ECE613 / CHE613: Electronic Materials Characterization  
Spring 2020  
Homework 2 - Solutions  
Due at the beginning of class Friday April 24th

Question 1 [9 marks]:

a) The occupancy of deep traps \(f_T\) at temperature \(T\), is described by the Fermi-Dirac distribution:

\[
f_T = \frac{1}{1 + \exp \left( \frac{E_T - E_F}{k_B T} \right)}
\]  
(1)

Where \(E_T\) and \(E_F\) are the energies of the trap level and the Fermi level respectively. \(k_B\) is the Boltzmann Constant.

The capture rate of holes is labeled \(r_c\) and expressed in Equation 2:

\[
r_c = \sigma_p v_{th} p N_T f_T
\]  
(2)

Where \(\sigma_p\) is the hole capture cross-section, \(v_{th}\) is the thermal velocity of holes, \(p\) is the delocalized hole density in the valence band, and \(N_T\) is the number density of trap states.

The rate of hole emission is labeled \(r_d\) and expressed in Equation 3:

\[
r_d = e_p N_T (1 - f_T)
\]  
(3)

Where \(e_p\) is the hole emission coefficient for holes.

The density of delocalized holes in the valence band can be expressed as:

\[
p = N_V \exp \left( - \frac{E_F - E_V}{k_B T} \right)
\]  
(4)

Where \(E_V\) is the energy of the conduction band, and \(N_V\) is the number density of valence band states.

Using equations (1), (2), (3) and (4) above, and by considering conditions under which the trap occupancy is constant, show that emission coefficient for holes \((e_p)\) can be expressed via the following equation:[3 marks]

\[
e_p = \sigma_p v_{th} N_V \exp \left( - \frac{E_T - E_V}{k_B T} \right)
\]  

This just involves some basic re-arranging of equations. As we are told the trap occupancy is constant, the first thing we need to do is equate the rates for hole emission and capture:

\[
r_c = r_d
\]

From Equations (2) and (3) above, this gives us:

\[
\sigma_p v_{th} p N_T f_T = e_p N_T (1 - f_T)
\]

\[
\sigma_p v_{th} f_T = e_p (1 - f_T)
\]
Re-arrange in terms of $e_p$:

$$e_p = \sigma_p v_{th} p \frac{f_T}{(1 - f_T)}$$

Use the Fermi-Dirac distribution:

$$f_T = \frac{1}{1 + \exp \left( \frac{E_T - E_F}{k_B T} \right)}$$

Re-arrange:

$$1 + \exp \left( \frac{E_T - E_F}{k_B T} \right) = \frac{1}{f_T}$$

$$\exp \left( \frac{E_T - E_F}{k_B T} \right) = \frac{1}{f_T} - 1$$

$$\exp \left( \frac{E_T - E_F}{k_B T} \right) = \frac{1 - f_T}{f_T}$$

Flip:

$$\frac{f_T}{(1 - f_T)} = \exp \left( \frac{E_F - E_T}{k_B T} \right)$$

Substitute back into $e_p$:

$$e_p = \sigma_p v_{th} p \exp \left( \frac{E_F - E_T}{k_B T} \right)$$

Now substitute in Equation (4):

$$e_p = \sigma_p v_{th} N_V \exp \left( - \frac{E_F - E_V}{k_B T} \right) \exp \left( \frac{E_F - E_T}{k_B T} \right)$$

Now just split all the exponentials:

$$e_p = \sigma_p v_{th} N_V \exp \left( - \frac{E_F}{k_B T} \right) \exp \left( \frac{E_V}{k_B T} \right) \exp \left( + \frac{E_F}{k_B T} \right) \exp \left( - \frac{E_T}{k_B T} \right)$$

We can cancel the Fermi-level term, giving the final result:

