Lecture 8: Introduction to Metal Semiconductor Contacts

Sze And Ng: Chapter 3

Announcements

Homework 2/4:
• Is due now.
• Please get it to me as soon as possible if you have not already done so.
• Email it to me at john.labram@oregonstate.edu.
• I will return it on Thursday February 4th.
Announcements

Literature Report 1

• Will be online after this lecture.
• You will have 2 weeks to complete the report.
  • It is due Thursday February 11th at 8:30 am.
  • Email it to me at john.labram@oregonstate.edu.
• This report contributes 20% of the overall grade of the course.
• There are a total of 25 marks available.
• The report will consist of combination of short and long questions.
• An example of a short question: Provide the reference for the first reported Quantum Cascade Laser. [2 marks]

A longer question would be something like the following:

• Briefly summarize how effective HMDS is a passivation layer for SiO₂. 200 words maximum. [6 marks]

• I will give you some guidance and hints where appropriate.
• To complete Report 1 you will need to use Clarivate Web of Science.
• We covered this in Lecture 7.
• Any questions, don’t hesitate to email me!
Last Time

• We covered the basics of searching the literature.

Lecture 8

• Introduction to Metal Semiconductor Contacts.
• Ideal Theory.
• Non-Ideal Theory.
• Non-Ideal Parameters.
Extra Information

- In addition to the textbook, you may find the following video helpful:
- Part of a series on metal-semiconductor contacts from University of Colorado Boulder.
- Notation is different to us.

Metal Semiconductor Contacts
Contacts

• Sooner or later we must connect our semiconductor devices to the outside world.

• Today we will use band diagrams to describe what happens when we bring a metal into contact with a semiconductor and what sorts of electrical behaviors we can expect in the ideal case.

• We will also begin a discussion of non-ideal effects.

Ohmic Contacts

• When you put a metal on a semiconductor, there are two extremes of what can happen.

• The first is Ohmic (non-rectifying) contact.

• A non-injecting contact with an I-V curve that is linear in both directions.

• Ideally, the slope of the IV curve is very large so that the contact resistance $r_c$ is small.

$$r_c = \left[ \frac{dI}{dV} \right]_{V=0}^{-1}$$

$r_c$ has units of $\Omega \cdot \text{cm}^{-2}$

$(1)$
Ideal Schottky Barrier

- The second is an Ideal Schottky Barrier.
- The rectifying contact behaves like a diode.
- In reality, we typically obtain metal-semiconductor contacts which are not ideal.

\[ I = I_0 \left[ \exp\left( \frac{eV_D}{nk_BT} \right) - 1 \right] \]

- For example, the IV curve of an Ohmic contact may actually look like this.

Contacts

- Instead of insisting that an Ohmic contact have a perfectly linear IV curve in both directions with a large slope, a more realistic requirement for an Ohmic contact is that the voltage drop across the contact be much less than the voltage drop across the device.
- The purpose of an Ohmic contact is to provide an ample supply of carriers to the semiconductor upon application of a bias, and for the maintenance of space charge neutrality.
- Making a good Ohmic contact can be problematic for wide bandgap semiconductors and for small dimensional structures.
Metal-Semiconductor Interface

- The ideal theory of metal-semiconductor (MS) formation begins by first considering energy band diagrams of the metal and of the semiconductor in isolation from one another.
- Let’s Consider the simplest description of a metal and a semiconductor.
  - $E_{Fm}$ Fermi Energy of metal.
  - $E_C$ Conduction band minimum of semiconductor.
  - $E_V$ Valence band maximum of semiconductor.
  - $E_F$ Fermi Energy of SC.
Metal-Semiconductor Interface

- $E_{VAC}$: Vacuum level. The energy of an $e^-$ just outside of the surface of the solid (a convenient reference energy).

- $e\phi_M$: Metal work function. The energy required to remove an $e^-$ from the Fermi level in the metal to the vacuum level.

- $e\phi_S$: Semiconductor work function. The energy required to remove an $e^-$ from the Fermi level in the semiconductor to the vacuum level.

Note that all these parameters are normally quoted in eV.

