

PHYS-E0421 Solid-State Physics (5cr), Spring 2019
Exercise session 3
Model solutions

1. Silicon

- a) The diamond structure consists of two FCC-lattices that are shifted by $\frac{a}{4}(\vec{i} + \vec{j} + \vec{k})$ relative to each other, see figure below (Ibach-Lüth Fig. 2.12). The cubic cell contains 4 atoms inside, 6 atoms on faces and 8 atoms in corners. Atoms on faces are shared by two neighbouring cells, and atoms in corners by eight cells. Then, the number of atoms per cell is $4 + \frac{1}{2} \cdot 6 + \frac{1}{8} \cdot 8 = 8$.

The Bravais lattice basis consists of two atoms at $(0, 0, 0)$ and $(\frac{a}{4}, \frac{a}{4}, \frac{a}{4})$.

Alternatively: Get the number of atoms from knowledge of the basis. We know that there are two atoms in the primitive cell (from the basis). Calculate the volumes of the primitive cell and the cubic cell. This will give that the cubic cell volume is 4 times larger, which means that it must contain 8 atoms.

- b) Silicon has 4 valence electrons (outer shell $3s^2 3p^2$) and phosphorus 5 ($3s^2 3p^3$). The extra electron is loosely bound to the positive phosphorus ion. This means that the defect acts as a donor and the conductivity is n -type. The motion of the extra electron in the bound state can be described by the hydrogen-like atom model. Its energy spectrum is $E_n = \frac{m_e^* e^4}{2(4\pi\epsilon_0\hbar)^2} \frac{1}{n^2}$.

The parameters m_e^ and ϵ describe properties of the material and, in general, they are tensor quantities. The dielectric constant ϵ can be written as a scalar due to the cubic symmetry of silicon lattice, while the effective mass has different values in the transverse and longitudinal directions. In this exercise, we use just an average $m_e^* = 0.3m_e$.*

With the dielectric constant $\epsilon = 11.7$, the ionization energy $E_i = E_1 - E_\infty \approx 28$ meV.

- c) Similarly, the Bohr radius for hydrogen $a_0 = \frac{\epsilon_0 \hbar^2}{\pi m_e e^2}$ can be transformed into the expression valid for our model by making the following changes: $\epsilon_0 \rightarrow \epsilon\epsilon_0$ and $m_e \rightarrow m_e^*$:

$$r_0 = \frac{\epsilon\epsilon_0 \hbar^2}{\pi m_e^* e^2} = \frac{\epsilon}{m_e^*/m_e} a_0 \approx 20.6 \text{ \AA}. \quad (1)$$

Using the density of silicon atoms $n = \frac{8}{a^3}$ [8 atoms in a unit cell a^3 as we found in a], the number of atoms in a sphere of radius r_0 is $N = n \cdot \frac{4}{3}\pi r_0^3 \approx 1800$.

- d) The distance between impurities $4r_0$ corresponds to concentration $n = \frac{1}{(4r_0)^3} = 1.8 \cdot 10^{18} \text{ cm}^{-3}$. This is a large number compared to the intrinsic carrier concentration $n_i \approx 10^{10} \text{ cm}^{-3}$.

2. Intrinsic semiconductor

- a) For an intrinsic semiconductor

$$E_F = \frac{E_C + E_V}{2} + \frac{3}{4}kT \ln(m_p^*/m_n^*), \quad (2)$$

(see Ibach-Lüth 12.2 for the derivation). Inserting $m_p^*/m_n^* = \frac{1}{3}$ yields

$$E_F = \frac{E_C + E_V}{2} - 0.82kT \approx \frac{E_C + E_V}{2} - 1kT. \quad (3)$$

The expression for the Fermi energy was obtained using assumptions $E_C - E_F \gg kT$ and $E_F - E_V \gg kT$, which allow the approximation for the Fermi-Dirac distribution

$$f(E, T) = \frac{1}{e^{(E-E_F)/kT} + 1} \approx e^{-(E-E_F)/kT}. \quad (4)$$

This approximation is also called the *approximation of non-degeneracy*. Here, we estimate that " \gg " is equivalent to " > 3 ". So, we need to satisfy conditions

$$\begin{cases} E_C - E_F \gg kT \\ E_F - E_V \gg kT \end{cases} \Rightarrow \begin{cases} E_C - E_F > 3kT \\ E_F - E_V > 3kT \end{cases} \Rightarrow \begin{cases} E_C - E_V > 4kT \\ E_C - E_V > 8kT \end{cases}, \quad (5)$$

where we have used Eq. (3). For example, from the condition $E_F - E_V = \frac{E_V + E_C}{2} - E_V - 1kT > 3kT$ we get the final answer $E_C - E_V > 8kT$.