$$e_p = \sigma_p v_{th} N_V \exp \left( - \frac{E_F - E_V}{k_B T} \right)$$

b) We carry out a room temperature ($T = 300$ K) experiment on germanium, allowing us to measure the electron and hole emission times. With this information and the other parameters provided in the table below, determine the band gap of this semiconductor. Give your answer in eV.[6 marks]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value (holes)</th>
<th>Value (electrons)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emission Time</td>
<td>$\tau_{p,em} = 183$ ns</td>
<td>$\tau_{n,em} = 2$ ns</td>
</tr>
<tr>
<td>Thermal Velocity</td>
<td>$v_{th}^p = 1.9 \times 10^7$ cm/s</td>
<td>$v_{th}^n = 3.1 \times 10^7$ cm/s</td>
</tr>
<tr>
<td>Band State Density</td>
<td>$N_V = 5.64 \times 10^{18}$ cm$^{-3}$</td>
<td>$N_n = 1.02 \times 10^{19}$ cm$^{-3}$</td>
</tr>
<tr>
<td>Capture Cross-Section</td>
<td>$\sigma_p = 5 \times 10^{-12}$ cm$^2$</td>
<td>$\sigma_n = 2 \times 10^{-15}$ cm$^2$</td>
</tr>
</tbody>
</table>
First, we identify the band gap \((E_G)\) as the difference in energy between the conduction band and valence band:

\[
E_G = E_C - E_V
\]

Next look at our two equations for emission coefficient:

\[
e_n = \sigma_n v_{th}^n N_C \exp \left( - \frac{E_C - E_T}{k_B T} \right)
\]

\[
e_p = \sigma_p v_{th}^p N_V \exp \left( - \frac{E_T - E_V}{k_B T} \right)
\]

Note thermal velocity now has a superscript to identify carrier type. It is clear we need to rearrange these equations to determine the difference \(E_C - E_V\). We can also identify that we have not been told the trap energy \(E_T\), so we can start by attempting to eliminate this variable.

Start with the equation for electrons:

\[
e_n = \sigma_n v_{th}^n N_C \exp \left( - \frac{E_C - E_T}{k_B T} \right)
\]

\[
\frac{e_n}{\sigma_n v_{th}^n N_C} = \exp \left( - \frac{E_C - E_T}{k_B T} \right)
\]

Take (natural) logs:

\[
\ln \left( \frac{e_n}{\sigma_n v_{th}^n N_C} \right) k_B T = E_T - E_C
\]

Express as a function of the trap energy:

\[
E_T = \ln \left( \frac{e_n}{\sigma_n v_{th}^n N_C} \right) k_B T + E_C
\]

Repeat this process for holes:

\[
e_p = \sigma_p v_{th}^p N_V \exp \left( - \frac{E_T - E_V}{k_B T} \right)
\]

\[
\frac{e_p}{\sigma_p v_{th}^p N_V} = \exp \left( - \frac{E_T - E_V}{k_B T} \right)
\]

\[
\ln \left( \frac{e_p}{\sigma_p v_{th}^p N_V} \right) k_B T = E_V - E_T
\]

\[
\ln \left( \frac{e_p}{\sigma_p v_{th}^p N_V} \right) k_B T = E_V - E_T
\]

\[
E_T = E_V - \ln \left( \frac{e_p}{\sigma_p v_{th}^p N_V} \right) k_B T
\]

Equate the trap energies:
\[ \ln \left( \frac{e_n}{\sigma_n v_{th}^n N_C} \right) k_B T + E_C = E_V - \ln \left( \frac{e_p}{\sigma_p v_{th}^p N_V} \right) k_B T \]

Now re-arrange to get the band gap:

\[ E_G = E_C - E_V = -\ln \left( \frac{e_p}{\sigma_p v_{th}^p N_V} \right) k_B T - \ln \left( \frac{e_n}{\sigma_n v_{th}^n N_C} \right) k_B T \]

\[ E_G = -k_B T \left[ \ln \left( \frac{1}{\sigma_p v_{th}^p N_V \tau_{p,em}} \right) + \ln \left( \frac{1}{\sigma_n v_{th}^n N_C \tau_{n,em}} \right) \right] \]

Recall we are told the emission times \((\tau_{i,em})\) rather than emission coefficients. The two are the inverse of each other:

\[ \tau_{i,em} = \frac{1}{\alpha_i} \]

Re-writing our expression for the band-gap in terms of emission times:

\[ E_G = -k_B T \left[ \ln \left( \frac{1}{\sigma_p v_{th}^p N_V \tau_{p,em}} \right) + \ln \left( \frac{1}{\sigma_n v_{th}^n N_C \tau_{n,em}} \right) \right] \]

We can use some laws of logarithms to tidy this up a little

\[ \ln A^n = n \ln A \]

I.e.:

\[ \ln \left( \frac{1}{A} \right) = \ln A^{-1} = -\ln A \]

So for our equation:

\[ E_G = k_B T \ln \left( \sigma_p v_{th}^p N_V \tau_{p,em} \right) + \ln \left( \sigma_n v_{th}^n N_C \tau_{n,em} \right) \]

