PHYS-E0421 - Solid State Physics Spring 2019

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Exercise session 4 - April 5, 2019	2	2	1
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1. p-n-junction

(a)

We will start with Eq. (6.246) from Elliot which gives the temperature dependence of the chemical potential

$$\mu_n = E_C - k_B T \ln \frac{N_C}{N_d}, \tag{1}$$

where N_d is the donor concentration in n-type semiconductor and N_c is the effective concentration of states at the conduction band edges. Energy E_C is the energy of the conduction belt. Similar equation can be written for p-type semiconductor so that

$$\mu_p = E_V + k_B T \ln \frac{N_V}{N_a}, \tag{2}$$

where E_V is the valence band energy and N_V is the effective concentration of the valence band and N_A the acceptor concentration.
When then junction is formed, different sides of the junction have different chemical potentials,difference between chemical potentials is called as the contact potential

$$\begin{aligned}
e\phi_c = \mu_n - \mu_p &= E_C - E_V - k_B T \ln \frac{N_C}{N_d} - k_B T \ln \frac{N_V}{N_a} \\
&= E_C - E_V - k_B T \left(\ln \frac{N_C}{N_d} + \ln \frac{N_V}{N_a} \right) \\
&= E_C - E_V - k_B T \ln \frac{N_C N_V}{N_d N_a}
\end{aligned}$$

The law of mass action is given by

$$\begin{gathered}
n_i^2 = N_C N_V e^{-E_g/kT} \\
\Leftrightarrow \\
N_C N_V = e^{E_g/kT} n_i^2,
\end{gathered}$$

where band gap energy is $E_g = E_C - E_V$.

By substituting this to previously obtained equation we can derive the result.

$$\begin{aligned}
e\phi_c &= E_C - E_V - k_B T \ln \frac{N_C N_V}{N_d N_a} \\
&= E_C - E_V - k_B T \ln \frac{e^{E_g/kT} n_i^2}{N_d N_a} \\
&= E_C - E_V - k_B T \ln \frac{n_i^2}{N_d N_a} - k_B T \frac{E_g}{k_B T} \\
&= E_C - E_V - k_B T \ln \frac{n_i^2}{N_d N_a} - E_C + E_V \\
&= k_B T \ln \frac{N_d N_a}{n_i^2},
\end{aligned}$$

so we obtain Elliot's Eq. (8.38a)

$$\phi_c = \frac{k_B T}{e} \ln \frac{N_d N_a}{n_i^2}. \tag{3}$$

(b)

Poisson's equation is given by

$$\frac{\partial^2 \phi(z)}{\partial^2 z} = -\frac{\rho(z)}{\epsilon_r \epsilon_0}, \tag{4}$$

where ρ is the charge density, and $\epsilon_r \epsilon_0$ is the permittivity.
In IL the Schottky model the charge density is shown in the $p-n$ junction at $z = 0$.