- b) Inserting numbers into Eq. (2), we get $E_F - E_V = E_g/2 = 0.115$ eV for $T = 0$ K and $E_F - E_V = E_g/2 + 0.065$ eV = 0.18 eV for $T = 300$ K. The electron and hole concentrations are

$$n = 2 \left(\frac{2\pi m_n^* kT}{h^2} \right)^{3/2} \exp\left(-\frac{E_C - E_F}{kT}\right) \quad (6)$$

and

$$p = 2 \left(\frac{2\pi m_p^* kT}{h^2} \right)^{3/2} \exp\left(\frac{E_V - E_F}{kT}\right), \quad (7)$$

respectively. For $T = 0$ K, $n = p = 0$. For $T = 300$ K, $n = p = 6.7 \cdot 10^{21} \text{ m}^{-3}$. Recall that in an intrinsic semiconductor the number of electrons in the conduction band is equal to the number of holes in the valence band.

3. Doped semiconductors

Assuming non-degeneracy, the Maxwell-Boltzmann statistics can be applied. Then, $n = N_{\text{eff}}^C e^{-(E_C - E_F)/kT} = N_d$. Solving the equation for E_F yields

$$E_F = E_C - kT \ln \frac{N_{\text{eff}}^C}{N_d}. \quad (8)$$

As in Exercise 2, the nondegeneracy condition can be written as $E_C - E_F > 3kT$. Then, $\ln \frac{N_{\text{eff}}^C}{N_d} > 3$ and $N_d < N_{\text{eff}}^C e^{-3} \approx 0.05 N_{\text{eff}}^C$. Inserting $N_{\text{eff}}^C = 2 \left(\frac{2\pi m_n^* kT}{h^2} \right)^{3/2}$, the maximum defect concentrations can be evaluated. For silicon ($m_n^* = 0.3m_e$), at 300 K $N_d = 2.1 \cdot 10^{17} \text{ cm}^{-3}$, at 77 K $N_d = 2.7 \cdot 10^{16} \text{ cm}^{-3}$. For GaAs ($m_n^* = 0.07m_e$), at 300 K $N_d = 2.2 \cdot 10^{16} \text{ cm}^{-3}$, at 77 K $N_d = 2.8 \cdot 10^{15} \text{ cm}^{-3}$.

4. Density of charge carriers

- (a) Intrinsic conductivity at $T = 300$ K? We use the law of mass action and the equality $n_i = p_i$,

$$p_i = \sqrt{N_{\text{eff}}^C N_{\text{eff}}^V} e^{-E_g/2kT} = 2 \left(\frac{kT}{2\pi\hbar^2} \right)^{3/2} (m_n^* m_p^*)^{3/4} e^{-E_g/2kT}. \quad (9)$$

We can evaluate the constants and write the equation in the following convenient numerical form [see A&M Eq. (28.20)]

$$p_i = 2.5 \left(\frac{m_p^*}{m_e} \right)^{3/4} \left(\frac{m_n^*}{m_e} \right)^{3/4} \left(\frac{T}{300 \text{ K}} \right)^{3/2} e^{-E_g/2kT} \times 10^{19} \text{ cm}^{-3} \quad (10)$$

The intrinsic carrier concentrations we obtain, $p_i = n_i \approx 10^{11} \text{ cm}^{-3}$, are very small compared to the hole concentration we obtain in part (b) for the p -doped semiconductor. Therefore, also the intrinsic conduction is negligible at room temperature.

Figure 1: The hole concentrations as a function of inverse temperature.

- (b) What is the conductivity at 300 K when the hole mobility μ_p is 100 cm²/Vs? The fraction of ionized acceptors, N_a^- , can be estimated using [see I&L Eq. (12.25)]

$$p \approx 2N_A \left(1 + \sqrt{1 + 8 \frac{N_A}{N_{\text{eff}}^V} e^{E_a/kT}} \right)^{-1}, \quad (11)$$

where $E_a = E_A - E_V = 0.1$ eV. (This form applicable for p -type conductivity instead of the n -type one is similar to the one in the I&L book. Only the donor and conduction band indices are changed to acceptor and valence band ones, respectively. This can be justified by simply noting that for holes the energy axis points to opposite direction than for electrons. Note that here we have used modified Fermi-Dirac function, compare with I&L and see discussion there.)

We obtain $p = N_A^- + p_i \approx N_A^- \approx 9.6 \cdot 10^{15} \text{ cm}^{-3} \approx N_A$. The conductivity in terms of the carrier concentrations and mobilities is

$$\sigma = e(n\mu_n + p\mu_p) \quad (12)$$

Because $n = n_i \ll p$, we may approximate

$$\sigma \approx ep\mu_p \approx 160 (\Omega\text{m})^{-1}. \quad (13)$$

- (c) Logarithm of the hole concentration, $\ln p$, versus reciprocal temperature $1/T$? See Fig. 1. The following ranges can be observed (see I&L Fig. 12.10, p. 436):

- Freeze-out range (low T): not all acceptors are ionized. Equation (11) has the asymptotic form $p \approx \sqrt{N_A N_{\text{eff}}^V / 2} e^{-E_a/2kT}$, i.e., the plot displays the slope $-E_a/2k$.
- Saturation range (intermediate T): all acceptors ionized, Eq. (11) gives $p \approx N_A$.
- Intrinsic range (high T): thermal excitations across the energy band gap become possible. Slope of $-E_g/2k$, see Eq. (9).