We can also use \(\ln A + \ln B = \ln AB\):

\[ E_G = k_B T \ln \left( \sigma_p \sigma_n v_{th}^p v_{th}^n N_V N_C \tau_{p,em} \tau_{n,em} \right) \]

So now it is simply an exercise in entering all the numbers. There are no fundamental constants inside the logarithm, so we can stick with cm and s if we want:

\[ E_G = k_B T \ln \left( \sigma_p \sigma_n v_{th}^p v_{th}^n N_V N_C \tau_{p,em} \tau_{n,em} \right) \]

To help identify errors, the respective electron-hole parameter products are:

\[ \sigma_p \sigma_n = 5 \times 10^{-12} \times 2 \times 10^{-15} = 1 \times 10^{-26} \text{ cm}^4 \]

\[ v_{th}^p v_{th}^n = 1.9 \times 10^7 \times 3.1 \times 10^7 = 5.89 \times 10^{14} \text{ cm}^2 \text{s}^{-2} \]

\[ N_V N_C = 5.64 \times 10^{18} \times 1.02 \times 10^{19} = 5.75 \times 10^{-26} \text{ cm}^{-6} \]

\[ \tau_{p,em} \tau_{n,em} = 183 \times 10^{-9} \times 2 \times 10^{-9} = 3.66 \times 10^{-16} \text{ s}^2 \]

Putting the numbers in:

\[ E_G = 1.38 \times 10^{-23} \times 300 \times \ln \left( 1 \times 10^{-26} \times 5.89 \times 10^{14} \times 5.75 \times 10^{-26} \times 3.66 \times 10^{-16} \right) \]
\[ E_G = 4.14 \times 10^{-21} \times \ln(1.24 \times 10^{11}) \]
\[ E_G = 4.14 \times 10^{-21} \times 25.5 \]
\[ E_G = 41.06 \times 10^{-19} \text{ J} \]

Finally, convert to electron volts:
\[ E_G = 0.66 \text{ eV} \]

**Question 2 [4 marks]:**

a) The figure below shows the results from a deep level transient spectroscopy (DLTS) experiment. This data is available to download [here](#). It was carried out on a sample with a donor doping density of \( N_D = 10^{15} \text{ cm}^{-3} \). If the steady-state capacitance is \( C_0 = 1.60 \text{ nF} \), and the sample times were \( t_1 = 0.5 \text{ ms} \) and \( t_2 = 4 \text{ ms} \), determine the trap density in this material. [4 marks]

\[
N_T = - \frac{\delta C_{\text{max}}}{C_0} \frac{2N_DR^{r-r_1}}{1 - r}
\]

Where \( r = t_2/t_1 \).

The only thing we need to do is identify \( \delta C_{\text{max}} \) from the graph. As the variable suggests, we just take the maximum value. Hence \( \delta C_{\text{max}} = 8 \times 10^{-15} \text{ F} \). Equivalently we could use the formula \( =\text{MAX}(B2:B362) \) in Excel.

Now we can just enter values. Start with \( r \):
\[
r = \frac{4}{0.5} = 8
\]
\[
N_T = - \frac{8 \times 10^{-15} \times 2 \times 10^{15} \times 8^{B^{r-T}}}{1.6 \times 10^{-9} \times 1 - 8}
\]
\[ N_T = -5 \times 10^{-6} \frac{2 \times 10^{15} \times 8^{1.14}}{-7} \]

\[ N_T = 1.54 \times 10^{10} \text{ cm}^{-3} \]

**Question 3 [6 marks]:**

a) How many charge carriers (electrons or holes) are associated with Shockley-Read-Hall recombination?[1 mark]

Shockley-Read-Hall recombination involves **one charge carrier** and a trap.

b) How many charge carriers (electrons or holes) are associated with radiative recombination?[1 mark]

Radiative recombination involves the recombination of **two charge carriers** an electron and a hole.

c) How many charge carriers (electrons or holes) are associated with Auger recombination?[1 mark]

Auger recombination involves **three charge carriers**: either an electron and two holes, or a hole and two electrons. An electron-hole pair recombine, and the third carrier is involved in a transfer of momentum.

d) Various notations are used for recombination coefficients. Equation (1) is a simplified differential equation use to describe the rate of change of total carrier concentration in a solar cell. In this context, we conventionally use cm as the length dimension (for example carrier concentration, \( n \), is expressed in cm\(^3\)) and seconds as the time dimension. Using Equation (1), determine the standard units for the Auger recombination rate (\( k_3 \)).[3 marks]

\[
\frac{dn}{dt} = k_1 n + k_2 n^2 + k_3 n^3
\]  

(1)

In this context:

- \( n \) is total carrier concentration (holes and electrons).
- \( t \) is time.
- \( k_1 \) is the Shockley-Read-Hall (mono-molecular) recombination rate.
- \( k_2 \) is the radiative (bi-molecular) recombination rate.
- \( k_3 \) is the Auger (tri-molecular) recombination rate.

