Lecture 19

Metal-Semiconductors Interface

Almost any semiconductor device consists of three components: semiconducting material in which the carrier motion / generation / recombination is modulated, conducting material (metal) that used apply potential and conduct current, and insulating material to isolate different components / induce field effect. As a result, interfaces between different materials are unavoidable. In particular, the electronic properties at the metal-semiconductor interface is critical for the design of functional semiconductor devices, which we will discuss in this lecture.

19.1 Ohmic and Schottky contacts

Consider a 1D semiconducting bar that a voltage drop V is applied upon (Figure 19.1 left).

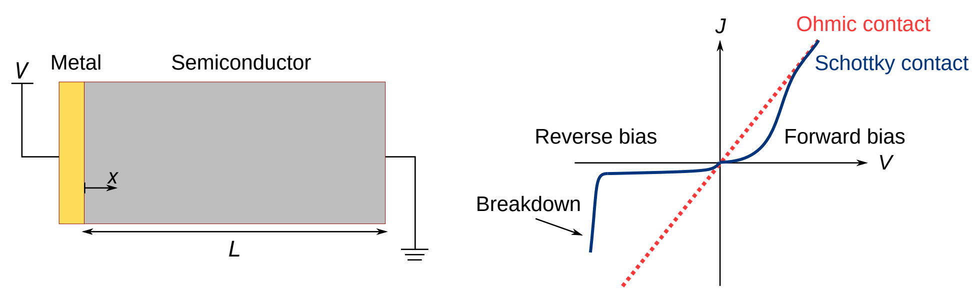

Figure 19.1: The metal-semiconductor interface. Left: scheme of the 1D M-S interface with a bias V applied. Right: J - V curves of two different types of M-S junction: the Ohmic contact (red line) and the Schottky contact (blue curve).

From the Drude model of conductivity in Lecture 18, the total drift current is $J_{\text{drift}} = (neu_{\text{n}} + peu_{p})\frac{\mathrm{d}\psi}{\mathrm{d}L}$. Ideally, the potential is linear across the semiconductor bar, which gives $\mathrm{d}\psi/\mathrm{d}x = V/L$, where L is the length of bar. The current density J_{drift} is thus linear with V:

$$J = J_{\text{drift}} = \underbrace{(\frac{neu_{\text{n}} + peu_{\text{p}}}{L})}_{\text{Const.}} V \tag{19.1}$$

which resembles the Ohm's law. Such kind of ideal metal-semiconductor is called the Ohmic contact, and the resistance is solely from the bulk semiconductor. However in reality, a large number of metal-semiconductor (M-S) interfaces have a non-linear J - V relation: the current density remains low when when $V_{\text{break}} < V < 0$ (breakdown voltage), where V_{break} is the breakdown voltage. When $V > 0$ (forward bias), the current increases rapidly with V (Figure 19.1 right). Such non-linear behavior of J-V is known as the Schottky contact, which indicates that a contact resistance exists at the M-S interface, especially within the reverse bias regime. The additional interfacial resistance, can be explained by the energy diagram of a M-S interface, which we will discuss in the next sections.

19.2 M-S interface without bias

First let's consider the case of a 1D M-S interface without applied bias, which consists of a metal with work function ϕ_{m} and a n-doped semiconductor with electron affinity χ (Figure 19.2).

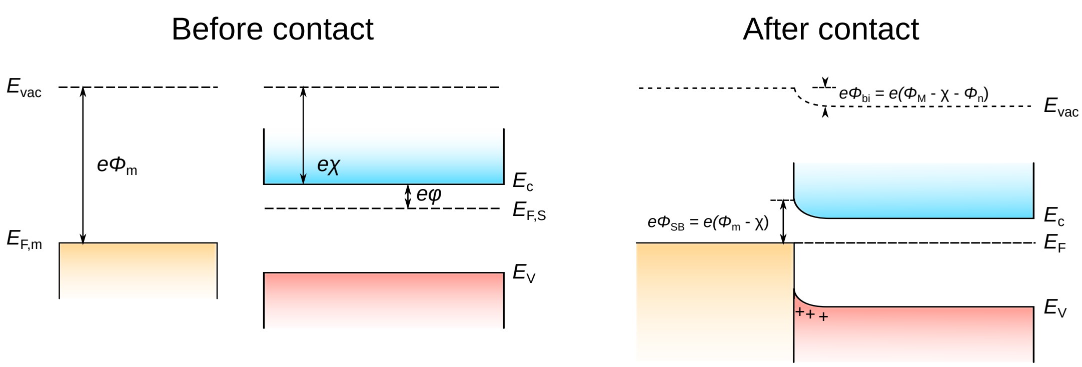

Figure 19.2: Metal and semiconductor in a Schottky barrier before (left) and after (right) contact. The mismatch between the energy levels causes the band bending in the semiconductor.

