Sample Solutions for HW5

14.June.2024

Q1 Exact Solution of Metal-Oxide-Silicon Junction

1. From the lectures (and the script), we know that:

$$n * p = N_C N_V exp\left(\frac{-E_g}{k_b T}\right) = n_i^2 \tag{1}$$

Since the question states that $N_C = N_V$, we have:

$$n * p = N_C^2 exp\left(\frac{-E_g}{k_b T}\right) = n_i^2 \tag{2}$$

$$N_C = n_i exp\left(\frac{E_g}{2k_b T}\right) = 2.56 * 10^{19}\, cm^{-3} \tag{3}$$

Moreover, since the number of intrinsic n-carriers is considerably smaller than the number of donor carriers introduced ($N_D \approx n$), we can calculate the energy gap as follows:

$$N_D \approx n = N_C exp\left(-\frac{E_C - E_F}{k_b T}\right) \tag{4}$$

$$ln\left(\frac{N_D}{N_C}\right) = -\frac{E_C - E_F}{k_b T} \tag{5}$$

$$ln\left(\frac{N_D}{N_C}\right) = -\frac{E_C - E_F}{k_b T} \tag{6}$$

$$E_C - E_F = K_b T ln\left(\frac{N_C}{N_D}\right) = 0.26\, eV \tag{7}$$

2. We start by writing down the 1D charge density in full form:

$$\rho = e\left[N_D - n(x) + p(x) - N_A\right] \tag{8}$$

Now we can introduce the electric potential dependency of the carrier concentrations by considering both the gate voltage as well as the field inherent to the junction:

$$\rho = e\left[N_D - N_C exp\left(\frac{-e(\phi_n - \psi(x)}{k_b T}\right) + N_V exp\left(\frac{e\phi_n - \psi(x) - E_g}{k_b T}\right) - N_A\right] \tag{9}$$

By observing that $n_0 = N_C exp\left(\frac{-e\phi_n}{k_b T}\right) = 1.02 * 10^{15}$ and $p_0 = N_V exp\left(\frac{e(\phi_n - E_g)}{k_b T}\right) = 9.85 * 10^4$, we can plug in the obtained charge density in the PBE, which leads us to the final result:

$$\frac{d^2\psi}{dx^2} = -\frac{e}{\epsilon_r \epsilon_0}\left[N_D - p_0 exp\left(\frac{-e\psi(x)}{k_b T}\right) - n_0 exp\left(\frac{e\psi(x)}{k_b T}\right)\right] \tag{10}$$

Here we note that $N_A = 0\,cm^{-3}$. Moreover, the boundary conditions are selected such that the potential at the interface corresponds to some initial value which decays to zero as the distance from said interface approaches infinity.

3. In the depletion layer layer of the semiconductor $n \approx p \approx 0$, thus in the case where the acceptor concentration is zero:

$$\rho = e\left[N_D - n(x) + p(x) - N_A\right] = eN_D \tag{11}$$

This leads to the following PBE:

$$\frac{d^2\psi}{dx^2} = -\frac{eN_D}{\epsilon_r\epsilon_0} \tag{12}$$

The solution of this equation has the following form:

$$\psi(x) = -\frac{eN_D}{\epsilon_r\epsilon_0}\frac{x^2}{2} + Ax + B \tag{13}$$

By considering the derivative of the potential at W, we obtain $A = \frac{eN_D}{\epsilon_r\epsilon_0}W$. Further, by evaluating the potential at $x = 0$, we get $B = \psi_0$. Finally, by considering the potential at $x = W$ and reducing back to a perfect square form, we arrive at the final form of the solution:

$$\psi(x) = -\frac{eN_D}{2\epsilon_r\epsilon_0}(x - W)^2 \tag{14}$$

4. The exact equation can be solved using a boundary value problem solver, such as finite element based methods or by applying the shooting method previously seen in past homework assignments. For the analytical solution of the approximate equation, all that is needed is a simple plotting library.

