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Problem Set 4

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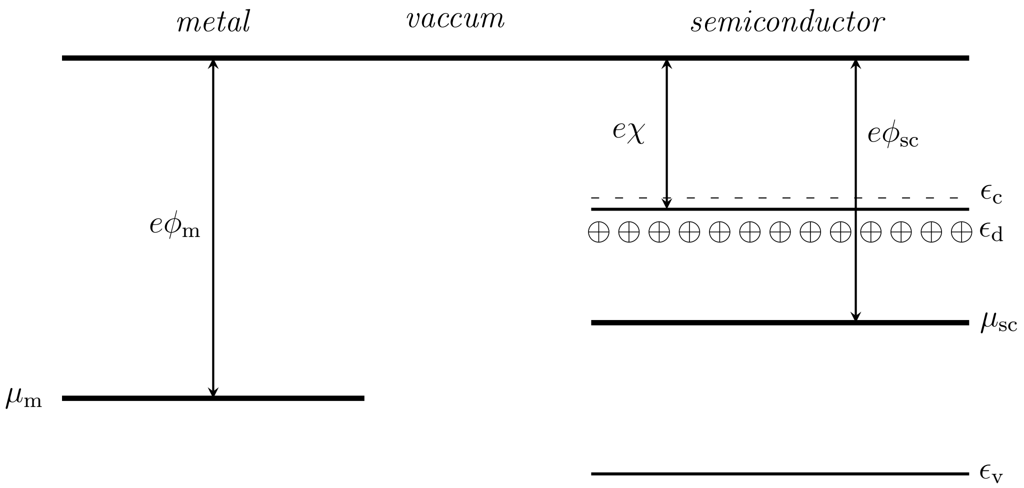
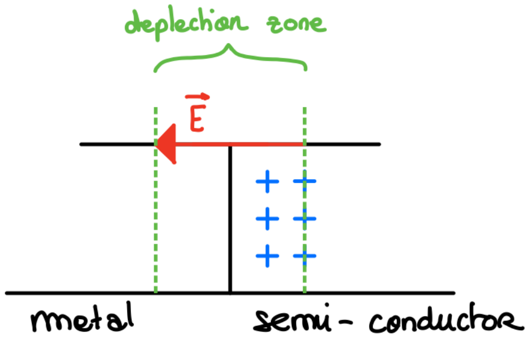
Exercise 1 : Schottky diode

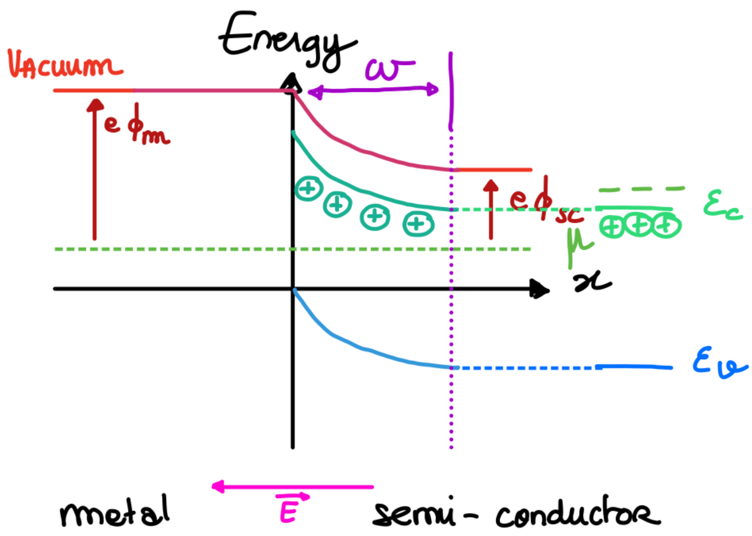
A Schottky diode can be formed at a metal-semiconductor interface. Let us consider a metal with work function $e\phi_m$, and an n-doped semiconductor with a dopant density N_d (assume that all dopants are ionized at room temperature), work function $e\phi_{sc}$ and electron affinity $e\chi$. The work function is the energy needed to extract an electron from the Fermi level towards the lowest vacuum state outside the ma- terial, while the electron affinity of a semiconductor describes the energy needed to extract an electron from the bottom of the conduction band. We assume the case $e\phi_m > e\phi_{sc}$. The energy diagram of the two materials before being in contact is sketched in the figure.