This question is asked because it the answer may be a little unintuitive. It can be solved via dimensional analysis. The easiest way to do it is just to look at the units on the left hand side first. \( n \) is a concentration and has units of cm\(^3\), and time has units s. Hence the derivative on the left hand side has units cm\(^{-3}\)s\(^{-1}\). Therefore every term on the right hand side must also have units of cm\(^{-3}\)s\(^{-1}\).

The first term relates to Shockley-Read-Hall (mono-molecular) recombination. \( k_1 n \) must have units of cm\(^{-3}\)s\(^{-1}\). Since carrier concentration, \( n \), has units of cm\(^3\), we can therefore deduce that \( k_1 \) must have units of s\(^{-1}\).
The second term relates to radiative (bi-molecular) recombination. \( k_2 n^2 \) also has units of \( \text{cm}^{-3} \text{s}^{-1} \). Carrier concentration squared \( (n^2) \) has units of \( \text{cm}^{-6} \). Therefore \( k_2 \) must have units of \( \text{cm}^3 \text{s}^{-1} \).

The final term relates to Auger (tri-molecular) recombination. \( k_3 n^3 \) also has units of \( \text{cm}^{-3} \text{s}^{-1} \). Carrier concentration squared \( (n^3) \) has units of \( \text{cm}^{-9} \). Therefore \( k_3 \) must have units of \( \text{cm}^6 \text{s}^{-1} \).

Question 4 [6 marks]:

The net capture rate for electrons \( (U_n) \) and holes \( (U_p) \) are given by the equations (2) and (3) below:

\[
U_n = \sigma_n v_{th} N_T [n(1 - f_T) - n_1 f_T] \tag{2}
\]

\[
U_p = \sigma_p v_{th} N_T [p f_T - p_1 (1 - f_T)] \tag{3}
\]

Where:
- \( \sigma_n, \sigma_p \) are the capture cross-sections of the trap for electrons and holes, respectively.
- \( v_{th} \) is the thermal velocity of electrons and holes (assumed to be equal).
- \( n, p \) are the delocalized electron and hole densities, respectively.
- \( N_T \) is the density of trap states.
- \( n_1, p_1 \) are the concentration of electrons in the conduction band or holes in the valence band, respectively, when the Fermi level is located at the trap energy level.

a) By considering the steady state situation where the net rate of electron and hole capture are identical, derive the steady-state trap occupancy factor \( (f_T) \) given by equation (4).[3 marks]

\[
f_T = \frac{\sigma_n n + \sigma_p p_1}{\sigma_n (n + n_1) + \sigma_p (p + p_1)} \tag{4}
\]

This is a reasonably straightforward derivation. All we have to do is equate the net capture rate for electrons and holes:

\[ U_n = U_p \]

Substitute from Equations (2) and (3):

\[
\sigma_n v_{th} N_T [n(1 - f_T) - n_1 f_T] = \sigma_p v_{th} N_T [p f_T - p_1 (1 - f_T)]
\]

Cancel the \( v_{th} N_T \) terms:

\[
\sigma_n [n(1 - f_T) - n_1 f_T] = \sigma_p [p f_T - p_1 (1 - f_T)]
\]

Multiply out:

\[
\sigma_n n - \sigma_n n f_T - \sigma_n n_1 f_T = \sigma_p p f_T - \sigma_p p_1 + \sigma_p p_1 f_T
\]