Before contact, the Fermi levels of the metal $\text{E}_{\text{F,m}}$ and semiconductor $E_{\text{F,s}}$ are not aligned, leading to a tendency of charge transfer (Figure 19.2 left). Upon contact, the Fermi level is aligned across the M-S interface. If the Fermi level of a n-type semiconductor, $E_{\text{F,s}}$, is higher than that of the metal, $E_{\text{F,m}}$, electrons have higher energy at the semiconductor interface, which tend to flow from the semiconductor to the metal, and *vice versa*. Since the system is at thermal equilibrium, using the relation $n = N_{\text{c}} \exp(-(E_{\text{C}} - E_{\text{F}})/k_{\text{B}}T)$, a decrease of electron concentration means the Fermi level at the interface, is moved away from E_{c}. This indicates that the band diagram of the semiconductor near the interface, is no longer a flat profile. To solve the x-dependent band diagram, we can make use of the Poisson equation for the semiconductor side:

$$\begin{aligned}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} &= -\frac{\rho(x)}{\varepsilon_0\varepsilon_\mathrm{r}} \\ &= -\frac{1}{\varepsilon_0\varepsilon_\mathrm{r}}[\underbrace{N_\mathrm{d} - N_\mathrm{a}}_{\text{immobile}} + \underbrace{p(x) - n(x)}_{\text{mobile}}]\end{aligned} \tag{19.2}$$

where ψ is the electrostatic potential, and follows $-e\psi = E_\mathrm{c}(x) - E_\mathrm{c}(x \to \infty) = E_\mathrm{v}(x) - E_\mathrm{v}(x \to \infty)$. Therefore the carrier concentrations are expressed by:

$$\begin{aligned}n(x) &= N_\mathrm{c}\exp(-\frac{E_\mathrm{c}(x) - E_\mathrm{F}}{k_\mathrm{B}T}) \\ &= N_\mathrm{c}\exp[-\frac{-e\psi(x) + E_\mathrm{c}(x \to \infty) - E_\mathrm{F}}{k_\mathrm{B}T}] \\ &= N_\mathrm{c}\exp[-\frac{e\phi_\mathrm{n} - e\psi(x)}{k_\mathrm{B}T}]\end{aligned} \tag{19.3}$$

and

$$\begin{aligned}p(x) &= N_\mathrm{v}\exp(-\frac{E_\mathrm{F} - E_\mathrm{v}(x)}{k_\mathrm{B}T}) \\ &= N_\mathrm{v}\exp(-\frac{E_\mathrm{F} - E_\mathrm{v}(x \to \infty) + e\psi(x)}{k_\mathrm{B}T}) \\ &= N_\mathrm{v}\exp[-\frac{E_\mathrm{g} - e\phi_\mathrm{n} + e\psi(x)}{k_\mathrm{B}T}]\end{aligned} \tag{19.4}$$

From the Poisson equation, we know that $\psi(x = 0)$ should be negative since positive charges are accumulated in the semiconductor. The band diagram of semiconductor is therefore bent upwards (Figure 19.2 right). To solve the potential profile, we need also the boundary conditions at the M-S interface. A often used assumption is the Schottky-Mott approximation,[1] that the vacuum level is continuous at the interface, which gives:

$$\psi(x = 0) = -(\phi_\mathrm{m} - \chi - \phi_\mathrm{n}) = -\phi_\mathrm{bi} \tag{19.5}$$

where ϕ_bi is known as the build-in potential. The difference between the work function of metal and electron affinity of semiconductor, is called the Schottky barrier height, $\phi_\mathrm{SB} = \phi_\mathrm{m} - \chi$. The Schottky-Mott assumption is very handy, but often fails to explain some real scenarios, due to the existence of surface states.[2] Nevertheless, we will use this theory to demonstrate some basic concepts of the M-S interface. Equations 19.2 - 19.5 can be numerically solved, but not too much insight can be given.