The contact between the two materials leads to the formation of a so-called Schottky diode.

a) Explain qualitatively what happens at the interface when the metal and the semiconductor are joined. Introduce the concept of a depletion zone (also called space charge region).





b) Assume that the carrier density vanishes in the depletion zone of width w and that the electric field vanishes in the semiconductor outside the depletion zone. Calculate the dependence of the electric field and the electrostatic potential $V(x)$ on the distance x from the interface. Choose the zero of the electrostatic potential at the interface ($V(O) = 0$).

$$\begin{cases} \vec{\nabla} \cdot \vec{E} = \dfrac{4\pi\rho}{\epsilon} \\ \vec{E} = -\vec{\nabla} V(x) \end{cases}$$

$$\implies \vec{\nabla}^2 V(x) = -\frac{4\pi\rho(x)}{\epsilon}$$

$$\rho(x) = \begin{cases} 0 \text{ if } x > w \\ -eN_d \text{ if } 0 < x < w \\ 0 \text{ if } x < 0 \end{cases}$$

$$\vec{\nabla}^2 V(x) = \begin{cases} 0 \text{ if } x > w \\ -\dfrac{4\pi e N_d}{\epsilon} \text{ if } 0 < x < w \\ 0 \text{ if } x < 0 \end{cases}$$

$$V(x) = \begin{cases} a_1 x + b_1 \text{ if } x > w \\ -\dfrac{4\pi e N_d}{2\epsilon} x^2 + a_2 x + b_2 \text{ if } 0 < x < w \\ a_3 x + b_3 \text{ if } x < 0 \end{cases}$$

$$V(0) = 0 \Longrightarrow b_3 = b_2 = 0$$

$$V(x) = \begin{cases} a_1 x + b_1 \text{ if } x > w \\ -\frac{4\pi e N_d}{2\epsilon} x^2 + a_2 x \text{ if } 0 < x < w \\ a_3 x \text{ if } x < 0 \end{cases}$$

$$V(w) = a_1 w + b_1 = w\left(-\frac{4\pi e N_d}{2\epsilon} w + a_2\right)$$

$$V'(x) = 0 \text{ if } x > w$$

Meaning we get $a_1 = 0$. If $x < w$, $V'(x) = 0$ and thus $a_3 = 0$.

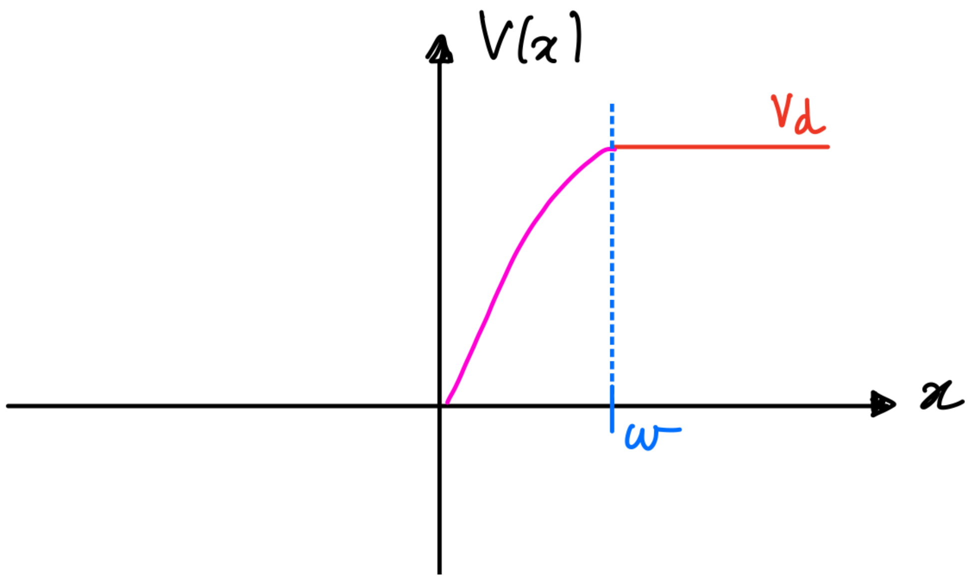
$$\begin{cases} V(w) = b_1 = w\left(-\frac{4\pi e N_d}{2\epsilon} w + a_2\right) \\ V'(w) = 0 = -\frac{4\pi e N_d}{\epsilon} w + a_2 \end{cases}$$

