Problem Set 4
Doped semiconductors

1 Occupation of dopant levels

Consider a nondegenerate doped semiconductor. The density n_d of neutral (not ionized), non-interacting donors is described by

$$n_\mathrm{d} = \frac{N_\mathrm{d}}{1 + \frac{1}{2}\,\mathrm{e}^{\beta(E_\mathrm{d}-\mu)}}, \tag{1}$$

where E_d is the energy level of the dopant and N_d the density of dopants, $\beta = 1/k_\mathrm{B}T$ with T the temperature, and μ the chemical potential.

(a) Assuming that the dopant level can be either empty (ionized dopant) or occupied by one electron (neutral dopant), derive Eq. (1) above using the general expression

$$\langle N \rangle = \frac{\sum_\lambda N_\lambda\,\mathrm{e}^{-\beta(E_\lambda-\mu N_\lambda)}}{\sum_\lambda \mathrm{e}^{-\beta(E_\lambda-\mu N_\lambda)}}$$

for the mean number of particles in a system (in the grand-canonical ensemble) from sums over all quantum states λ of the system, with E_λ and N_λ the energy and particle number in state λ.

(b) Deduce from Question (a) an expression for the density of ionized donors n_d^+.

(c) Draw a qualitative sketch of the behavior of n_d^+ as a function of the chemical potential μ, for $T = 0$ and for two different finite temperatures T_1 and T_2.

(d) Respond to the same questions as in (a), (b), and (c), but for the case of doping with acceptors, where the density of acceptor atoms is N_a. Assume that the acceptor levels, with energy E_a, can never be empty, and that they are occupied either by one (neutral dopant) or by two electrons (ionized dopant) [Why is that the case?]. Show that in such a situation the density of neutral (not ionized) acceptor atoms is given by

$$p_\mathrm{a} = \frac{N_\mathrm{a}}{1 + \frac{1}{2}\,\mathrm{e}^{\beta(\mu-E_\mathrm{a})}}.$$

2 Electrons in the conduction band of a doped semiconductor

We study the density of electrons in the conduction band of an n-doped semiconductor (donors with density N_d, but no acceptors, $N_\mathrm{a} = 0$). We call μ the corresponding chemical potential.

(a) Write the detailed expressions (in terms of an energy integral) for the densities n_c of electrons in the conduction band, and p_v of holes in the valence band.

(b) Suppose that the chemical potential μ is far away (several $k_\mathrm{B}T$) from both, the conduction and the valence band edges E_c and E_v, and write simplified approximate expressions for n_c and p_v.

(c) Using your results to Problem Set 3 and Question (b) above, show that $n_\mathrm{c}p_\mathrm{v} = n_\mathrm{i}^2$ regardless of the fact that the semiconductor is doped or not, where n_i is the intrinsic carrier density.

(d) Introducing $\Delta n = n_c - p_v$, show that

$$n_c = \sqrt{n_i^2 + \frac{\Delta n^2}{4}} + \frac{\Delta n}{2},$$
$$p_v = \sqrt{n_i^2 + \frac{\Delta n^2}{4}} - \frac{\Delta n}{2}.$$

(e) Let us denote μ_i the chemical potential in the intrinsic case. Determine the chemical potential μ of the doped semiconductor as a function of μ_i and Δn.

(f) Assume that all donor levels are ionized (due to high-enough temperature). Use charge conservation to relate Δn and N_d.

(g) Give n_c, p_v, and μ for the case $N_d \gg n_i$ (predominantly extrinsic behavior) and for the opposite case $N_d \ll n_i$ (predominantly intrinsic behavior). What is the transition temperature between the two regimes?

3 Holes in the valence band of a doped semiconductor

We now study the density of holes in the valence band of a p-doped semiconductor (acceptors with density N_a, but no donors, $N_d = 0$). At home, adapt the questions of Exercice 2 and reconsider your answers to them in such a situation.

4 At which energy are most of the carriers?

The electron density in the conduction band (the hole density in the valence band) is given by an integral over contributions from different energies. These contributions are given by the product of an increasing density of states with a decreasing occupation probability when the energy moves away from the band edge. The maximum contribution to the electron (hole) density occurs at a finite energy above (below) the conductance (valence) band edge.

(a) Use the Boltzmann approximation to determine the energy $E_{c,max}$ at which the contribution to the density of electrons in the conduction band assumes its maximum value.

(b) Determine in the same way the energy $E_{v,max}$ where the contribution to the density of holes in the valence band is maximum.