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3.23 Electrical, Optical, and Magnetic Properties of Materials

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Homework # 7

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Homework is due on Thursday November 8st, 5pm

1 Intrinsic semiconductor

Let us consider a 2 band intrinsic semiconductor. From the microscopic point of view this semiconductor is characterized by a **valence density of states**, $D_v(E)$, a **conduction density of states**, $D_c(E)$, and a band gap $E_g = E_c - E_v$. Using those density of states and the Fermi factor $f(T, E) = \frac{1}{1+e^{(E-\mu)/k_B T}}$, we can easily express the volumic density of electrons in the conduction band, $n_c(T, \mu)$, and the volumic density of holes in the valence band, $p_v(T, \mu)$:

$$n_c(T, \mu) = \int_{E_c}^{+\infty} f(T, E) D_c(E) dE \text{ and } p_v(T, \mu) = \int_{-\infty}^{E_v} (1 - f(T, E)) D_v(E) dE$$

Those formulas are extremely general and always applicable in practice. Now we will use the hypothesis of **non-degeneracy**, meaning that the chemical potential is far away in terms of thermal energy from the top of the valence band **and** the bottom of the conduction band:

$$\mu - E_v \gg k_B T \text{ and } E_c - \mu \gg k_B T \text{ non-degeneracy conditions}$$

For **intrinsic** semiconductors like Silicon, Germanium and Galium Arsenide those conditions of non-degeneracy are very well satisfied. Using this hypothesis, we see that the Fermi factor can be simplified to a Maxwell-Boltzmann factor (here in the case where $E > \mu$):

$$f(T, E) = \frac{1}{1+e^{(E-\mu)/k_B T}} \text{ becomes } f(T, E) \approx e^{-(E-\mu)/k_B T}$$

1.1 Some general results for any $D_c(E)$ and $D_v(E)$ and both intrinsic and extrinsic semiconductors

1) Using the non-degeneracy conditions, express the densities of electrons and holes, $n_c(T, \mu)$ and $p_v(T, \mu)$, as follows:

- $n_c(T, \mu) = N_c(T) e^{-(E_c-\mu)/k_B T}$
- $p_v(T, \mu) = P_v(T) e^{-(\mu-E_v)/k_B T}$

Find an integral expression for both $N_c(T)$ and $P_v(T)$. What happens when one multiplies $n_c(T)$ by $p_v(T)$?

Important Remark: This relation is called the **law of mass action**. It is satisfied for both intrinsic and extrinsic semiconductors. All the doping does is to introduce some states inside the band gap, and shift the chemical potential, but this does not change the densities of states $D_v(E)$ and $D_c(E)$ so it does not change the law of mass action.

2) Now if we consider an **intrinsic semiconductor**, what is the relationship between $n_c(T, \mu)$ and $p_v(T, \mu)$? Use this relationship to express the chemical potential as a function of T only. What is the chemical potential at $0K$? What is the order of magnitude of the chemical potential shift at finite T from its value at $T = 0K$? In which direction does the chemical potential shift from its value at $T = 0K$ when one increases the temperature?

1.2 Introducing the parabolic approximation for the valence and conduction bands

3) By using the following results from the parabolic approximation of the valence and conduction bands:

$$D_c(E) = \frac{1}{2\pi^2} \left(\frac{2m_c^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_c} \text{ and } D_v(E) = \frac{1}{2\pi^2} \left(\frac{2m_v^*}{\hbar^2} \right)^{3/2} \sqrt{E_v - E}$$

calculate explicitly $N_c(T)$ and $N_v(T)$. Then use this to calculate the chemical potential μ as a function of T , m_c^* , m_v^* , E_v and E_c . By taking the origin of the energy axis in the middle of the band gap, calculate the chemical potential shift in eV at 300K for GaAs ($m_c^* = 0.063 m$ and $m_v^* = 0.505 m$, where m is the mass of a free electron).

2 p-doped semiconductors

We will now consider a semiconductor homogeneously doped with acceptors. Those acceptors are what we call "shallow impurities" in the sense that their presence inside the host semiconductor is responsible for the appearance of allowed energy states for holes right above the top of the valence band. The concentration of acceptors is N_a and the binding energy of the holes is $\epsilon_a = E_a - E_v$.

2.1 qualitative description of the physics with increasing temperature

4) Describe qualitatively what happens to the majority carriers (in this p-doped semiconductor the majority carriers are the holes) as one increases slowly the temperature T from $0K$ to high temperature. Use the terms : freezing-out regime, saturation regime and intrinsic regime to specify the different behavior regimes of the doped semiconductor with temperature.

