Series 11 - The Schottky junction

Exercise

The aim of this series is to consider the case of metal - semiconductor contacts. As we will see, such a contact can exhibit a rectifying behavior originating from the potential barrier which is formed at the metal - semiconductor interface due to the presence of a space charge region on the semiconductor side. The model which results from this concept is the so-called Schottky barrier or Schottky junction. Metal - semiconductor contacts can also exhibit a non-rectifying behavior, i.e. the contact will have a negligible resistance whatever the applied potential. The latter case corresponds to the Ohmic contact and it is the type of contact which is required to connect a semiconductor device or an integrated circuit to other devices in an electronic system.

As quoted in the problem wording at the surface of a semiconductor the crystal periodicity is broken. The dangling bonds which result from this configuration are not fully hybridized. Qualitatively we can understand that the wave function associated with such a dangling bond will not possess the delocalized behavior of orbitals from a bulk material. We will rather speak of a localized state, i.e. such a state won't take part to the transport properties of a semiconductor material as it is usually the case for delocalized states. It will rather be a hindrance to the mobility of free carriers (electrons and holes). The corresponding electronic states will not contribute to the continuum of states of a bulk material. they will lie instead in the band gap of the semiconductor. The large surface density of states (i.e. dangling bonds) will provide to this two-dimensional system a continuum-like behavior on a given energy range.

②

1_ Poisson's equation applied to the vicinity of an n-type semiconductor surface such as the case displayed in Figure 1 will express as:

$\frac{d^2V}{dz^2} = -\frac{eN_D}{\varepsilon}$ (equation applied to the case of positive fixed charges of density equal to N_D)

i.e. $\frac{dV}{dz} = -E(z) = -\frac{eN_D}{\varepsilon}z + K_1$

Boundary conditions are such that in $z=0$ (origin of distances taken at the surface with the Oz axis oriented toward the semiconductor) $K_1 = E_0$. As a result, we get $V(z) = -\frac{eN_D}{2\varepsilon}z^2 + E_0 z + K_2$ (the electric field is pointing from positive charges to negative ones).

For $z=0$, $K_2 = V(0)$ so that $V(z) - V(0) = -\frac{eN_D}{2\varepsilon}z^2 + E_0 z$

We wish to determine the critical length L beyond which the potential difference $V(L) - V(0)$ is fully screened, i.e. the length leading to $E(z) = 0$.

From the expression of $E(z)$ derived above, we get:

$E_0 - \frac{eN_D L}{\varepsilon} = 0$ i.e. $L = \frac{\varepsilon E_0}{eN_D}$

In addition, $V(L) - V(0) = -\frac{eN_D}{2\varepsilon}L^2 + E_0 L$ and as $E_0 = \frac{eN_D L}{\varepsilon}$, we obtain:

$\Delta V\,(= V(L) - V(0)) = -\frac{eN_D L^2}{2\varepsilon} + \frac{eN_D L^2}{\varepsilon} = \frac{eN_D L^2}{2\varepsilon}$

so that $\boxed{L = \left(\frac{2\varepsilon \Delta V}{eN_D}\right)^{1/2}}$ It is seen that $\Delta V \propto \frac{\rho}{\varepsilon}L^2$ where ρ is the fixed charge density

ΔV will also be called V_d (potential drop) in the next exercises

~~2~~_ For a non-degenerate semiconductor in absence of any external perturbation, the average electron density in the conduction band is given by: $n_0 = N_c \exp(-(E_c - E_F)/k_B T)$ (Boltzmann approximation)

If now we add a slowly varying electrostatic potential $V(z)$ at the crystal lattice scale, each electron along z will possess, in addition to its energy arising from the crystal network, a potential energy $-eV(z)$. We can then understand that the whole conduction band will be shifted in energy by a quantity $-eV(z)$. As at thermal equilibrium the Fermi energy is constant throughout the material, the electron density will vary like:

$$n(z) = N_c \exp\left(-\frac{(E_c - eV(z) - E_F)}{k_B T}\right) \quad \text{i.e.} \quad n(z) = n_0 \exp\left(\frac{eV(z)}{k_B T}\right)$$

The charge induced by the potential is given by: $\rho_{ind}(z) = -e(n(z) - n_0)$

i.e. $\rho_{ind}(z) = -en_0\left[\exp\left(\frac{eV(z)}{k_B T}\right) - 1\right] \approx -\frac{e^2 n_0}{k_B T} V(z) = -\varepsilon q_D^2 V(z)$

$\hookrightarrow$ valid in the limit of weak potentials!

