Problem Set 3 Intrinsic and extrinsic homogeneous semiconductors

1 Carrier density in a semiconductor

Consider electrons in the conduction band of a semiconductor with anisotropic dispersion relation

$$E_{\mathbf{k}} = E_{\mathbf{c}} + \frac{\hbar^2}{2} \left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z} \right), \tag{1.1}$$

where $\mathbf{k} = (k_x, k_y, k_z)$ is the crystal momentum and E_c the energy of the bottom of the conduction band.

(a) Show that the dispersion relation (1.1) can be written as

$$E_{\mathbf{q}} = E_{\mathbf{c}} + \frac{\hbar^2 \mathbf{q}^2}{2m_{\mathbf{c}}^*}$$

with the effective mass $m_c^* = (m_x m_y m_z)^{1/3}$. Express the components q_α ($\alpha = \{x, y, z\}$) of the momentum $\mathbf{q} = (q_x, q_y, q_z)$ as functions of k_α , m_α and m_c^* .

- (b) Determine the density of states per unit volume $g_c(E)$ in such a conduction band. Compare to the free-electron density of states discussed in Problem Set 1.
- (c) Express the finite-temperature carrier density $n_{\rm c}(T)$ in terms of the density of states $g_{\rm c}(E)$ and as a function of the chemical potential μ and the temperature T. Show that for $E_{\rm c} - \mu \gg k_{\rm B}T$, the carrier density can be approximated by $n_{\rm c}(T) \simeq N_{\rm c}(T) e^{-\beta(E_{\rm c}-\mu)}$ with

$$N_{\rm c}(T) = \int_{E_{\rm c}}^{\infty} \mathrm{d}E \, g_{\rm c}(E) \, \mathrm{e}^{-\beta(E-E_{\rm c})},$$

where $\beta = 1/k_{\rm B}T$ is the inverse temperature. Using that $\int_0^\infty dx \sqrt{x} \exp(-x) = \sqrt{\pi}/2$, show that

$$N_{\rm c}(T) = \frac{1}{4} \left(\frac{2m_{\rm c}^*k_{\rm B}T}{\pi\hbar^2}\right)^{3/2}$$

- (d) Apply the same reasoning to holes in the valence band, and derive the approximation for the hole density $p_{\rm v}(T) = P_{\rm v}(T) e^{-\beta(\mu E_{\rm v})}$, where $E_{\rm v}$ is the energy corresponding to the top of the valence band. Give the expression for $P_{\rm v}(T)$ and the condition for the validity of the approximation.
- (e) Show that within the above approximations, the product of n_c and p_v is independent of the chemical potential. Express it in terms of the energy gap $E_g = E_c E_v$ of the semiconductor.

2 Intrinsic semiconductors

- (a) Explain the meaning of "intrinsic semiconductor".
- (b) Assume low enough temperature and use the approximate results for the carrier and hole densities of Exercise 1. Express the intrinsic carrier density $n_{\rm i} = n_{\rm c} = p_{\rm v}$ in terms of the energy gap $E_{\rm g}$.
- (c) Derive an expression for the chemical potential μ from the condition of charge conservation (equal number of electrons in the conduction band and holes in the valence band).
- (d) Take an energy gap $E_{\rm g} = 0.6 \,\mathrm{eV}$, and an effective mass $m_{\rm c}^*$ in the conduction band which is three times the effective mass $m_{\rm v}^*$ in the valence band. Calculate the temperature for which the chemical potential μ is located at $E_{\rm v} + E_{\rm g}/3$.

3 Doped semiconductors

The semiconductor InSb has a gap $E_{\rm g} = 0.18 \,{\rm eV}$. The dielectric constant of the material is $\epsilon = \epsilon_0 \epsilon_{\rm r}$ with $\epsilon_{\rm r} = 17$). The effective mass is $m_{\rm c}^* = 0.014 \, m_{\rm e}$, where $m_{\rm e}$ is the free electron mass. Some of the In atoms (group III of the periodic table) are replaced by Si donor atoms (group IV), with a donor dopant density $N_{\rm d} = 10^{18} \,{\rm cm}^{-3}$. Let us treat a donor atom as a positively charged Si atom with a weakly bound electron in a hydrogen-like state.

(a) The energy levels of a hydrogen atom are given by

$$E_n = -\frac{m_e e^4}{8\epsilon_0^2 h^2} \frac{1}{n^2} \quad \text{with} \quad n \in \mathbb{N}^*.$$

Calculate the ground state energy E_1 of the hydrogen atom in eV and determine the ionization energy (Rydberg constant Ry).

- (b) In analogy with the previous case, express the ionization energy of a donor in a semiconductor in units of Ry and calculate its value for Si donors in InSb.
- (c) Compare the ionization energy to the thermal energy at room temperature and to the energy gap of the semiconductor.
- (d) The typical distance between the electron and the nucleus in a hydrogen atom is given by the Bohr radius

$$a_0 = \frac{h^2 \epsilon_0}{\pi m_{\rm e} e^2} \simeq 53 \,\mathrm{pm}.$$

Estimate the distance between a Si donor atom and the weakly bound electron.

(e) Estimate the critical dopant concentration above which the distance between dopants is small enough to allow for the hopping of electrons between the lowest bound states on neighboring dopants. At what temperatures is this effect expected to be important?

4 Some simple calculations

- (a) Estimate the slope of the temperature dependence of the intrinsic carrier concentration in the vicinity of room temperature, for the semiconductors InAs, Si and GaAs. Intrinsic carrier concentrations at room temperature (300 K) are for InAs: $8.6 \times 10^{14} \,\mathrm{cm^{-3}}$, Si: $1.0 \times 10^{10} \,\mathrm{cm^{-3}}$, GaAs: $1.8 \times 10^6 \,\mathrm{cm^{-3}}$. The corresponding energy gaps are for InAs: $0.36 \,\mathrm{eV}$, Si: $1.1 \,\mathrm{eV}$, GaAs: $1.43 \,\mathrm{eV}$.
- (b) Take the case of doped silicon with an electron density in the conduction band $n_c = 10^{16} \text{ cm}^{-3}$ at T = 300 K. Using the value $N_c = 7.28 \times 10^{19} \text{ cm}^{-3}$ at T = 300 K, determine the value of the chemical potential with respect to the bottom of the conduction band E_c .
- (c) Calculate the mean distance between dopants in silicon for dopant concentrations of (i) 10^{16} cm^{-3} ; (ii) 10^{18} cm^{-3} ; and (iii) 10^{20} cm^{-3} .