2.2 quantitative calculation of the majority carrier density with temperature

5) Let us now construct the curve $\ln(p_v(T))$ as a function of $1/k_B T$. We will study the different regimes that you outlined above and find the expression for the chemical potential and the volumic density of holes in the valence band at different temperatures. To do this we will establish a **general balance equation** for the charges in the system. We denote by $P(E_a, T)$ the probability for a hole to occupy an acceptor level at temperature T. Show that we have the following equation between the total density of electrons in the conduction band $n_c(T, \mu)$, the total density of holes in the valence band $p_v(T, \mu)$ and the concentration of acceptor impurities N_a :

$$n_c(T, \mu) + N_a(1 - P(E_a, T)) = p_v(T, \mu) \quad \text{balance equation}$$

6) **At very low temperature**, which term in the balance equation can we safely neglect and why? The probability $P(E_a, T)$ is given by $P(E_a, T) = \frac{1}{\frac{1}{2}e^{\frac{\mu - E_a}{k_B T}} + 1}$. In the low temperature limit the chemical potential sits between the top of the valence band E_v and the acceptor level E_a . Simplify the term $1 - P(E_a, T)$ to a single exponential term up to a constant in front, and then use this simplified expression to show that the chemical potential can be written as follows (to obtain this expression you need to use the general expression for $p_v(T, \mu)$ found in the first part of the problem set):

$$\mu(T) = \frac{E_a + E_v}{2} - \frac{1}{2}k_B T \ln\left(\frac{N_a}{2P_v(T)}\right)$$

7) Using the expression for the chemical potential in 6), express $\ln(p_v(T, \mu))$ as a function of T only. What is the coefficient of the linear dependance of $\ln(p_v(T, \mu))$ with $1/k_B T$? This regime is called the **freezing-out regime**.

8) **At intermediate temperatures**, where all the impurities have been ionized but no electrons have been promoted from the valence to the conduction band, simplify the balance equation and find an expression for the chemical potential. Show that in this regime called the **saturation regime**, $\ln(p_v(T, \mu))$ is independant of the temperature. Define a temperature that will characterize this intermediate regime.

9) **At very high temperature**, electrons get promoted from the valence band to the conduction band. The density of impurities is then negligible. Use the balance equation to calculate the chemical potential. Using this expression, calculate $\ln(p_v(T, \mu))$ as a function of T only. This regime is called the **intrinsic regime**. What is the obvious reason for this? What is the coefficient of the linear dependance of $\ln(p_v(T, \mu))$ with $1/k_B T$?

10) Draw a schematic diagram of $\ln(p_v(T, \mu))$ as a function of $1/k_B T$.

3 The p-n junction

We discussed the physics of what's happening when one joins a p-type semiconductor and an n-type semiconductor together. After a very small amount

of time, a built-in potential is created and a space charge region at the metallurgical junction appears. We consider both doped semiconductor to be homogeneously doped with impurity concentrations N_a and N_d . We choose an x axis perpendicular to the pn junction and going from the p-side to the n-side. At equilibrium, the drift currents and the diffusion currents balance each other. The drift currents are given by the standard Ohm's law:

$$J_n^{drift}(x) = n_c(T, \mu)e\mu_n E \text{ and } J_p^{drift}(x) = p_v(T, \mu)e\mu_p E \text{ drift currents for electrons and holes}$$

In those expressions, μ_n and μ_p are the electron and hole mobilities. The diffusion currents are given by Fick's law:

$$J_n^{diff}(x) = -(-e)D_n \frac{dn_c(T, \mu)}{dx} = eD_n \frac{dn_c(T, \mu)}{dx} \text{ and}$$

$$J_p^{diff} = -(+e)D_p \frac{dp_v(T, \mu)}{dx} = -eD_p \frac{dp_v(T, \mu)}{dx}$$

Remember that electrons have a negative charge $-e$ and the holes have a positive charge $+e$, hence the above equations. Because of the space charge region, an electrical potential $\phi(x)$ is created, and its effect is to shift rigidly the band structure at point x by an amount $-e\phi(x)$ which represents the amount of supplemental potential energy of an electron due to the electric field. We will study the behavior of the pn junction at room temperature which is about 300K.