The linearization of the built-in charge allows defining the Debye wave vector q_D and thus the Debye screening length $\ell_D = \frac{1}{q_D}$.

As a result, we get $\boxed{\ell_D = \left(\frac{\varepsilon k_B T}{e^2 n_0}\right)^{1/2}}$ ℓ_D corresponds to the length scale beyond which an electron gas can fully screen an external potential.

For silicon exhibiting a doping level of $10^{17}\,cm^{-3}$ at room temperature, we get ($\varepsilon_r \sim 12$): $\ell_D = \left(\frac{12 \times 8.82 \times 10^{-12} \times 1.38 \times 10^{-23} \times 300}{(1.6 \times 10^{-19})^2 \times 10^{23}}\right)^{1/2} \sim 13.1\,nm$

I. Surface phenomena

2. From Figure 1, we can immediately deduce that σ is given by

$$\boxed{\sigma = -eN_{ss}(E_F - e\phi_0 - E_V(0))}$$

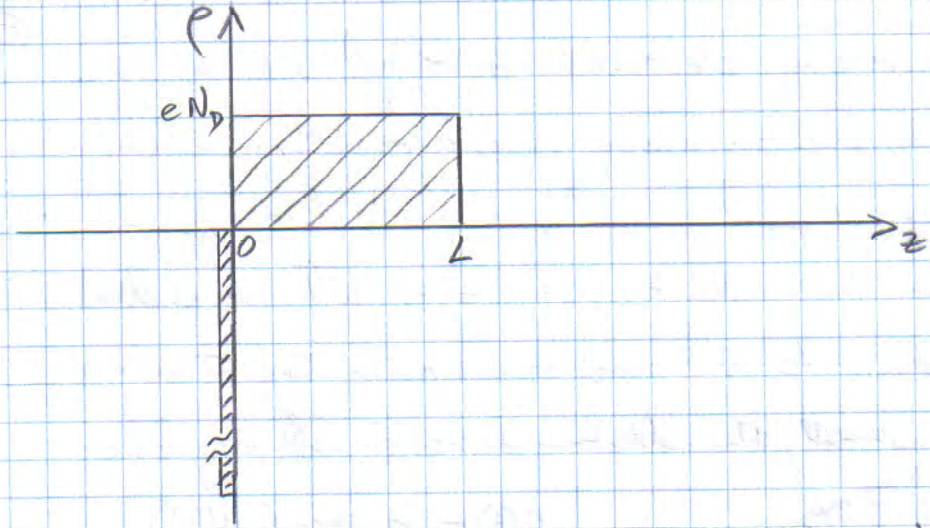
3. As we must satisfy electrical neutrality, the surface charge σ will correspond to the charge spread over the space charge region so that

$-\sigma = eN_D L$ and thus $\boxed{V_d = -\frac{\sigma L}{2\varepsilon}}$

$\hookrightarrow$ as seen on the figure hereafter!

to find it, express the result of Ex.1 to find Vd= ...

and indentify the presence of σ



4- From previous questions, we can derive that

$$V_d = \frac{L}{2\varepsilon} e N_{ss} \left(E_F - e\phi_0 - E_V(0) \right)$$

Moreover, $E_V(0) = E_V(+\infty) + eV_d$ so that

$$V_d = \frac{L}{2\varepsilon} e N_{ss} \left(E_F - e\phi_0 - E_V(+\infty) - eV_d \right)$$

i.e. $$V_d \left(1 + \frac{e^2 L}{2\varepsilon} N_{ss}\right) = \frac{eL}{2\varepsilon} N_{ss} \left(E_F - e\phi_0 - E_V(+\infty) \right)$$

In the limit of a large surface density, V_d will not depend on N_{ss} so that

$$eV_d = E_F - e\phi_0 - E_V(+\infty)$$

i.e. $E_c(+\infty) - E_g + eV_d = E_F - e\phi_0$ and since $E_c(0) = E_c(+\infty) + eV_d$

we finally get $\boxed{E_c(0) - E_F = E_g - e\phi_0}$

II_ The ideal Schottky junction

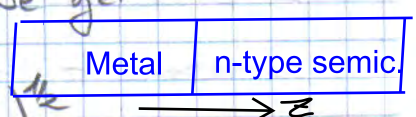
5- By analogy with question 2, we can write $n(0) = N_c \exp\left(-\frac{(E_c(0) - E_F)}{k_B T}\right)$.