Gather \( f_T \) terms:
\[
\sigma_n n - f_T (\sigma_n n + \sigma_p n_1) = f_T (\sigma_p p + \sigma_p p_1) - \sigma_p p_1 \\
\sigma_n n + \sigma_p p_1 = f_T (\sigma_p p + \sigma_p p_1) + f_T (\sigma_n n + \sigma_n n_1) \\
f_T (\sigma_p p + \sigma_p p_1 + \sigma_n n + \sigma_n n_1) = \sigma_n n + \sigma_p p_1 \\
f_T = \frac{\sigma_n n + \sigma_p p_1}{\sigma_p p + \sigma_p p_1 + \sigma_n n + \sigma_n n_1} \\
f_T = \frac{\sigma_n n + \sigma_p p_1}{\sigma_n (n + n_1) + \sigma_p (p + p_1)}
\]

b) Using the equation for \( f_T \) given in Equation (4) above, show that the Shockley-Read-Hall capture rate \( (U_{SRH}) \) can be given by the following expression.[3 marks]

\[
U_{SRH} = \frac{\sigma_n \sigma_p v_{th} N_T (pn - n_i^2)}{\sigma_n (n + n_1) + \sigma_p (p + p_1)} \\
(5)
\]

You will need to use the relationship: \( n_i p_1 = n_i^2 \), and the definition of the Shockley-Read-Hall capture rate \( (U_{SRH}) \) as the steady-state situation in which the net rates of electron and hole capture are equal:

\[
U_n = U_p = U_{SRH} \\
(6)
\]

To start, we will use Equation (2):

\[
U_{SRH} = U_n = \sigma_n v_{th} N_T [n(1 - f_T) - n_i f_T] \\
\]

It is easier to re-arrange this slightly before we substitute in \( f_T \):

\[
U_{SRH} = \sigma_n v_{th} N_T [n - n f_T - n_i f_T] \\
U_{SRH} = \sigma_n v_{th} N_T [n - f_T (n + n_i)]
\]

Now substitute in \( f_T \):

\[
U_{SRH} = \sigma_n v_{th} N_T \left[ n - \frac{\sigma_n n + \sigma_p p_1}{\sigma_n (n + n_1) + \sigma_p (p + p_1)} (n + n_i) \right]
\]

Re-write \( n \) as:

\[
n = \frac{n\sigma_n (n + n_1) + n\sigma_p (p + p_1)}{\sigma_n (n + n_1) + \sigma_p (p + p_1)}
\]

Then substitute into \( U_{SRH} \):

\[
U_{SRH} = \sigma_n v_{th} N_T \left[ \frac{n\sigma_n (n + n_1) + n\sigma_p (p + p_1)}{\sigma_n (n + n_1) + \sigma_p (p + p_1)} - \frac{\sigma_n n + \sigma_p p_1}{\sigma_n (n + n_1) + \sigma_p (p + p_1)} (n + n_i) \right]
\]
\[ U_{SRH} = \sigma_n v_{th} N_T \left[ \frac{n\sigma_n(n + n_1) + n\sigma_p(p + p_1) - (\sigma_n n + \sigma_p p_1)(n + n_1)}{\sigma_n(n + n_1) + \sigma_p(p + p_1)} \right] \]

Multiply out the top of the fraction:
\[
= n\sigma_n(n + n_1) + n\sigma_p(p + p_1) - (\sigma_n n + \sigma_p p_1)(n + n_1)
\]
\[
\text{top} = n^2\sigma_n + nn_1\sigma_n + np\sigma_p + np_1\sigma_p - \sigma_n n^2 - nn_1\sigma_n - \sigma_p p_1 n - \sigma_p p_1 n_1
\]
We can cancel the \(n^2\sigma_n\) terms:
\[
\text{top} = nn_1\sigma_n + np\sigma_p + np_1\sigma_p - \sigma_p p_1 n - \sigma_p p_1 n_1
\]
Also cancel \(nn_1\sigma_n\) terms:
\[
\text{top} = np\sigma_p + np_1\sigma_p - \sigma_p p_1 n - \sigma_p p_1 n_1
\]
And finally we can also cancel \(np_1\sigma_p\) terms:
\[
\text{top} = np\sigma_p - \sigma_p p_1 n_1
\]
Putting back into \(U_{SRH}\):
\[ U_{SRH} = \sigma_n v_{th} N_T \left[ \frac{np\sigma_p - \sigma_p p_1 n_1}{\sigma_n(n + n_1) + \sigma_p(p + p_1)} \right] \]
Finally, we use the relationship \(n_1 p_1 = n_1^2\) to put the equation into its final form:
\[ U_{SRH} = \sigma_n v_{th} N_T \left[ \frac{np\sigma_p - \sigma_p n_1^2}{\sigma_n(n + n_1) + \sigma_p(p + p_1)} \right] \]
\[ U_{SRH} = \frac{\sigma_n \sigma_p v_{th} N_T (pn - n_1^2)}{\sigma_n(n + n_1) + \sigma_p(p + p_1)} \]