int_{-W_{dn}}^{0} N_D d\tilde{x} \quad (22)$$

• We made use of the depletion approximation which states:
  • Only fixed (localized) charge is important in determining the electrostatics of the depletion region. Mobile (delocalized) charge is neglected.
  • Also:
    • Carrier concentrations are negligible in depletion region. Charge density is zero ($\rho = 0$) outside of depletion region.
**Maximum Electric Field**

- From the diagram we plotted earlier, we also see that alternatively, we could just evaluate $\mathcal{E}(0)$.

- For $-W_{dp} < x < 0$:
  \[
  \mathcal{E}(x) = -\frac{eN_A}{\varepsilon_r \varepsilon_0} (x + W_{dp})
  \]
  \[
  \mathcal{E}(0) = -\frac{eN_A W_{dp}}{\varepsilon_r \varepsilon_0} \tag{23}
  \]

- For $0 < x < W_{dn}$:
  \[
  \mathcal{E}(x) = \frac{eN_D}{\varepsilon_r \varepsilon_0} (x - W_{dn})
  \]
  \[
  \mathcal{E}(0) = -\frac{eN_D W_{dn}}{\varepsilon_r \varepsilon_0} \tag{24}
  \]

**Built-In-Potential**

- The built-potential is defined as the total amount of band bending in equilibrium:
  \[
  \phi_{bi} = \frac{1}{2} \mathcal{E}_{max} W \tag{25}
  \]

- Where $W$ is the total width of the depletion region:
  \[
  W = W_{dp} + W_{dn} \tag{26}
  \]
Depletion Width

• We can evaluate the total depletion width \( W \):

\[
W = W_{Dp} + W_{Dn} \\
W = \left[ \frac{2\varepsilon_r \varepsilon_0}{e} \frac{N_A + N_D}{N_A N_D} \, \Phi_{bi} \right]^{1/2}
\]  

(28)

• The is a very important equation: it gives the equilibrium depletion layer width in terms of the total band bending and doping.

Summary

• pn-junction formation.
  • Mobile carriers vs. ionized dopants.
  • Equilibrium band diagram.
• Intro to pn junction electrostatics
  • Poisson's equation.
  • Charge density.
  • Electric field.
  • Electrostatic potential or voltage.
  • Potential energy.
  • Band Energy.
Next Time...

• More pn-junctions.
• Generalizations.
• Equilibrium band diagram.
• Capacitance vs Voltage.

• Reading: Sze & Ng Chapter 2 p85-90.