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## 1 Overview

In this lecture, we discuss MS junctions. MS junctions are interfaces between metals and semiconductors, hence the “MS” notation. MS junctions are important since every electronic device has electrical contacts in which a metal is in intimate contact with a semiconductor.

Nearly every metal contact to is an MS junction.

MS contacts allow one to make good electrical contacts to semiconductors and manipulate their properties by applying external potentials and are therefore a critical component in device fabrication and characterization. Furthermore, MS junctions can be made intentionally into a new form of diode which we have not yet discussed – a Schottky diode.

A Schottky diode is similar to a one-sided pn junction diode.

Schottky diodes are conceptually similar to a pn-junction diode in which one of the sides of the junction is degenerately doped to be “metallic”. Review the electrostatics of pn-junctions if this is not clear. Schottky contacts are rectifying, electrical contacts are Ohmic. A Schottky contact can be used to make a diode that functions in the same way as a pn-junction diode in terms of its rectifying characteristics.

Key topics to cover include:

- **Ohmic Contacts**: for making low-resistance electrical contact to semiconductors. Can occur due to carrier accumulation at contacts or due to quantum mechanical tunneling.
- **Schottky Contacts**: May arise due to imperfect contact formation or intentionally due to formation of a Schottky diode.

## 2 Ideal MS Contacts

The ideal MS contact has the following assumptions:

- The metal and semiconductor are in intimate contact, forming a clean, atomically precise, defect free interface between them.
- The interface is abrupt, there is no inter-diffusion between the metal and the semiconductor.
2.1 Schottky Barriers

A Schottky barrier is an energy barrier formed at the interface between a metal and semiconductor having different work functions. As shown in Figure 1, an energy barrier can arise, preventing electron or hole flow towards or away from the junction. As shown, the barrier for electrons is denoted $\Phi_{Bn}$ and the barrier for holes is denoted $\Phi_{Bp}$. Similar to a pn-junction, a depletion region forms where the concentration of charge carriers is reduced.

A Schottky barrier is an energy barrier preventing carrier transport across the junction.

For electrons, the barrier height is given by the following:

$$\Phi_{Bn} = \Phi_M - \chi$$

...and for holes:

$$\Phi_{Bp} = E_g + \chi - \Phi_M$$

From this we see that the barrier heights approximately sum to the bandgap energy in the ideal case.

$$\Phi_{Bn} + \Phi_{Bp} \approx E_G$$

Measured data for the Schottky barrier heights of electrons and holes in n-type Silicon is shown...
in Figure 2. Evidently, and as expected from the definitions of the barrier heights, there is a strong work function dependence of the barrier heights. In practice, the linear trend with the barrier heights and work function is rarely followed due to the formation of interface dipoles as shown in Figure 3, resulting in what is known as Fermi level pinning. To design an ideal MS junction, in which Fermi level pinning is neglected, we need only compare the work functions of the semiconductor to that of the metal. As can be deduced by visual inspection of the band diagrams:

- **N-Type Semiconductors:**
  - If $\Phi_M > \Phi_S$, a Schottky contact will be formed.
  - If $\Phi_M < \Phi_S$, an Ohmic contact will be formed.

- **P-Type Semiconductors:**
  - If $\Phi_M > \Phi_S$, an Ohmic contact will be formed.
  - If $\Phi_M < \Phi_S$, a Schottky contact will be formed.

These relations simply restate a fact that should be obvious at this point: in order to create an Ohmic contact, the carrier concentration at the junction should be increased. If the opposite is true, a Schottky barrier will be formed. This comes down to basic thermodynamics – electrons and holes will prefer the lowest energy state. Under such considerations, the relative difference in the work functions of the metal and the semiconductor define the direction in which electron/hole diffusion will occur during initial interface formation. For example, in an n-type semiconductor in contact with a metal:

- if $\Phi_M > \Phi_S$: Electron diffusion occurs from the semiconductor to the metal, thus depleting electrons from the semiconductor near the interface and forming a Schottky barrier. $E_F$ on the metal is lower in energy!

- if $\Phi_M < \Phi_S$: Electron diffusion occurs from the metal to the semiconductor, thus accumulating electrons in the semiconductor near the interface and forming an Ohmic contact. $E_F$ on the semiconductor is lower in energy!

As a good exercise, apply the same logic to a p-type semiconductor and note the distinctions if any.

### 2.2 Schottky Diodes

In this section, we derive quantitative relationships defining the expected current-voltage characteristics of an ideal MS junction composed of a metal and an n-type semiconductor.