In addition, $E_c(0) - E_F = E_g - e\phi_0 = e\phi_B$ (cf. Figs. 1 and 2)

So that $\boxed{n(0) = N_c \exp\left(-\frac{e\phi_B}{k_B T}\right)}$

6 When considering Boltzmann velocity distribution we get

$$\langle v_z \rangle = \frac{\int_{-\infty}^{0} v_z \exp(-m_c^* v_z^2 / 2k_B T)\, dv_z}{\int_{-\infty}^{0} \exp(-m_c^* v_z^2 / 2k_B T)\, dv_z} = -\left(\frac{2k_B T}{\pi m_c^*} \right)^{1/2}$$

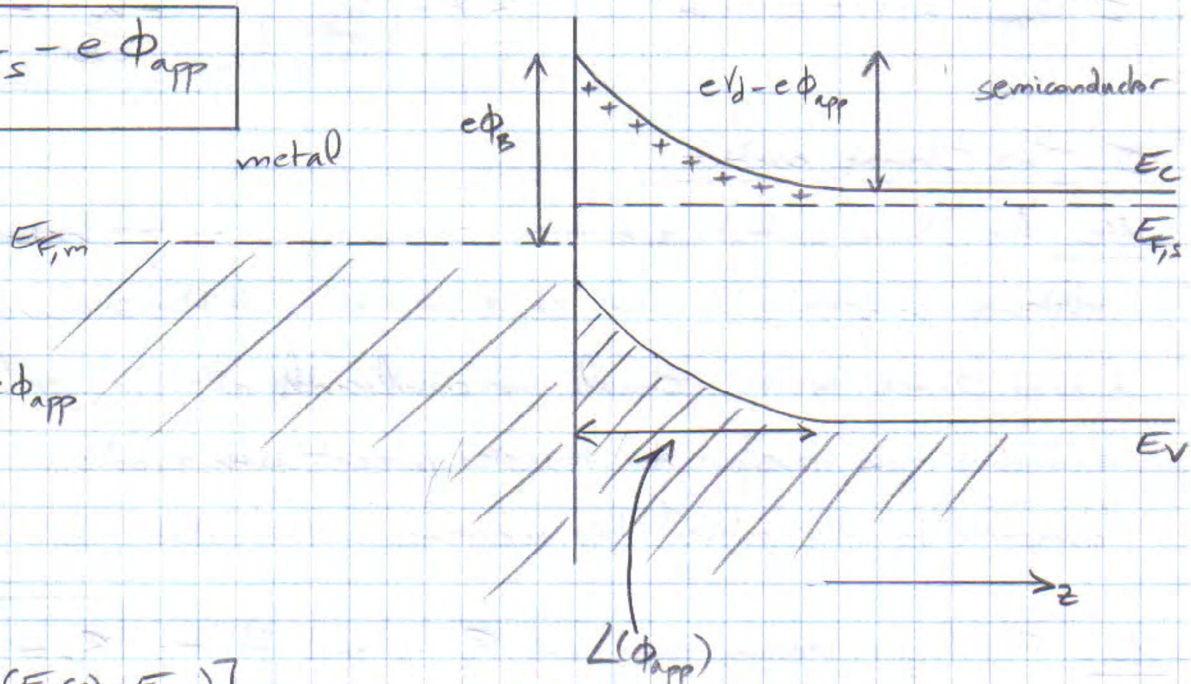


Average v_z of carriers travelling towards the left

7 The expression of $j_{s\to m}$ is given by $j_{s\to m} = -e\dfrac{n(0)}{2}\langle v_z\rangle$

so that $\boxed{j_{s\to m} = e\left(\dfrac{k_B T}{2\pi m_c^*}\right)^{1/2} N_c \exp\left(-\dfrac{e\phi_B}{k_B T}\right)}$