In fact, if the doping density is not large (i.e., $E_\mathrm{F,s} \approx E_i$), we can use a even simpler model, the abrupt junction assumption, for the M-S interface. The merit of such assumption, is that within $0 \le x \le x_\mathrm{d}$, the concentration of mobile carriers can be neglected, due to the charge transfer process. Such region is called the depletion layer, with a thickness x_d. Inside the depletion layer, the charge density is $\rho \approx eN_\mathrm{d}$ and is constant. The Poisson equation is then simplified to:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\frac{eN_\mathrm{d}}{\varepsilon_0\varepsilon_\mathrm{r}} \tag{19.6}$$

We further assume that the potential profile is flat outside the depletion layer, giving the new set of boundary conditions:

$$\begin{aligned} \psi(x=0) &= -\phi_{\mathrm{bi}} \\ \psi(x=x_{\mathrm{d}}) &= 0 \\ \frac{\mathrm{d}\psi}{\mathrm{d}x}(x=x_{\mathrm{d}}) &= 0 \end{aligned} \tag{19.7}$$

Solving Equation 19.6 with the new BCs leads to a linear electric field inside the depletion layer:

$$E(x) = -\frac{\mathrm{d}\psi}{\mathrm{d}x} = \frac{eN_{\mathrm{d}}}{\varepsilon_0\varepsilon_{\mathrm{r}}}(x - x_{\mathrm{d}}) \tag{19.8}$$

and a parabolic potential profile:

$$\psi(x) = -\frac{eN_{\mathrm{d}}}{\varepsilon_0\varepsilon_{\mathrm{r}}}(x - x_{\mathrm{d}})^2 \tag{19.9}$$

where x_{d} is further solved as:

$$x_{\mathrm{d}} = \sqrt{\frac{2\varepsilon_0\varepsilon_{\mathrm{r}}\phi_{\mathrm{bi}}}{eN_{\mathrm{d}}}} \tag{19.10}$$

The potential, electric field, and charge density profile of the abrupt junction approximation, can be seen in Figure 19.3.

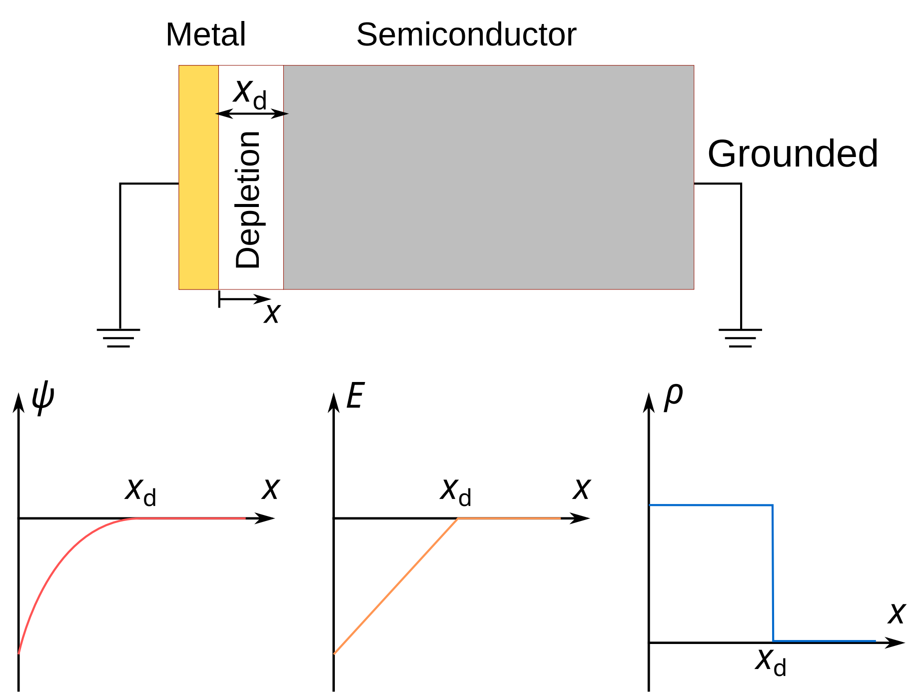

Figure 19.3: Profiles of ψ, $\mathcal{E}$, and ρ using the abrupt junction approximation.