<table>
<thead>
<tr>
<th>Metal</th>
<th>Mg</th>
<th>Ti</th>
<th>Cr</th>
<th>W</th>
<th>Mo</th>
<th>Pd</th>
<th>Au</th>
<th>Pt</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_Bn$ (V)</td>
<td>0.4</td>
<td>0.5</td>
<td>0.61</td>
<td>0.67</td>
<td>0.68</td>
<td>0.77</td>
<td>0.8</td>
<td>0.9</td>
</tr>
<tr>
<td>$\phi_Bp$ (V)</td>
<td>0.61</td>
<td>0.50</td>
<td>0.42</td>
<td>0.3</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Work Function $\psi_M$ (V)</td>
<td>3.7</td>
<td>4.3</td>
<td>4.5</td>
<td>4.6</td>
<td>4.6</td>
<td>5.1</td>
<td>5.1</td>
<td>5.7</td>
</tr>
</tbody>
</table>
Figure 3: Comparison of (a) ideal and (b) non-ideal Schottky barrier due to interface dipole formation. Image from Hu, 1st edition.
2.2.1 Electrostatics

Referring to Figure 3 (a), the built-in potential can be written down by inspection as:

\[
\phi_{bi} = \frac{1}{e} (\Phi_{B,n} - (E_C(\infty) - E_F)) \\
= \frac{1}{e} (\Phi_M - \chi - (E_C(\infty) - E_F))
\]

The term, \( E_C(\infty) \), corresponds to the conduction band evaluated at an infinite distance away from the junction, where there is no curvature (i.e. electric field) due to the presence of space-charge. This is referred to as the “flat-band” region. Since the semiconductor is n-type in this example, we can derive the electrostatics following the same procedure as we applied to pn-junctions. The p-side in this case is replaced by the metal. Since metals do not have internal electric fields or space-charge, all of the depletion region will drop across the n-type semiconductor and not in the metal.

\[
W = x_n
\]

\[
\rho = eN_D^+ \quad \ldots \quad 0 \leq x \leq W
\]

Applying Poisson’s equation to calculate the electric field, we obtain:

\[
\varepsilon'(x) = -\frac{eN_D^+}{\epsilon_s} (W - x) \quad \ldots \quad 0 \leq x \leq W
\]

And, using the definition of the electric field in terms of potential, we compute the electrostatic potential as:

\[
\phi(x) = -\frac{eN_D^+}{2\epsilon_s} (W - x)^2 \quad \ldots \quad 0 \leq x \leq W
\]

Using the expression for the depletion width in a one-sided junction that we arrived for a pn-junction, we can write the depletion width as follows:

\[
W = \sqrt{\frac{2\epsilon_s (\phi_{bi} - V_A)}{eN_D^+}}
\]

2.3 IV Characteristics

2.3.1 Why Minority-Carrier Diffusion Does Not Occur

So far, there is no fundamental difference between an MS junction and a one-sided pn junction in terms of electrostatics. Current flow, on the other hand, is very different. In a pn junction current flows due to a steady-state diffusion of minority carriers away from the depletion region on both sides of the junction, moving towards the contacts. As carriers diffuse, they recombine, provided that the length of the quasi-neutral region is longer than a few diffusion lengths. Applying the same logic to an MS junction would suggest that holes supplied by the metal are injected at the junction, and diffuse away from the junction towards \( \infty \), recombining with electrons in the semiconductor. A valid question arises – do metals have holes? The answer is simple: Metals are not a source of holes. Metals are composed of a large number of electrons, close to the atomic density \( \approx 1 \times 10^{22} \text{ cm}^{-3} \).
At these high electron densities, recombination rates would be anticipated to be quite large, based on Shockley Read Hall statistics. If a hole were to somehow enter the metal, it would recombine almost instantly. Therefore, the steady-state hole population in a metal can be taken to be 0 for all practical purposes. What about electrons injected from the semiconductor to the metal? This would be equivalent to adding a drop of water to the ocean and asking if we increased the size of the ocean. Technically yes but practically no. Semiconductors would reach dopant solubility limits before ever acquiring enough dopants to make their resulting electron concentration comparable to a metal. Therefore, injection of electrons to the metal is always negligible from the perspective of creating a diffusion current. Without a viable means of generating or sustaining minority carriers, it becomes difficult to support a theory for conduction based on minority carrier diffusion.