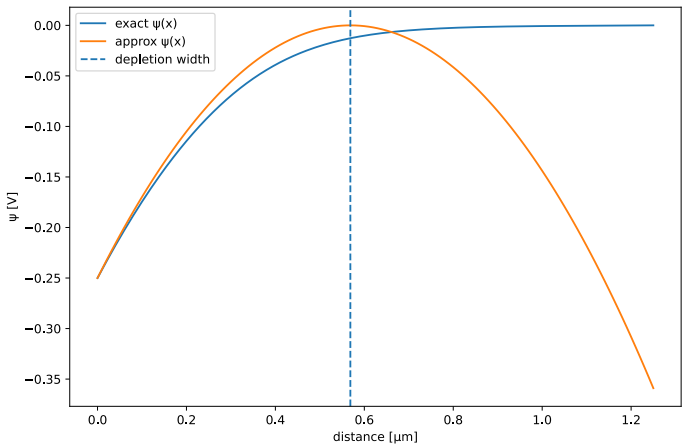

Figure 1: Potential profile as a function of distance from the insulator-semiconductor interface for an initial surface potential of -0.25V. The analytical solution of the approximate PBE shows the expected parabola behavor which is only physically meaningful until the depletion width is reached (see B.C.), whereas the numerical solution of the exact equation results in a profile that is sensible within the whole plotted range.

5. In order to determine ψ_0 as a function of V_G, we start by considering charge neutrality, which, in this case, can be reduced to a surface charge form due to the geometry of the problem and of the charge distribution.

$$\sigma_c + \sigma_d = 0 \tag{15}$$

Where σ_c and σ_d are the surface charges due to the gate voltage (in the metal) and due to the difference in Fermi energy (in the semiconductor). Since the gate voltage is applied such that it forms a capacitor, we get:

$$-(\psi_0 - V_G)\frac{\epsilon_d \epsilon_0}{d} + \int_0^\infty \rho_d(x)\, dx = 0 \tag{16}$$

$$-(\psi_0 - V_G)\frac{\epsilon_d \epsilon_0}{d} - \int_0^\infty \epsilon_0 \epsilon_r \frac{d^2\psi}{dx^2}\, dx = 0 \tag{17}$$

The final expression can then be solved numerically to obtain $\psi(V_G)$ for the desired voltage range.

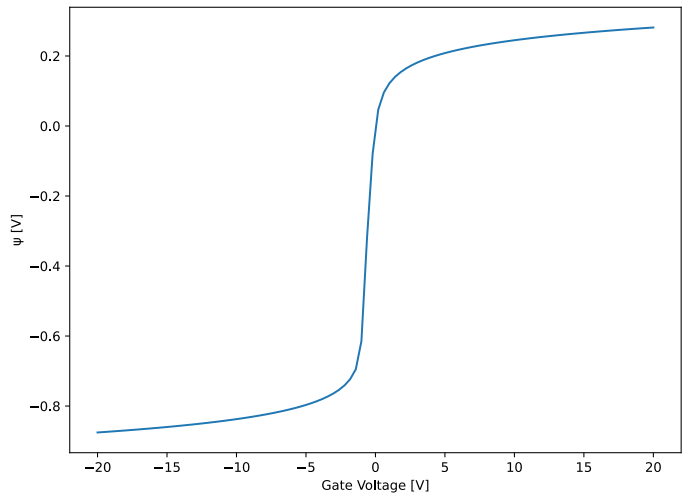

Figure 2: Potential profile as a function of the gate voltage.

Q2 Examining the Shockley-Queisser Limit

1. Spectral radiance of black body

   The spectral radiance of black body can be seen in Fig. 3.

   The maximal radiance occurs at $\partial B/\partial \nu = 0$:

$$\frac{\partial B}{\partial \nu} \propto \frac{\nu^2}{(e^{\beta\nu} - 1)^2}[e^{\beta\nu}(e^{\beta\nu} - 3) + 3] = 0 \tag{18}$$

   where $\beta = h/k_B T$. The solution is $\beta\nu_{\max} \approx 2.82$, corresponding to $\nu_{\max} = 3.87 \times 10^{14}$ Hz, or 1.60 eV or 773.7 nm.