Chi (pronounced Kai)

- $e\chi_S$: Semiconductor electron affinity. The energy required to remove an $e^-$ from the bottom of the conduction band in the semiconductor to the vacuum level (a much more convenient semiconductor reference energy than $e\phi_S$).

- $eIP_S$: Semiconductor ionization potential. The energy required to remove an $e^-$ from the top of the valence band in the semiconductor to the vacuum level.
Evaluating Energies

- How do we evaluate these parameters?
- Normally via some sort of photo-emission experiment.

\[ E_{\text{vacuum}} \]

\[ h\nu \]

\[ V_{B} \]

\[ V_{B} - 1 \]

- Photons is incident on sample, emitted electrons detected.

UPS Data

- This is an example of real data.
- We are looking for the energy after which no electrons are emitted → top of valence band.
- This can be tricky and subjective.
- Note VBE here is relative to Fermi Energy.

\[ \text{Work Function} \]

\[ V_{B E} \]

\[ E_{\text{Fermi}} \]

\[ E_{\text{vac}} \]
Metal-Semiconductor Interface

- What happens when we bring the metal and semiconductor in to contact?
  - Start with the case that $\phi_M > \phi_S$:

  Before Contact
  - $E_{Fm}$
  - $E_C$
  - $E_V$

  After Contact
  - $E_{Fm}$
  - $E_F$

  I.e. when $E_{Fm}$ is lower than $E_F$

- What happens to our parameters after contact?
  - All of the band-bending occurs in the semiconductor.
  - The vacuum level is continuous across the interface, which establishes barrier heights and band-bending.
Metal-Semiconductor Interface

- Note:
  - $\chi_S$, $IP_S$, $\phi_M$ stay the same.
  - $\phi_S(x)$ is a function of position $x$.
  - $\phi_{bi} = \phi_M - \phi_S$(bulk).
  - $\phi_{Bi} = \phi_M - \chi_S$.

We have three new variables as the interface is created:

- $E_{LVAC}$: Local vacuum level. The apparent vacuum level within the solid, as if each interior distance into the solid constitutes the surface.
- $\phi_{bi} = \phi_M - \phi_S$(bulk). Built-in Potential. The equilibrium energy barrier seen by an $e^-$ at the bottom of the conduction band in the semiconductor bulk.
- $\phi_{Bi} = \phi_M - \chi_S$. Schottky barrier height for an n-type semiconductor. The equilibrium energy barrier seen by an $e^-$ at the Fermi level in the metal.
- Since $\phi_{bi} \neq \phi_{Bi}$, this is a rectifying interface.
Metal-Semiconductor Interface

- Band-bending is due to electron transfer from the semiconductor to the metal.
- The direction of electron transfer is established by the relative energy of the metal and the semiconductor Fermi levels when these materials are isolated from one another.
- Electron transfer from the semiconductor leads to the formation of a depletion layer.

Ideal Theory

- We can refer to this ideal theory of interface formation mechanism as Fermi-level mediated charge transfer, giving rise to a macroscopic dipole.
- By enforcing charge balance, we can state the charge density at the interface as:

\[ Q_M + Q_{SC} = 0 \]

- Where:
  - \( Q_M \) is charge per unit area associated with the metal.
  - \( Q_{SC} \) is charge per unit area associated with the semiconductor space charge region.
Ideal Theory

- What does the charge distribution look like?
- We hence have an electric dipole across the interface pointing from right to left.
- Since depletion width dimensions are typically ~0.01-10μm, this charge distribution can be described as a macroscopic dipole.
- That is, the dipole distance between the sheet of negative charge at the metal-semiconductor interface and the centroid of the positive depletion region charge is macroscopic, compared to atomic dimensions.

