Homework # 13

Exercise 1: As-doped germanium

Impurities that contribute to the carrier density of a semiconductor are called *donors* if they supply additional electrons to the conduction band, and *acceptors* if they supply additional holes (i.e. capture electrons from) the valence band. Here we consider the case of substitutional impurity—an arsenic atom—that replace occasionally a germanium atom. Arsenic is a neighbour of germanium in the periodic table, hence it carries an additional valence electron. To a first approximation, we can model this system with a pure germanium crystal where the germanium atom is not removed, but an additional fixed positive charge of e is placed at its site, along with an additional electron. This is the general model for a semiconductor doped with donor impurities[1].

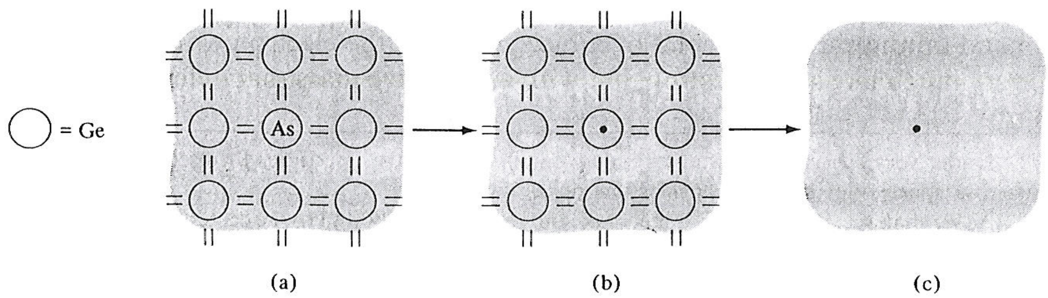

Figure 1: Schematic representation of a substitutional arsenic donor impurity in a germanium crystal.

In a very simplified picture, the extra electron from a donor impurity can be modeled as a charged particle moving in a coulomb potential $\frac{e}{\epsilon r}$ due to the impurity ion, where ϵ in a covalent crystal is the static dielectric constant of the medium. The factor $1/\epsilon$ takes into account the screening of the Coulomb interaction due to the electronic polarization of the medium. We can estimate the energy level of the donor using the Bohr theory of the hydrogen atom. The theory has to be modified to take into account the dielectric constant of the medium and the effective mass of an electron in the crystal periodic potential. Replacing e^2 with e^2/ϵ and the mass of the free electron m with the effective mass m_d^* in the expression for the energy level of an hydrogen atom we obtain:

$$\varepsilon_c - \varepsilon_d = \frac{m_d^*}{m}\frac{1}{\epsilon^2}\,(\mathrm{Ry}) \tag{1}$$

and

$$r_d = \frac{m}{m_d^*}\epsilon\,(\mathrm{Bohr}) \tag{2}$$

where ε_c is the energy at the conduction band minimum, ε_d is the energy of the donor level, r_d the radius of the ground-state Bohr orbit of the donor, and m is the free-electron mass. The static dielectric constant of germanium is $\epsilon \approx 16$ and m_d^* can be approximated with m_c ($m_c = 0.22m$).

1. Estimate the binding energy of an arsenic substitutional impurity and compare it with the band gap of pure germanium ($E_g = 0.67eV$).

[1] For a detailed discussion of the physics of homogeneous and inhomogeneous semiconductors we make reference to the classic book by Ashcroft and Mermin, *Solid State Physics*, 1976.

2. Estimate the radius of the ground-state orbit an compare it with the germanium lattice constant ($a \approx 5.7 \AA$).

Exercise 2: P-doped silicon

Consider silicon doped with phosphorous at room temperature. Answer the following questions.

A) In this case is it a n-doped or p-doped semiconductor?

B) Compute the electrical conductivity σ when the concentration of P impurities is $N_d = 10^{16}$ cm^{-3} (assume the extrinsic regime). Compare the obtained conductivity with the conductivity in the intrinsic regime.

Hint: In Si the effective mass at the bottom of the conduction band is $m_c/m = 0.3$ and the effective mass at the top of valence band is $m_v/m = 0.55$. The band gap in Si is 1.12 eV. Remember also that silicon has six equivalent conduction band minima inside the Brillouin zone. You can find the values of carrier mobilities in the table shown in the slides of week 13.

Exercise 3: non-degeneracy condition in doped silicon

In the case of the n-type doping (*i.e.* the semiconductor has a predominance of negatively charged carriers (electrons)) the chemical potential is (see lectures):

$$\mu_{n-type}(T) = \mu_i(T) + k_B T \ln\left(\frac{N_D}{n_i(T)}\right) \,, \tag{3}$$

where $\mu_i(T)$ is the chemical potential in the intrinsic case (see lectures), N_D is the density of donors, and $n_i(T)$ is the density of carriers in the conduction bands in the intrinsic case

$$n_i(T) = N_c(T)\, e^{-(\varepsilon_c - \mu_i(T))/k_B T} \,. \tag{4}$$

Here ε_c is the energy at the bottom of the conduction band, and $N_c(T)$ is the density of available states in the conduction bands. By substituting the expression for $n_i(T)$ from Eq. (4) into Eq. (3) we obtain that the chemical potential for the n-type doped semiconductors is given by

$$\mu_{n-type}(T) = \varepsilon_c + k_B T \ln\left(\frac{N_D}{N_c(T)}\right) \,. \tag{5}$$

In the case of p-type doping (*i.e.* the semiconductor has a predominance of positively charged carriers (holes)) it can be similarly shown that the chemical potential reads:

$$\mu_{p-type}(T) = \varepsilon_v - k_B T \ln\left(\frac{N_A}{P_v(T)}\right) \,, \tag{6}$$

where ε_v is the energy at the top of the valence band, N_A is the density of acceptors, and $P_v(T)$ is the density of available states in the valence bands.

Consider a silicon semiconductor in the *extrinsic case*, namely the n-type doped case and p-type doped case, at room temperature (T = 300 K). Using Eqs. (5) and (6), and using the expressions for $N_c(T)$ and $P_v(T)$ from lectures, determine the maximum doping concentrations of donors ($N_D^{\max}$ =?) and acceptors ($N_A^{\max}$ =?) that preserve the *non-degeneracy condition* (i.e. $\mu_{n-type} \leq \varepsilon_c - 3k_B T$ for the n-type doping; $\mu_{p-type} \geq \varepsilon_v + 3k_B T$ for the p-type doping).

Hint: Use the values of the effective masses for Si from the Exercise 2.

Exercise 4: p-n **junction**

Consider a p-n junction of GaAs. An example can be a diode in which a p-type material is made of GaAs doped by Be, and a n-type material is made of GaAs doped by Si.

Determine the built-in voltage at $T = 300$ K in the case when the density of donors (i.e. of Si) is $N_d = 10^{15}$ cm^{-3} and the density of acceptors (i.e. of Be) is $N_a = 10^{16}$ cm^{-3}.

Hint: In GaAs, the effective masses are $m_c/m = 0.063$ and $m_v/m = 0.51$, and the band gap energy is $E_g = 1.43$ eV.