The idea of depletion layer is similar to the Debye length we introduced for electric double layer, however its thickness is dependent on both the dopant concentration, and the surface potential. The capacitance of the depletion layer is: $C = \varepsilon_0\varepsilon_r/x_d$. Since x_d is further related with ϕ_{bi}, we can calculate the build-in potential by measuring the differential capacitance of the M-S junction.

19.3 M-S interface with bias

The discussion about the potential profile without bias is helpful to understand the nonlinear J - V behavior of the Schottky contact. If a bias V is applied on the metal of a Schottky junction with barrier height ϕ_{SB}, the variation of E_c and E_v, ϕ_b, becomes: $\phi_b = \phi_{bi} - V$. Similar to Equation 19.10, the depletion length x_d is expressed as:

$$x_d = \sqrt{\frac{2\varepsilon_r\varepsilon_0\phi_b}{eN_d}} = \sqrt{\frac{2\varepsilon_r\varepsilon_0(\phi_{bi} - V)}{eN_d}} \tag{19.11}$$

which is also dependent on V. Two scenarios can be distinguished:

1. $V > 0$, forward bias

   The Fermi level at the metal side is lowered ($\Delta E_F = -eV$). The depletion length x_d decreases.

2. $V < 0$, reverse bias

   The Fermi level at the metal side is raised. The depletion length x_d increases.

Since we also know that the differential capacitance $C \propto x_d^{-1} \propto 1/\sqrt{\phi_{bi} - V}$, we can plot the measured value of $1/C^2$ against the voltage $-V$, and extrapolate the curve to $y = 0$. Its intercept with the x-axis is ϕ_{bi}, as shown in Figure 19.4.

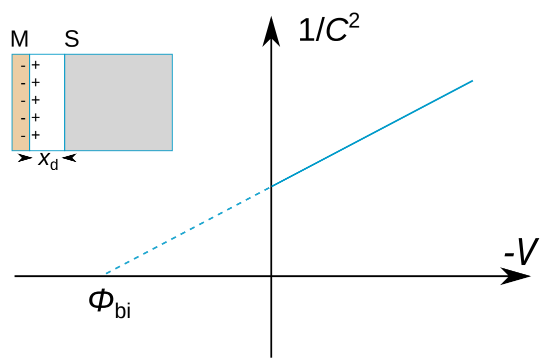

Figure 19.4: Plot of $1/C^2$ vs V for a S-M interface. The extrapolated intercept with x-axis equals the value of ϕ_{bi}.

Intuitively, when a reverse bias is applied, the increased depletion length causes resistance to the current. A quantitative explanation of the nonlinear current behavior can be made by the thermionic emission theory, which assumes the thermal emission of carrier over the barrier dominates the current density. The total current density across the S-M interface, can be divided into the left-going electrons J_{L}, from semiconductor to metal, and the right-going electrons J_{R} from metal to semiconductor. The thermionic emission theory shows that for one direction, the current that across an energy barrier of ΔE, is calculated by:[3]

$$J = A^* T^2 \exp(-\frac{\Delta E}{k_{\mathrm{B}} T}) \tag{19.12}$$

where A^* is the Richardson constant[4] of a semiconductor. When no bias is applied across the S-M interface (Figure 19.5a), the barrier height in both directions is $e\phi_{\mathrm{SB}}$, thus $J_{\mathrm{L}} = -J_{\mathrm{R}} = A^* T^2 \exp(-\frac{e\phi_{\mathrm{SB}}}{k_{\mathrm{B}} T}) = J_0$ (here we assume the left-going electrons give positive current), and the net current is zero. When the bias changes, the value of J_{R} remains constant at $-J_0$, while J_{L} becomes: $J_{\mathrm{L}} = A^* T^2 \exp(-e(\phi_{\mathrm{SB}} - V)/k_{\mathrm{B}} T) = J_0 \exp(eV/k_{\mathrm{B}} T)$. This means in the forward bias regime ($V > 0$, Figure 19.5b), J_{L} is enhanced, while in the reverse bias regime ($V < 0$, Figure 19.5c), J_{L} almost vanishes. The overall current density is then:

$$J = J_{\mathrm{L}} + J_{\mathrm{R}} = J_0[\exp(\frac{eV}{k_{\mathrm{B}} T}) - 1] \tag{19.13}$$

As can be seen in Figure 19.5d, the current remains almost constant at -J_0 within the reverse bias regime, which explains the non-linear J - V behavior shown in Figure 19.1. The magnitude of J_0 is then dominated by ϕ_{SB}. With a larger ϕ_{SB}, the reverse bias current is suppressed.