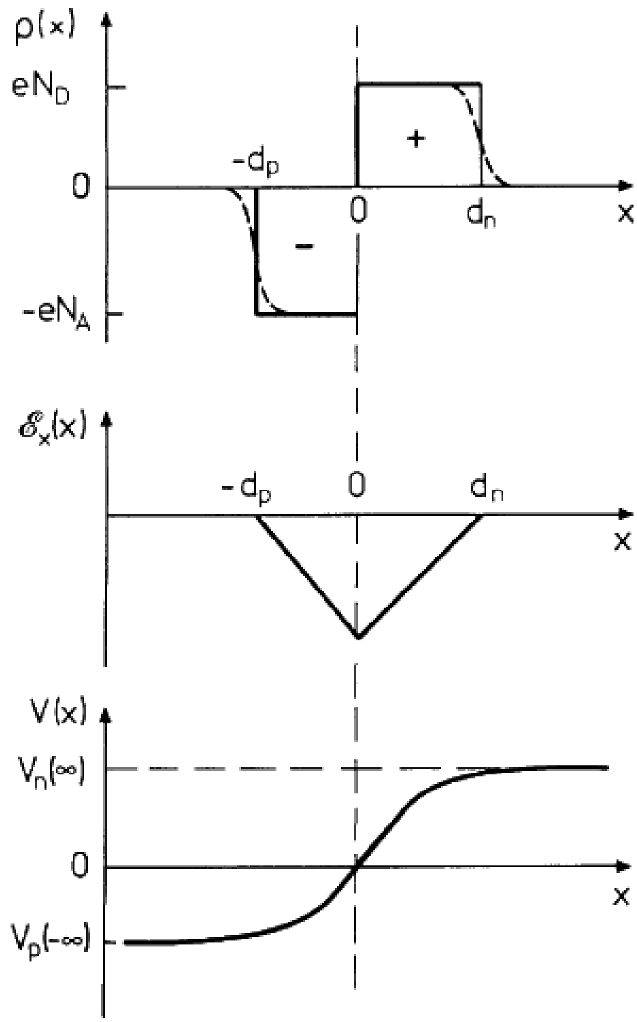

Figure 1: Spatial variation of the charge density. The depletion region for different for the n- and p-type of semiconductor.

The charge density can be approximated so that it is

$$\rho(z) = \begin{cases} -eN_a & -d_p < z < 0 \\ eN_d & 0 < z < d_n \end{cases}$$

Gauss' law in one dimension can be written as

$$\nabla \cdot E(z) = \frac{\partial E(z)}{\partial z} = \frac{\rho(z)}{\epsilon_r \epsilon_0}$$

and we can see that electric field $E(z) = -\frac{\partial \phi(z)}{\partial z}$. Electric field form is shown in Fig. 1 where we can see that it is linear in both regions and $E(-d_p) = E(d_n) = 0$.
Now we can integrate the Gauss' law over the depletion region when assuming the approximation for the charge density. We can divide the integration into two parts so that

$$\begin{aligned}
\int_0^{d_n} \frac{\partial E(z)}{\partial z} \mathrm{d}z &= \int_0^{d_n} \frac{\rho(z)}{\epsilon_r \epsilon_0} \mathrm{d}z \\
E(d_n) - E(0) &= \frac{1}{\epsilon_r \epsilon_0} \int_0^{d_n} e N_d \mathrm{d}z \\
E(0) &= -\frac{e N_d d_n}{\epsilon_r \epsilon_0}
\end{aligned}$$

similarly

$$\begin{aligned}
\int_{-d_p}^{0} \frac{\partial E(z)}{\partial z} \mathrm{d}z &= \int_{-d_p}^{0} \frac{\rho(z)}{\epsilon_r \epsilon_0} \mathrm{d}z \\
E(0) - E(-d_p) &= \frac{1}{\epsilon_r \epsilon_0} \int_{-d_p}^{0} -e N_a \mathrm{d}z \\
E(0) &= \frac{e N_a d_p}{\epsilon_r \epsilon_0}
\end{aligned}$$

when knowing that the form is linear in those regions we can formulate the electric field so that

$$E(z) = \begin{cases} -\frac{e N_a}{\epsilon_r \epsilon_0}(z + d_p) & -d_p < z < 0 \\ \frac{e N_d}{\epsilon_r \epsilon_0}(z - d_n) & 0 < z < d_n \end{cases}$$

Now when we know the relation between the potential and electric field we can integrate again in the two regions to obtain.

$$\begin{aligned}
\phi_n(z) &= \int E(z)\mathrm{d}z = \int \frac{e N_d}{\epsilon_r \epsilon_0}(z - d_n)\mathrm{d}z = \frac{e N_d}{2\epsilon_r \epsilon_0}(z - d_n)^2 \\
\phi_p(z) &= \int E(z)\mathrm{d}z = \int -\frac{e N_a}{\epsilon_r \epsilon_0}(z + d_p)\mathrm{d}z = -\frac{e N_a}{2\epsilon_r \epsilon_0}(z + d_p)^2
\end{aligned}$$

When looking at the form given in Fig. 1 we can obtain actual definition of the potential in both sides of the junction

$$\phi(z) = \begin{cases} \phi_n(\infty) - \phi_n(z) = \phi_n(\infty) - \frac{e N_d}{2\epsilon_r \epsilon_0}(z - d_n)^2 & 0 < z < d_n \\ \phi_p(-\infty) - \phi_p(z) = \phi_p(-\infty) + \frac{e N_a}{2\epsilon_r \epsilon_0}(z + d_p)^2 & -d_p < z < 0 \end{cases}$$