Ideal Theory

- Let’s estimate the relative width of the depletion regions in the metal and the semiconductor.
- The following values are reasonable:
  - \( N_D \approx 10^{17} \text{ cm}^{-3} \).
  - \( n_{\text{metal}} \approx 10^{22} \text{ cm}^{-3} \).
  - From \( q \)-balance we say:
    \[
    N_D W_{dn} = n_{\text{metal}} W_{\text{metal}} \tag{2}
    \]
    \[
    \frac{W_{\text{metal}}}{W_{dn}} = \frac{N_D}{n_{\text{metal}}} \approx 10^{-5} \tag{3}
    \]
- Thus, it is safe to conclude that the vast majority of the Schottky barrier depletion layer width resides in the semiconductor, not in the metal.
\[ \phi_M = \phi_S \]

- If the Fermi Energies (work functions) are equal, the semiconductor should in theory experience no band bending:

Before Contact

After Contact

\[ E \]

\[ E_V \]

\[ E_{VAC} \]

\[ e\phi_M \]

\[ e\phi_S \]

\[ E_F \]

\[ E_C \]

\[ E_V \]

\[ \phi_M < \phi_S \]

- If the Fermi Energies of the metal is higher than that of the semiconductor, we get the following situation:

Before Contact

After Contact

\[ E \]

\[ E_{VAC} \]

\[ e\phi_M \]

\[ e\phi_S \]

\[ E_F \]

\[ E_C \]

\[ E_F \]

\[ E_V \]
\( \phi_M < \phi_S \)

- In more detail:

- In this case electrons flow from the metal to the semiconductor.
- Electrons accumulate at interface.

• This band diagram corresponds to an Ohmic contact.
• The interface is accumulated with electrons and there is no appreciable barrier so that current will easily flow.
• Carriers (electrons in this case) may be easily supplied with application of a bias of either polarity.
• The Schottky barrier energy for an Ohmic contact is very small and can be negative.
Metal-Semiconductor Contacts

Accumulation

Neutral

Depletion

\[ \phi_M < \phi_S \]

\[ \phi_M = \phi_S \]

\[ \phi_M > \phi_S \]

P-Type Semiconductors

• For the p-type semiconductors the situation is analogous.

\[ \phi_M > \phi_S \]

\[ \phi_M < \phi_S \]
Summary

- The relevant barrier equations are as follows.
- **N-Type:**
  \[ \phi_{Bn} = \phi_M - \chi_S \quad (4) \]
  \[ \phi_{bi,n} = \phi_M - \phi_S \quad (5) \]
- **P-Type:**
  \[ \phi_{Bp} = IP_S - \phi_M \quad (6) \]
  \[ \phi_{bi,p} = \phi_S - \phi_M \quad (7) \]

Work Functions

Sze & Ng Fig. 3.2, pg. 137
Non-Ideal Theory

- In reality the Ideal Theory does not predict proper barrier heights for a given M-S system.
- Intuitively, we might expect this theory to fail for the following reasons:
  - Ideal theory assumes that the individual properties of the M and S alone determine barrier heights.
  - Ideal theory ignores interfacial chemical reactions.
  - In actuality, $\phi_M$ and $\chi_S$ depend upon surface cleanliness and crystal orientation.
  - Real material interfaces contain impurities, interfacial oxides, and perhaps non-stoichiometry.
Interface States

- Bardeen resolved this ideal theory M-S problem by invoking surface states (or interface states) and asserting that they are partially responsible for determining barrier heights.
- **Interface States** constitute the fundamental hypothesis leading to non-ideal theory.
- Interface states are localized electronic states within the bandgap (with decaying wavefunctions, which are chargeable, and may be donor- or acceptor-like (discussed later).

- Interface states can be:
  - Associated with defects (e.g. vacancies, interstitials, anti-sites, interfacial inter-diffusion).
  - Associated with incomplete bonding (dangling bonds).
  - Associated with impurities.
  - Exponentially attenuated evanescent wave associated with the physical termination of a surface.
Interface States

- Diagrammatically, we picture the inclusion of interface states something like this:

![Interface States Diagram](image)

Non-Ideal Theory

- The Non-Ideal Theory is most simply approached via charge balance as expressed by the following equation:

  \[ Q_M + Q_{SC} + Q_{SS} = 0 \]  

  (8)

- Where \( Q_{SS} \) is the charge per unit area associated with interface states.
- Interface state charge transfer is handled via the charge neutrality level \( E_{CNL} \), a branch point within the semiconductor band gap
  - Above which: an interface state is predominantly conduction band derived and acceptor-like.
  - Below which: an interface state is predominantly valence band derived and donor-like.
**Charge Neutrality Level**

- We describe these surface trap states as being a continuum in the semiconductor band gap:

- The states are classified relative to the Charge Neutrality Level ($E_{CNL}$).
- **Acceptor-like states** are neutral when empty and negatively charged when occupied.
- **Donor-like states** are positively charged when empty and neutral when occupied.