Schottky junctions are a consequence of the energy level mismatch between the metal and semiconductor, and is often undesired for a semiconductor design. Using the Schottky-Mott rule, the Schottky barrier height is:

$$\begin{aligned} \phi_{\mathrm{SB}}^{\mathrm{n}} &= \phi_{\mathrm{m}} - \chi, && \text{n-doped} \\ \phi_{\mathrm{SB}}^{\mathrm{p}} &= \frac{E_{\mathrm{g}}}{e} - \phi_{\mathrm{m}} + \chi, && \text{p-doped} \end{aligned} \tag{19.14}$$

therefore to reduce ϕ_{SB}, we can choose a metal with small ϕ_{m} (such as Al, ~4.0 V) for n-doped semiconductor, or a metal with large ϕ_{m} (such as Au, ~5.0 V). However as discussed previously, the actual value of the Schottky barrier height is also dependent on the surface states, which still poses as a major challenge for the circuit design of new semiconductors.

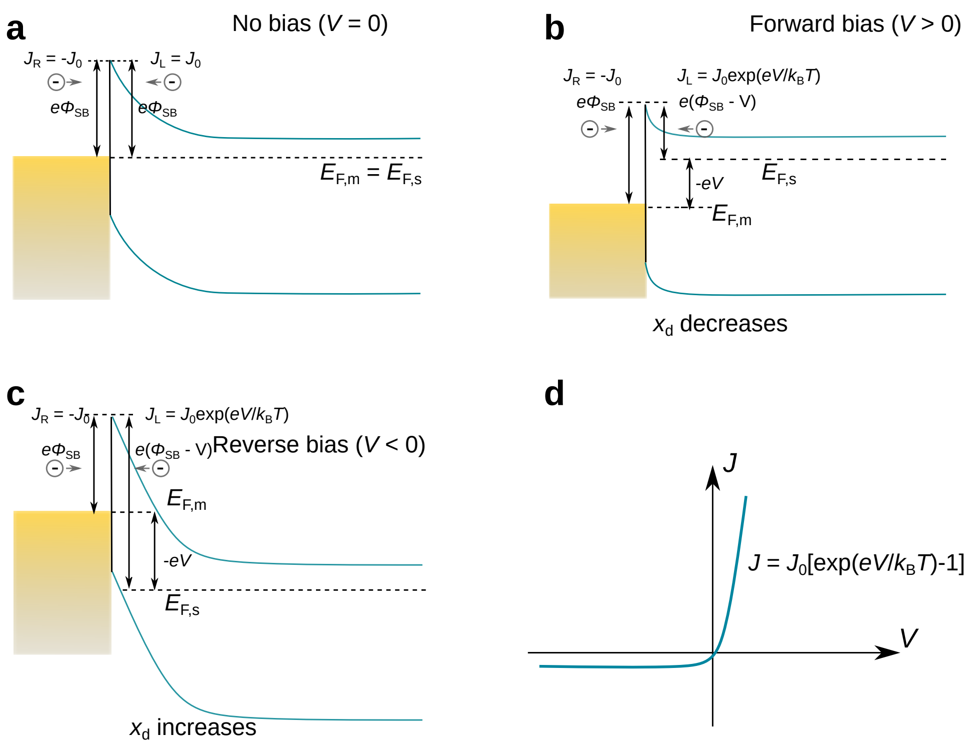

Figure 19.5: Thermionic emission theory of the current across the Schottky barrier. (a) No bias ($V = 0$), the currents from left-going and right-going electron cancel out. (b) Forward bias ($V > 0$), the barrier of left-going electron is reduced. (c) Reverse bias ($V < 0$), the barrier of right-going electron is increased. (d) Overall current density from the thermionic emission theory.

References

(1) Sze, S.; Ng, K. K. In *Physics of Semiconductor Devices*; John Wiley & Sons, Inc.: 2006, pp 134–196.

(2) Tung, R. T. *Phys. Rev. B* **2001**, *64*, 205310.

(3) Murphy, E. L.; Good, R. H. *Phys. Rev.* **1956**, *102*, 1464–1473.

(4) Crowell, C. *Solid State Electronics* **1965**, *8*, 395–399.