8 $\boxed{E_{F,m} = E_{F,s} - e\phi_{app}}$



$E_c(0) - E_c(+\infty) = eV_d - e\phi_{app}$

9 $n(0) = N_c \exp\left[-\dfrac{(E_c(0) - E_{F,s})}{k_B T}\right]$

i.e. $n(0) = N_c \exp\left[-\dfrac{(e\phi_B - e\phi_{app})}{k_B T}\right]$ and thus we get:

$$\boxed{j_{s\to m} = e\left(\frac{k_B T}{2\pi m_c^*}\right)^{1/2} N_c \exp\left(-\frac{e\phi_B}{k_B T}\right)\exp\left(\frac{e\phi_{app}}{k_B T}\right)}$$

10 $j(\phi_{app}) = j_{s\to m} + j_{m\to s}$

because the two currents at equilibrium have opposite signs

so that $\boxed{j(\phi_{app}) = e\left(\dfrac{k_B T}{2\pi m_c^*}\right)^{1/2} N_c \exp\left(-\dfrac{e\phi_B}{k_B T}\right)\left[\exp\left(\dfrac{e\phi_{app}}{k_B T}\right) - 1\right]}$

$j(\phi_{app})$ can thus be expressed as $j(\phi_{app}) = j_{sat}\left[\exp\left(\dfrac{e\phi_{app}}{k_B T}\right) - 1\right]$ i.e. it exhibits a rectifying dependence and j_{sat} is given by:

$j_{sat} = A^* T^2 \exp\left(-\dfrac{e\phi_B}{k_B T}\right)$ since $N_c = \dfrac{1}{4}\left(\dfrac{2 m_c^* k_B T}{\pi \hbar^2}\right)^{3/2}$ with $A^* = \dfrac{4 e k_B^2 \pi m_c^*}{h^3}$

11 $A^* = \dfrac{4 \times 1.6\times 10^{-19} \times (1.38\times 10^{-23})^2 \times \pi \times 9.1\times 10^{-31}}{(6.62\times 10^{-34})^3} \approx 120 \text{ A cm}^{-2}\text{K}^{-2}$

2 $j_{sat} = A^* \frac{m_c^*}{m_0} T^2 \exp\left(-\frac{e\phi_B}{k_B T}\right)$ i.e. $j_{sat} = 120 \times 0.067 \times 300^2 \exp\left(-\frac{0.7}{0.025}\right) = 0.5\,\mu A/cm^2$

$I_{sat} = 0.05\ nA$, $I(\phi_{app} = 0.2V) = I_s\left[\exp\left(\frac{0.02}{0.025}\right) - 1\right] = 0.15\,\mu A$

$I(\phi_{app} = 0.4V) = 0.44\ mA$ $\qquad R_0 A = \left(\frac{\partial j}{\partial \phi_{app}}\right)^{-1}_{\phi_{app}=0} = \frac{k_B T}{e\, j_{sat}} = \frac{0.025}{0.5 \times 10^{-6}} = 50\,k\Omega\, cm^2$

and $R_0 = 500\,M\Omega$

III - The Ohmic contact

3 An Ohmic contact is a metal-semiconductor contact having a negligible contact resistance compared with the series resistance of the semiconductor. As a result, a good Ohmic contact should not significantly alter the performances of a device and thus can transfer the requested current with a potential drop which is small compared to the potential drop occurring in the active region of the device.

4 For light doping conditions R_c is such that: $\boxed{R_c = \frac{k_B}{eA^*T} \exp\left(\frac{e\phi_B}{k_B T}\right)}$

To obtain a low R_c value a metal-semiconductor contact exhibiting a small Schottky barrier height is to be preferred.

5 For heavy doping conditions the barrier thickness becomes relatively thin and is dominated by tunneling.

$$I \sim \exp\left[-2L\left(2m_c^*(e\phi_B - e\phi_{app})/\hbar^2\right)^{1/2}\right] \text{ and } L^2 \sim \frac{2\varepsilon}{eN_D}(\phi_B - \phi_{app})$$

so that $I \sim \exp\left[-\frac{4(m_c^*\varepsilon)^{1/2}(\phi_B - \phi_{app})}{\hbar N_D^{1/2}}\right]$

and $\boxed{R_c \sim \exp\left[\frac{4(m_c^*\varepsilon)^{1/2}\phi_B}{\hbar N_D^{1/2}}\right] \propto \exp\left(\frac{\phi_B}{N_D^{1/2}}\right)}$

R_c exhibits a strong dependence on the doping level