And so we get

$$a_2 = \frac{4\pi e N_d}{\epsilon} w$$

So,

$$V(x) = \begin{cases} \frac{4\pi e N_d w^2}{2\epsilon} \text{ if } x > w \\ -\frac{4\pi e N_d}{2\epsilon}\left(x^2 - 2wx\right) \text{ if } 0 < x < w \\ 0 \text{ if } x < 0 \end{cases}$$



So the energies go as $\epsilon \to \epsilon - eV(x)$.

c) The voltage resulting from the difference of the work functions in the metal and the semiconductor is the so-called diffusion voltage $V_\mathrm{d} = \phi_\mathrm{m} - \phi_\mathrm{sc}$. This diffusion voltage corresponds also to the voltage drop in the depletion zone ($V_\mathrm{d} = V(w) - V(0)$). Use this relation to express w as a function of the work functions.

$$\begin{aligned} V_d &= V(w) - V(0) \\ &= V(w) \end{aligned}$$

$$eV_d = e\phi_m - e\phi_{sc}$$

$$V(w) = \frac{4\pi e N_d w^2}{2\epsilon} = \phi_m - \phi_{sc}$$

So we get,

$$w = \sqrt{\frac{(\phi_m - \phi_{sc})2\epsilon}{4\pi e N_d}}$$

d) The total energy of a charge carrier in a semiconductor (in our case an electron in the conduction band) at a distance x from the interface depends not only on the band structure of the bulk semiconductor, but also on the electrostatic potential $V(x)$. Determine the resulting curbature of the band edges close to the metal-semiconductor interface.

We have $E \to E - eV(x)$,

$$E'' = \frac{4\pi e^2 N_d}{\epsilon} = -eV''$$

e) The junction is now biased by the application of a voltage difference between the two materials, with the semiconductor side grounded. Express the barrier height at the interface and the width of the depletion zone as a function of the applied voltage. Describe the different behavior in the cases of positive and negative voltage.

Now,

$$V(x) = \begin{cases} & \text{idem} \\ & \text{idem} \\ V_1 & x < 0 \end{cases}$$

And so,

$$w = \sqrt{\frac{(\phi_m - \phi_{sc} - V_1)2\epsilon}{4\pi e N_d}}$$

$$eV_d = e\phi_m - e\phi_{sc} - eV_1$$

f) Consider the thermionic current at temperature T through the junction that is given by the carriers whose energy is sufficient to overcome the barrier. The currents from the metal to the semiconductor $I_{\mathrm{m}\to\mathrm{sc}}$ and from the semi- conductor to the metal $I_{\mathrm{sc}\to\mathrm{m}}$ can be written as $|I_{\mathrm{m}\to\mathrm{sc}}| = A^*T^2\mathrm{e}^{-E_\mathrm{b}/k_\mathrm{B}T}$ and $|I_{\mathrm{sc}\to\mathrm{m}}| = A^*T^2\mathrm{e}^{-E'_\mathrm{b}/k_\mathrm{B}T}$ where A^* is the so-called Richardson constant, and E_b and E'_b, is the barrier height seen by electrons traveling from the metal towards the semiconductor and from the semiconductor towards the metal, respectively. Define $e\phi_\mathrm{F} = \epsilon_{\mathrm{c},\infty} - \mu$, where $\epsilon_{\mathrm{c},\infty}$ is the conduction band edge in the semiconductor far from the junction, and describe the relations between $E_\mathrm{b}, V_\mathrm{d}$ and ϕ_F. Consider first the unbiased system and show that the currents through the junction can be expressed in terms of the carrier density in the conduction band of the semiconductor $n_\mathrm{c} = N_\mathrm{c}\mathrm{e}^{-e\phi_\mathrm{F}/k_\mathrm{B}T} = N_\mathrm{d}$ and N_c. Use the result to describe and sketch the voltage dependence of the current through the junction.

For unbiased,

$$E_B = eV_d + e\phi_F = E'_B$$

Biased,arr

$$E_B = e(V_d + \phi_F + V_1)$$

In the unbiased case, $I_{m\to sc} + I_{sc\to m} = 0$.
With voltage , we have

$$\begin{aligned}
I_{\text{tot}} &= A^*T^2 e^{-E_B/k_BT} - A^*T^2 e^{-E'_B/k_BT} \\
&= A^*T^2 \left(e^{-E_B/k_BT} - e^{-E'_B/k_BT} \right) \\
&= A^*T^2 e^{-E'_B/k_BT} \left(e^{-eV_1/k_BT} - 1 \right) \\
&= -I_{m\to sc} \left(e^{V_1/k_BT} - 1 \right)
\end{aligned}$$