**Non-Ideal Theory**

- Let’s add a few more variables to our band diagram:
Non-Ideal Theory

Where:

- $E_{VAC}$: Vacuum level.
- $e\phi_M$: Metal work function.
- $eE_F$: Fermi Energy.
- $e\phi_{Bn}$: Barrier height.
- $Q_M$: Charge per unit area associated with the metal.
- $D_{it}$: Interface trap density.
- $\delta$: Thickness of interfacial layer.
- $Q_{SS}$: Interface trap charge.
- $Q_{SC}$: Charge per unit area associated with the semiconductor space charge region.

Units of e.g. states / cm$^2$eV

Non-Ideal Theory

Where:

- $e\phi_0$: Neutral level (above $E_V$) of interface states.
- $e\phi_{bi}$: Built-in potential.
- $\chi$: Electron affinity.
- $\Delta$: Potential across interfacial layer.
- $E_g$: Band gap.
- $E_C$: Conduction band minimum.
- $E_{CNL}$: Charge Neutrality Level.
- $E_V$: Conduction band minimum.
Non-Ideal Theory

- The textbook has slightly different notation:

\[ \begin{align*}
\phi_m & = \text{Work function of metal} \\
\phi_{m0} & = \text{Barrier height (without image-force lowering)} \\
\phi_b & = \text{Neutral level (above } E_F \text{) of interface states} \\
\Delta & = \text{Potential across interfacial layer} \\
\chi & = \text{Electron affinity of semiconductor} \\
\psi_{bi} & = \text{Built-in potential} \\
\delta & = \text{Thickness of interfacial layer} \\
Q_n & = \text{Space-charge density in semiconductor} \\
Q_{nt} & = \text{Interface-trap charge} \\
Q_m & = \text{Surface-charge density on metal} \\
D_a & = \text{Interface-trap density} \\
\varepsilon_i & = \text{Permittivity of interfacial layer (vacuum)} \\
\varepsilon_r & = \text{Permittivity of semiconductor}
\end{align*} \]

Fermi Level Pinning

- Interface states can be due to a number of sources.
- For this thought experiment, consider them as incomplete / different bonds.
- In silicon the density of surface states is \( \sim 10^{15} \text{ cm}^{-2} \).
- Consider the semiconductor in isolation from the metal:
Fermi Level Pinning

- Electrons close to the interface fill these empty interface states and create stored charge.
- Depletion region also occurs observed in the semiconductor close to the interface
  - Self-doping the semiconductor at the interface.

In reality the electrons from the metal fill a lot more of these traps, since the free carrier concentration is so much higher.

- The result is a barrier height which is a lot-less dependent on the metal than in should be.
- Makes it harder to engineer interface to our specification.
Non-Ideal Theory Parameters

Interface Dipoles

• We can describe this non ideal interface formation mechanism as charge neutrality level mediated charge transfer, giving rise to a microscopic dipole.

• We assume that $\delta \sim$ atomic dimensions. I.e. $\delta \approx 4$-5 Å.
Ideal Injection Barriers

- When it comes to injection and transport we are concerned with barrier heights.
- We saw earlier, that for the ideal barriers:
  - **N-Type:**
    \[
    \phi_{Bn} = \phi_M - \chi_S \tag{4}
    \]
    \[
    \phi_{bi,n} = \phi_M - \phi_S \tag{5}
    \]
  - **P-Type:**
    \[
    \phi_{BP} = IP_S - \phi_M \tag{6}
    \]
    \[
    \phi_{bi,p} = \phi_S - \phi_M \tag{7}
    \]