2.3.2 Thermionic Emission

Current flows in an MS junction due to thermionic emission, which is a term describing the physics of carriers hopping over a barrier. Unlike tunneling, thermionic emission is a classical effect. Being a classical effect, we require that the kinetic energy of charge carriers exceed the potential energy barrier limiting their motion.

$$\frac{1}{2}m_n^* v_x^2 \geq e(\phi_{bi} - V_A)$$

Equivalently, this relation can be expressed in terms of a minimum velocity, which is more portable since the velocity directly relates to the current.

$$v_x \geq v_{min}$$

$$v_{min} \equiv \sqrt{\frac{2e}{m_n^*}}(\phi_{bi} - V_A)$$

To compute the current, we need to evaluate the velocities of all electrons and add up all of the current components corresponding to those having velocity high enough to exceed the barrier, as indicated in Figure 4. Since the velocity of electrons is negative (right to left), we have the
following:

\[ I_{S\rightarrow M} = -eA \int_{-\infty}^{v_{\text{min}}} n(v_x) dv_x \]

It can be shown that the electron concentration as a function of velocity is given by:

\[ n(v_x) = \left( \frac{4\pi k_b T m_n^*}{\hbar^3} \right) \exp \left( \frac{E_F - E_C}{k_b T} \right) \exp \left( -\frac{-m_n^* v_x^2}{2k_b T} \right) \]

Substituting this expression into the expression for the current and performing the integration yields the following:

\[ I_{S\rightarrow M} = A \mathcal{G}^* T^2 \exp \left( -\frac{\phi_B n}{k_b T} \right) \exp \left( \frac{eV_A}{k_b T} \right) \]

...where the constants are defined as follows:

\[ \mathcal{G}^* = \left( \frac{m_n^*}{m_e} \right) \mathcal{G} \]
\[ \mathcal{G} \equiv \frac{e m_e k_b^2}{2\hbar^3 \pi^2} = \text{Richardson’s Constant} \]

For the current flowing in the opposite direction, due to electrons injected from the metal to the semiconductor, they always see the same barrier height. Therefore, we can write:

\[ I_{M\rightarrow S} = I_{M\rightarrow S}(V_A = 0) \]

At equilibrium, the current components must vanish, such that:

\[ I_{M\rightarrow S}(V_A = 0) + I_{S\rightarrow M}(V_A = 0) = 0 \]

This leads to the following:

\[ I_{M\rightarrow S} = -I_{S\rightarrow M}(V_A = 0) = -A \mathcal{G}^* T^2 \exp \left( \frac{\phi_B n}{k_b T} \right) \]

Combining the results under non-equilibrium conditions, is then:

\[ I = I_S \left( \exp \left( \frac{eV_A}{k_b T} \right) - 1 \right) \]
\[ I_S \equiv A \mathcal{G}^* T^2 \exp \left( -\frac{\Phi_B n}{k_b T} \right) \]

This expression is functionally equivalent to the pn-junction ideal diode equation we derived in previous lectures, and summarized in Figure 5. The key difference is that the reverse saturation current of the MS junction is much larger than the reverse saturation current of a pn-junction diode. This leads to larger currents, faster switching transients, etc...
Figure 5: Summary of the conduction processes in an MS junction.  
(a) Equilibrium \( I_{M \rightarrow S} = -I_0 \), \( I_{S \rightarrow M} = I_0 \) \( E = E_F = q\phi_B \) \( q\phi_B \) \( E_F \)  
(b) Forward bias. Metal is positive wrt Si. \( I_{S \rightarrow M} = I_0 e^{qV/kT} \) \( <q\phi_B \) \( >q\phi_B \) \( qV \) \( E_V \)  
(c) Reverse bias. Metal is negative wrt Si. \( I_{M \rightarrow S} = -I_0 \), \( I_{S \rightarrow M} = 0 \) \( qV \) \( E_F \)  
(d) Schottky diode IV.  

Reverse bias \( \rightarrow \) Forward bias

Image from Hu, 1st edition
2.4 Tunneling Ohmic Contacts

We have seen how quantum-mechanical tunneling can lead to current flow. This fact can be exploited in the fabrication of low-resistance Ohmic contacts by ensuring that the semiconductor is degenerately doped. Doping of the semiconductor reduces the depletion region width. The depletion region width is the width of the energy barrier preventing tunneling from the metal to the semiconductor and vice versa. This is visualized in Figure 6, which shows how tunneling occurs in the case of a metal in contact with an n-type semiconductor (degenerately doped).