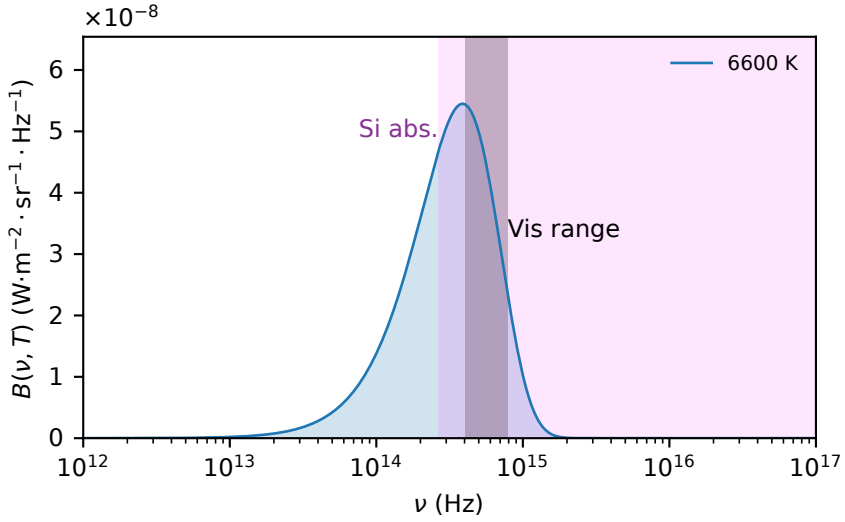

Figure 3: Spectral radiance $B_{\nu,T}$ of black body with $T = 6600$ K. The absorption by Si is indicated by magenta, and the visible light range is marked in gray.

2. Light absorption by Si

   See the magenta region marked in Fig. 3. The total solar energy absorbed is about 83 %.

3. Light conversion in Si

   The high-energy photons excite electron-hole pairs into "deep levels" away from the conduction band / valence band minima (CBM / VBM). The excited electron / holes have momentum $p = \sqrt{2m^*\Delta E}$ where ΔE of deep level away from band minima and m^* is the effective mass. When the carriers relaxed to the band minima, due to the conservation of momentum, their momentum are transferred to a phonon which causes energy loss. After a very short time ($\sim$ fs), all the photo-excited electron-hole pairs fall into the states at the band edge, having an energy associated with the silicon band gap. The onset energy is the bandgap of Si.

4. Theoretical limit

   For any photon with $h\nu > E_g$, the maximum output energy is E_g. Therefore the theoretical upper limit is

$$\eta_{\text{upper}} = \frac{\int_{E_g/h}^{\infty} \frac{E_g}{h\nu} B(\nu, T)\mathrm{d}\nu}{\int_0^{\infty} B(\nu, T)\mathrm{d}\nu} \tag{19}$$

   where $E_g = 1.1$ eV is the bandgap of Si. Using the bandgap of Si, η_{upper} is estimated to be about 43 %.

5. Gap-dependent efficiency limit

   The theoretical upper limit of solar energy conversion as function of bandgap can be seen in Fig. 4. Si is very close to the theoretical optimal bandgap. In addition, the theoretical upper limit calculated using the AM1.5 global spectrum are also plotted for comparison. Note the limit we obtained only considered the bandgap mismatch between a semiconductor and solar spectrum. The actual Shockley-Quessier limit of Si is

calculated to be about 33% which considered more effects. You can access their original paper for more details.

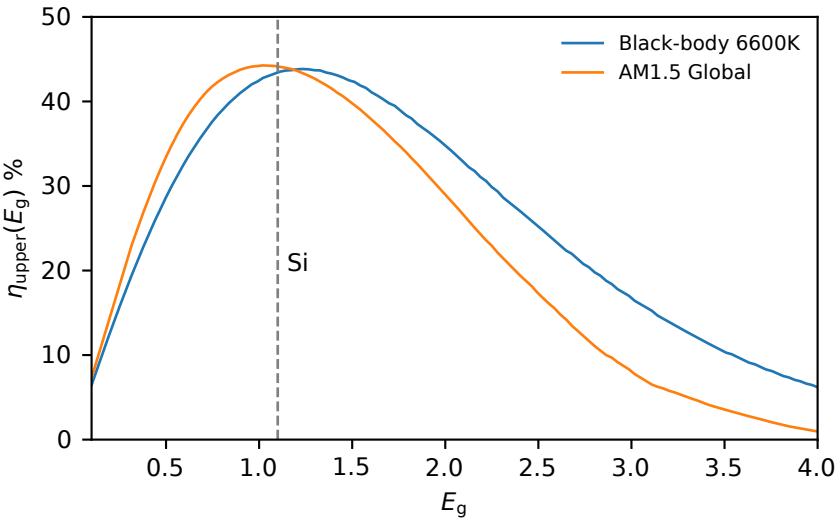

Figure 4: Bandgap-dependent theoretical upper limit of an ideal solar cell with black body radiation at 6600 K and AM1.5 global spectrum.