3.1 calculation of the built-in potential

11) With what has been done in the previous part of the homework, conclude about the behavior regime of the p-side and the n-side at 300K. What is the expression for the chemical potential on the p-side, $\mu_L(T)$, previous to the formation of the junction? Identically one can show that the chemical potential on the n-side previous to the formation of the junction is:

$$\mu_R(T) = E_c + k_B T \ln\left(\frac{N_d}{N_c(T)}\right)$$

where E_c is the bottom of the conduction band, N_d is the concentration of donor impurities on the n-side and $N_c(T)$ is the effective density of states in the conduction band.

12) By definition the built-in potential is given by $e\phi_b = E_v(+\infty) - E_v(-\infty) = E_c(+\infty) - E_c(-\infty)$. By observing that the distance between the chemical potential and the top of the valence band must not change on both the p-side and the n-side in the respective limits $x \rightarrow -\infty$ and $+\infty$ even after the junction has been created, prove that the built-in potential is given by:

$$e\phi_b = \mu_R(T) - \mu_L(T)$$

and calculate explicitly this built-in potential as a function of E_g , T , N_a , N_d , $N_c(T)$ and $P_v(T)$. What is the built-in potential at 0K? What is the built-in potential for GaAs at 0K and 300K with uniform doping of $N_a = N_d = 10^{22} m^{-3}$? The band gap for GaAs at 300K is 1.43 eV.

3.2 electrical potential profile and size of the depletion region

Let us now focus on the depletion region. We would like to calculate the size of the depletion region as a function of some fundamental physical constants of the pn junction. For this we will consider that the charge density $\rho(x)$ looks like the following:

$$\rho(x) = -eN_a \text{ for } -d_p < x < 0 \text{ and } \rho(x) = +eN_d \text{ for } 0 < x < d_n$$

where d_p and d_n denote the size of the depletion region on respectively the p-side and the n-side. The way to find the electrical potential is to use the Poisson equation with the appropriate boundary conditions. The Poisson equation in the international system of units is:

$$\frac{d^2\phi(x)}{dx^2} = -\frac{\rho(x)}{\epsilon}$$

where ϵ is the dielectric constant of the medium (here some GaAs with $\epsilon = 13.2 * \epsilon_0$) and ϵ_0 is the vacuum dielectric permittivity $\epsilon_0 = 8.854 * 10^{-12} F.m^{-1}$.

13) Find the boundary conditions that $\phi(x)$ must satisfy and solve the Poisson equation explicitly using the given shape for the charge density $\rho(x)$.

14) Using the continuity of the electrical potential and its first derivative (the electric field) at $x = 0$, find two equations that will link the variables N_a , N_d , ϵ , d_p , d_n , e and ϕ_b together. From those expressions, give the values for d_n , d_p and $w = d_p + d_n$ as functions of N_d , N_a , e , ϵ and ϕ_b only. Find the numerical values for each of those length in the case of a GaAs pn junction with $\phi_b = 1V$, $N_a = N_d = 10^{22} m^{-3}$.

3.3 pn junction under bias an I(V) curve

When one apply a potential difference V between the two ends of a pn junction one can easily realize that **forward bias** and **reverse bias** are not symmetrical. Let us investigate why. For this we will use two relationships linking the carrier densities at different points x that may easily be obtained from what we have seen before. Those relations are the following:

$$\text{For electrons, } n_c(T, x_1) = n_c(T, x_2)e^{e(\frac{\phi(x_1) - \phi(x_2)}{k_B T})}$$

and

$$\text{For holes, } p_v(T, x_1) = p_v(T, x_2)e^{-e(\frac{\phi(x_1) - \phi(x_2)}{k_B T})}$$

15) What is the relationship between the electron density at $x = -d_p$ and $x = d_n$ when no bias exists? Same question for the hole density.

16) When one applies a bias V, it tends to favor the flowing of charges under **forward bias** and unfavour it under **reverse bias**. So we will take V to be positive when it is a forward bias and negative when it is a reverse bias. With this convention how will the built-in potential ϕ_b change when an arbitrary bias

V is applied? Explain what happens to the depletion region size when a forward and reverse bias is applied to the junction and conclude about the asymmetry between forward and reverse bias.

17) Using the above results, show that the change in **electron** density Δn_c at $x = -d_p$ between a configuration where no bias is applied and a configuration where a bias V is applied can be written as:

$$\Delta n_c = n_c^0 (e^{\frac{eV}{k_B T}} - 1)$$

Same question for the change in **hole** density Δp_v at $x = d_n$.

Concluding remark: This change in the concentration of **minority carriers** on both side of the pn junction is responsible for a minority carrier diffusion current that behaves like:

$$J(V) = J_s (e^{\frac{eV}{k_B T}} - 1)$$

This current is responsible for the $I(V)$ response curve of a pn junction.