When taking into account the charge neutrality of the homojunction we can write $N_a d_p = N_d d_n$ and solving the derived potential at $z = 0$ we have

$$\phi(0) = \phi_p(-\infty) + \frac{e N_a}{2\epsilon_r \epsilon_0} d_p^2 = \phi_n(\infty) - \frac{e N_d}{2\epsilon_r \epsilon_0} d_n^2$$

Contact potential is therefore

$$\phi_c = \phi_n(\infty) - \phi_p(-\infty) = \frac{e}{2\epsilon_r \epsilon_0}(N_a d_p^2 + N_d d_n^2) \tag{5}$$

(c)

Using the charge neutrality $N_d d_n = N_a d_p$ and previous equation we can derive

$$\begin{aligned}
N_a d_p^2 + N_d d_n^2 &= \frac{2\phi_c \epsilon_r \epsilon_0}{e} \\
N_a d_p^2 + N_d \left(\frac{N_a}{N_d}\right)^2 d_p^2 &= \frac{2\phi_c \epsilon_r \epsilon_0}{e} \\
d_p^2 \frac{N_a N_d + N_a^2}{N_d} &= \frac{2\phi_c \epsilon_r \epsilon_0}{e} \\
d_p^2 &= \frac{2\phi_c \epsilon_r \epsilon_0 N_d}{e N_a (N_d + N_a)} \\
d_p &= \left[\frac{2\phi_c \epsilon_r \epsilon_0 N_d}{e N_a (N_d + N_a)}\right]^{1/2}
\end{aligned}$$

same for d_n can be obtained by just changing indices so that

$$d_n = \left[\frac{2\phi_c \epsilon_r \epsilon_0 N_a}{e N_d (N_d + N_a)}\right]^{1/2},$$

which form together Eg. (8.41) in Elliot's book.

2. p-n-junction

We know values

$$\begin{aligned}
n_i &\approx 1.5 \times 10^{10} \text{cm}^{-3} \\
\epsilon_r &= 11.7 \\
\epsilon_0 &= 8.854 \times 10^{-12} \text{F/m} \\
A &= 0.508 \text{mm}^2 \\
N_a &= 4 \times 10^{18} \text{cm}^{-3} \\
N_d &= 10^{16} \text{cm}^{-3} \\
T &= 300K \\
k_B &= 8.617 \times 10^{-5} \text{eV/K} \\
e &= 1.602 \times 10^{-19} \text{C}
\end{aligned}$$

Equation for potential difference over the junction was derived in exercise 1. so that

$$\phi_c = \frac{k_B T}{e} \ln \frac{N_d N_a}{n_i^2} = \frac{8.617 \times 10^{-5} \text{eV/K} \ \times 300K}{e} \ln \left(\frac{4 \times 10^{18} \text{mm}^{-3} \times 10^{16} \text{mm}^{-3}}{(1.5 \times 10^{10} \text{mm}^{-3})^2}\right) = 0.848 \text{V}.$$

Depletion area widths were also derived and we obtain

$$d_n = \left[\frac{2\phi_c \epsilon_r \epsilon_0 N_a}{e N_d (N_d + N_a)}\right]^{1/2} = \left[\frac{2 \times 0.848 \text{V} \times 11.7 \times 8.854 \times 10^{-12} \text{F/m} \times 4 \times 10^{24} \text{m}^{-3}}{1.602 \times 10^{-19} \text{C} \times 10^{22} \text{m}^{-3} (10^{22} \text{m}^{-3} + 4 \times 10^{24} \text{m}^{-3})}\right]^{1/2} = 3.3 \times 10^{-7} \text{m}$$

$$d_p = \left[\frac{2\phi_c \epsilon_r \epsilon_0 N_d}{e N_a (N_d + N_a)}\right]^{1/2} = \left[\frac{2 \times 0.848 \text{V} \times 11.7 \times 8.854 \times 10^{-12} \text{F/m} \times 10^{22} \text{m}^{-3}}{1.602 \times 10^{-19} \text{C} \times 4 \times 10^{24} \text{m}^{-3} (10^{22} \text{m}^{-3} + 4 \times 10^{24} \text{m}^{-3})}\right]^{1/2} = 8.3 \times 10^{-10} \text{m}$$