Non-Ideal Injection Barriers

- When considering interface states we need to account for the potential dropped across the interface layer as well:
- We hence say:
  - **N-Type:**
    \[
    \phi_{Bn} = \phi_M - \chi_S - \Delta \tag{9}
    \]
    \[
    \phi_{bi,n} = \phi_M - \phi_S - \Delta \tag{10}
    \]
  - **P-Type:**
    \[
    \phi_{BP} = IP_S - \phi_M + \Delta \tag{11}
    \]
    \[
    \phi_{bi,p} = \phi_S - \phi_M + \Delta \tag{12}
    \]
**Potential Across Interface**

- So we need to determine the potential dropped across the interfacial layer ($\Delta$) to evaluate barrier heights.
- We will just quote some formulae today.
  - The textbook provides more detail.
  
  $$\Delta = -\frac{\delta Q_M}{\epsilon_0 \epsilon_{ri}} \quad (12)$$

- Where:
  - $\Delta$ is the potential across the interfacial layer.
  - $\delta$ is the thickness of the interfacial layer.
  - $Q_M$ is the surface charge density (e.g. C/cm$^2$).
  - $\epsilon_0 \epsilon_{ri}$ is the relative permittivity of the insulator.

**Corrected Barrier Height**

- From Equation (8) we can say:
  
  $$Q_M + Q_{sc} + Q_{ss} = 0$$

  $$\Delta = \frac{\delta (Q_{sc} + Q_{ss})}{\epsilon_0 \epsilon_{ri}} \quad (13)$$

- We are told the interfacial trap density in term of $D_{it}$.
- We can hence write this in terms of charge density:
  
  $$Q_{ss} = -eD_{it} \left(E_g - e\phi_0 - e\phi_{Bn}\right) \quad (14)$$

- We are also told the charge associated with the semiconductor depletion region is:
  
  $$Q_{ss} = eN_D W_D = \sqrt{2e\epsilon_0 \epsilon_{rs} N_D \left(\phi_{Bn} - \phi_n - \frac{k_B T}{e}\right)} \quad (15)$$

  where $\phi_n = \phi_{Bn} - \phi_{bi}$.
Corrected Barrier Height

- Combining equations (9), (13), (14) and (15):
  \[ \phi_{Bn} = c_2(\phi_M - \chi_S) + (1 - c_2)\left(\frac{E_g}{e} - \phi_0\right) \]  
  (16)

- Where:
  \[ c_1 = \frac{2e\epsilon_0\epsilon_{rs}N_D\delta^2}{(\epsilon_0\epsilon_{ri})^2} \]  
  (17)
  \[ c_2 = \frac{\epsilon_0\epsilon_{ri}}{\epsilon_0\epsilon_{ri} + e^2\delta D_{it}} \]  
  (18)

- \( c_1 \) and \( c_2 \) can be evaluated experimentally.
- We can also write:
  \[ \phi_{Bn} = c_2\phi_M + c_3 \]  
  (19)
  \[ c_3 = (1 - c_2)\left(\frac{E_g}{e} - \phi_0\right) - c_2\chi_S \]  
  (20)

Various metals on silicon
Corrected Barrier Height

\[ \phi_{Bn} = c_2 \phi_M + c_3 \]

- Reasonable behavior is observed experimentally:

Electronegativity

- For ionic semiconductors (CdS and ZnS), the barrier height has been observed to be dependent on the electronegativity of the metal.
- Electronegativity \((X_m)\) of the metal is it’s the “pulling power” for an atom to pull electrons to it.
- Note:
  - \(X_m\) is a relative (dimensionless) parameter.
  - \(\chi_s\) has units of volts and measures the energy involved in adding or removing an electron in gaseous form.
- Be aware: Different textbooks use \(\chi\)’s and \(X\)’s for different parameters (often interchangeably).
**Electronegativity**

- Pauling’s Electronegativity Scale:

![Electronegativity Scale Diagram](image)

- Sometimes the relationship is quantified through the slope of barrier height to electronegativity:

\[ S = \frac{\Delta \phi_{Bn}}{\Delta X_m} \]  

(21)
Summary

• We looked at what happens when you bring a semiconductor into contact with a metal:

• We also dealt with issues relating to interface states:

Next Time…

• Electrostatics and capacitance of metal-semiconductor junctions.