Homework Assignment 5

Due date: 14.June.2024

Q1 Exact Solution of Metal-Oxide-Silicon Junction

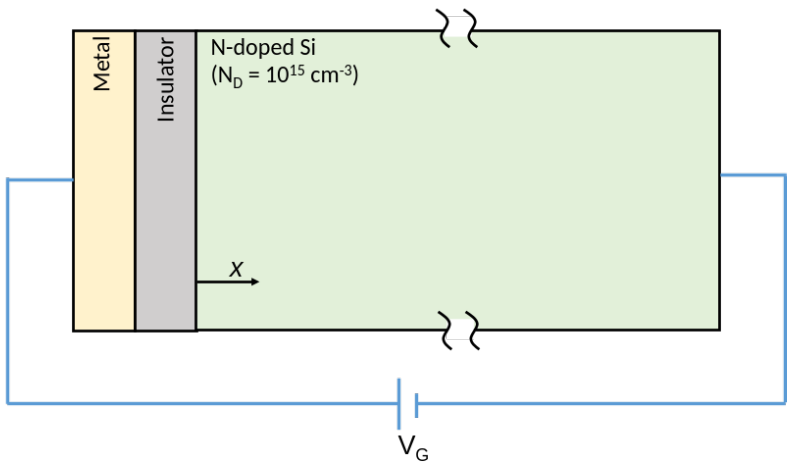

Figure 1: Schematic diagram for a metal-insulator-silicon interface.

In Lecture 19, we discussed the 1D profile of the electric potential ψ at a metal-semiconductor junction without bias. Consider now a metal-insulator-semiconductor interface system, where the semiconductor is n-doped silicon with a donor concentration of $N_d = 10^{15}$ cm^{-3}. Similar to what you did in HW4, by applying a gate voltage between metal and semiconductor electrodes, V_G, one can control the surface potential at the insulator-semiconductor surface at $x = 0$, ψ_0, as shown in Fig. 1. The thickness of the insulating layer is d =100 nm, and the relative permittivities of the insulator and silicon are $\varepsilon_d = 3.9$ and $\varepsilon_r = 11.7$, respectively. The self-ionization of electrons and holes in the semiconductor follows $n \cdot p = n_i^2 = 10^{20}$ cm^{-6}. The bandgap for silicon is $E_g = 1.12$ eV. The total number of states in the conduction band valence band are identical, or namely $N_C = N_V$. Under the assumption that at $V_G = 0$, the semiconductor conduction and valence bands are flat without bending, so the bulk electron concentration $n_0 \approx N_D$. Please answer the following questions.

1. Please calculate (i) the total number of states in the conduction band N_C and (ii) the energy difference between the conduction band minimum E_C and the Fermi energy E_F, $E_C - E_F$.

2. Please show that the 1D Poission-Boltzmann equation for the semiconductor layer is given by:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \frac{-\rho}{\varepsilon_r\varepsilon_0} = -\frac{e}{\varepsilon_r\varepsilon_0}[N_\mathrm{d} + p_0 \exp\left(\frac{-e\psi(x)}{k_\mathrm{B}T}\right) - n_0 \exp\left(\frac{e\psi(x)}{k_\mathrm{B}T}\right)] \tag{1}$$

And the boundary conditions $\psi(x=0) = \psi_0$; $\frac{d\psi}{dx}(x \to \infty) = \psi(x \to \infty) = 0$. Please calculate the values for p_0.

3. Consider $\psi_0 = -0.25$ V, please derive the analytical solution for the 1D PBE using the abrupt junction approximation. Please show how the governing equation and boundary conditions can be simplified as follows:

$$\frac{d^2\psi}{dx^2} = \frac{-eN_d}{\varepsilon_r\varepsilon_0}$$
$$\psi(x=0) = \psi_0$$
$$\frac{d\psi}{dx}(x=W) = \psi(x=W) = 0$$

   Please derive also the expression for the depletion width W.

4. Please solve the initial value problem in Q1.2 numerically for $\psi_0 = -0.25$ V and compare the $\psi - x$ profile to the approximated solution from Q1.3.

5. Using your numerical solution from Q1.4, please solve and plot the surface potential ψ_0 as a function of V_G, for $-20 \le V_G \le 20$.

Q2 Examining the Shockley-Queisser Limit

Assuming sunlight emission follows the black-body radiation from a point source given by (see `https://en.wikipedia.org/wiki/Black-body_radiation`):

$$B(\nu, T) = \frac{2h\nu^3}{c^2} \frac{1}{\exp(\frac{h\nu}{k_B T}) - 1} \tag{2}$$

where B is the spectral radiance (the power per unit solid angle per unit area normal to the light propagation direction), c is the speed of light, $\nu = \frac{c}{\lambda}$ is the light frequency, λ is the light wavelength, $T = 6600$ K is the black body temperature. Please answer the following questions. (hint: all calculations will become easier if you define a new variable $\chi = \frac{h\nu}{k_B T}$.)

1. Please plot B as a function of ν (from 10^{12} to 10^{17} Hz) and numerically determine the value of ν_{max}, which is the frequency reaching the B maximum. What are the corresponding photon energy and wavelength at this point?

2. By using Silicon, with a bandgap energy of 1.1 eV, as the solar cell material, please indicate the light frequency range in your plot in Q2.1 which can be absorbed by Silicon. Please numerically calculate the percentage of solar energy being absorbed. (hint: total radiation power of the blackbody is $\int_0^\infty B(\nu)d\nu$.)

3. Within the absorbing frequency region, please explain how the high-energy photons being converted and relaxed to electron/hole pairs in the Silicon conduction/valence bands having a lower energy, and what is the energy level?

4. Assuming that all absorbed photons become electron-hole pairs, please calculate the theoretical upper limit of the power conversion efficiency for the Silicon-based solar cell upon absorbing the blackbody radiation. (hint: You will need to first calculate the number of photons radiated from the blackbody per unit time per unit solid angle per unit area normal to the light propagation direction as a function of frequency, which are all absorbed by the solar cell, followed by relaxation to a constant energy level given in Q2.3.)

5. Following the same procedure, please plot the theoretical upper limit for the solar cell power conversion efficiency as a function of bandgap energy of the absorbing semiconductor. The procedure follows the way Shockley and Queisser established the solar cell theoretical efficiency limit.