Also the electric field was derived in ex 1. to be

$$E(z=0) = -\frac{e N_a}{\epsilon_r \epsilon_0} d_p = -\frac{1.602 \times 10^{-19} \text{C} \times 4 \times 10^{24} \text{m}^{-3}}{11.7 \times 8.854 \times 10^{-12} \text{F/m}} \times 8.3 \times 10^{-10} \text{m} = -5.13 \times 10^6 \ \text{V/m}$$

Capacitance can be shown to be

$$C = \left|\frac{\mathrm{d}Q}{\mathrm{d}V}\right| = \left|\frac{eN_d A \ \mathrm{d}d_n}{\mathrm{d}V}\right|.$$

I found from Ref. [1] how potential V affects depletion width

$$\frac{\mathrm{d}d_n}{\mathrm{d}V} = \frac{\mathrm{d}}{\mathrm{d}V}\left[\frac{2\epsilon_r\epsilon_0 N_a(\phi_c - V)}{eN_d(N_d + N_a)}\right]^{1/2} = -\frac{1}{2}\left[\frac{2\epsilon_r\epsilon_0 N_a}{eN_d(N_d + N_a)}\right]^{1/2}(\phi_c - V)^{-1/2}.$$

since we know that

$$(\phi_c - V)^{1/2} = \left[\frac{2\epsilon_r\epsilon_0 N_a}{eN_d(N_d + N_a)}\right]^{-1/2} \times d_n,$$

we can plug this back to previous equation to obtain

$$\frac{\mathrm{d}d_n}{\mathrm{d}V} = -\frac{1}{2d_n}\left[\frac{2\epsilon_r\epsilon_0 N_a}{eN_d(N_d + N_a)}\right],$$

which can be plugged to the equation of conductivity to obtain

$$\begin{aligned} C &= \frac{A\epsilon_r\epsilon_0 N_a}{d_n(N_a + N_d)} \\ &= \frac{0.508 \times 10^{-6}\mathrm{m}^2 \times 11.7 \times 8.854 \times 10^{-12}\mathrm{F/m} \times 4 \times 10^{24}\mathrm{m}^{-3}}{3.3 \times 10^{-7}\mathrm{m}(4 \times 10^{24}\mathrm{m}^{-3} + 10^{22}\mathrm{m}^{-3})} \\ &= 1.59 \times 10^{-10}\mathrm{F} \end{aligned}$$

Since $C \propto (\phi_c - V)^{-1/2}$ we obtain a curve which looks something like in Fig. 2. I set $\phi = 1$ which is noticed in the plot as a great increase in capacitance as $V \to 1$.

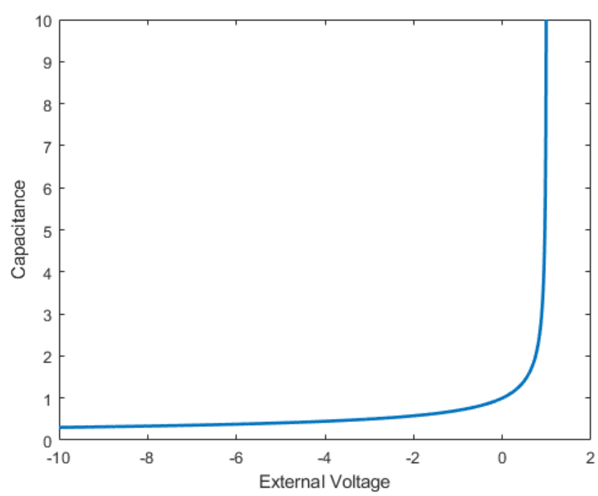

Figure 2: Capacitance dependency on external voltage.

3. I-V characteristic

We assume that a silicon solar cell has the I-V characteristics (Eq. (8.89) in Elliott) as

$$I = I_0(\exp[eV/k_BT] - 1) - I_S, \tag{6}$$

where $I_0 = 10^{-12}$A and under illumination $I_S = 10$mA. The open circuit voltage is determined from Eq. (6) by setting $I = 0$, so that

$$V_{oc} = \frac{k_BT}{e} \ln\left(\frac{I_s}{I_0} + 1\right) \approx \frac{k_BT}{e} \ln\left(\frac{I_s}{I_0}\right). \tag{7}$$

The short circuit current is now obtained by setting $V = 0$ so that $I_{sc} = I_S$. Theoretical maximum power is $P^{th}_{max} = V_{oc}I_{sc}$, which won't be obtained due to the I-V characteristic. Realistic maximum power is the area of the largest rectangle presented in Elliott's book Fig. 8.82 shown below.

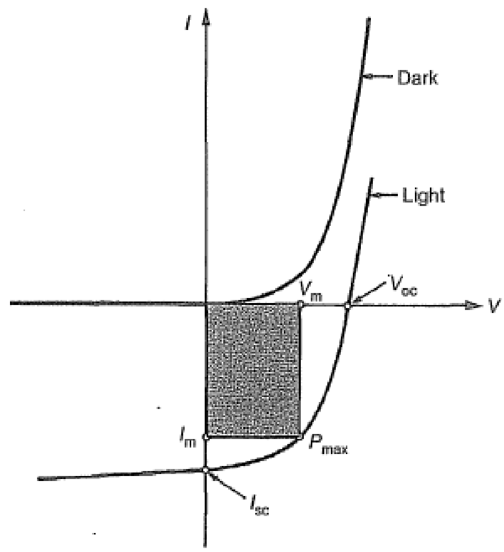

Figure 3: C-V characteristics under illumination I_S. Maximum power corresponding to the dark square.

Power is obtained by

$$P = IV = (I_0(\exp[eV/k_BT] - 1) - I_S)\, V.$$

To maximise this we solve when the derivative in respect to V is zero.

$$\begin{aligned}\frac{\partial P}{\partial V} &= \frac{\partial}{\partial V}\left(I_0(\exp[eV/k_BT] - 1) - I_S\right) V \\ &= I_0(\exp[eV/k_BT] - 1) - I_s + I_0\frac{eV}{k_BT}\exp[eV/k_BT] = 0.\end{aligned}$$

Since $I_0 \ll I_s$, we can estimate

$$I_s \approx I_0 \exp[eV_{max}/k_BT]\left(1 + \frac{eV_{max}}{k_BT}\right).$$

For open circuit voltage we found that $I_s = I_0 \exp[eV_{oc}/k_BT]$ which we can substitute here so that

$$I_0 \exp[eV_{oc}/k_BT] = I_0 \exp[eV_{max}/k_BT]\left(1 + \frac{eV_{max}}{k_BT}\right)$$
$$\Leftrightarrow$$
$$V_{oc} = V_{max} + \frac{k_BT}{e}\ln\left(1 + \frac{eV_{max}}{k_BT}\right)$$
$$\Leftrightarrow$$
$$V_{max} = V_{oc} - \frac{k_BT}{e}\ln\left(1 + \frac{eV_{max}}{k_BT}\right)$$

Since logarithm is not that strict to the changes of argument we can do last approximation that

$$V_{max} \approx V_{oc} - \frac{k_BT}{e}\ln\left(1 + \frac{eV_{oc}}{k_BT}\right).$$

With this maximum voltage we can obtain maximum current by plugging this to the IV-relation

$$I_{max} = I_0(\exp[eV_{max}/k_BT] - 1) - I_s$$
$$I_{max} \approx -I_s$$

by assuming that $k_BT/eV_{max} \ll 1$. Now we can write maximum power by multiplying obtained voltage and current

$$P_{max} = V_{max}I_{max} = -I_s\left[V_{oc} - \frac{k_BT}{e}\ln\left(1 + \frac{eV_{oc}}{k_BT}\right)\right] \quad (8)$$

Total power is given by

$$P_T = I_{sc}V_{oc} = I_s\frac{k_BT}{e}\ln\left(\frac{I_s}{I_0}\right)$$

Fill factor is given by

$$FF = \frac{P_{max}}{P_T} = \frac{-V_{oc} + \frac{k_BT}{e}\ln\left(1 + \frac{eV_{oc}}{k_BT}\right)}{\frac{k_BT}{e}\ln\left(\frac{I_s}{I_0}\right)}$$

Lastly the load resistance is defined as

$$R_{load} = \frac{V_{max}}{I_{max}} = \frac{\left[V_{oc} - \frac{k_BT}{e}\ln\left(1 + \frac{eV_{oc}}{k_BT}\right)\right]}{-I_s}$$

Negative sign in these equations depends on how charge is defined as can be seen from Fig. 3.

References

[1] https://ecee.colorado.edu/ bart/book/book/chapter4/ch4_3.htm