### T10. Semiconductor band gap

In this problem we will consider the structure of semiconductors from the point of view of solid-state physics and explain the temperature dependences of the concentration of electrons and holes. To describe the electrons on the upper shells of the atoms in a crystal lattice, we consider the problem of electron motion in the effective periodic potential  $U(\vec{r})$ , which models the interaction of the electron with the nuclei and the surrounding low-energy electrons in the nodes of the crystal lattice.



Figure 1. The crystal lattice of silicon. Wen, Mingjian et. all (2021).

Let us simplify the problem to the Cronig-Penny model (1931). Let us consider a one-dimensional problem: let non-interacting electrons move in the electric field of a chain of stationary charges located at a distance a from each other. Let U(x) be the periodic potential, modeling the interaction of the electron with the crystal lattice, consist of rectangular wels of depth  $U_0$  and width b.



From the point of view of quantum mechanics, to describe the behavior of electrons, we need to find the wave functions  $\Psi(x)$  and their corresponding energies E satisfying the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\Psi''(x) + U(x)\Psi(x) = E\Psi(x).$$

Quantum mechanics requires that the derivative  $\Psi'(x)$  of the wave function has no discontinuities.

Bloch's theorem allows us to significantly narrow down the set of functions among which we will search for solutions. According to this theorem, the solutions to the equation in the periodic potential U(x) can only be a function of the following form:

$$\Psi(x) = e^{ikx/a}u(x/a),$$

where  $k \in [-\pi, \pi]$  is a dimensionless constant called quasimomentum, and u(y) is a periodic function with unit period, i.e., u(y+1) = u(y).

A1 Substitute  $\Psi(x) = e^{ikx/a}u(x/a)$  into the Schrödinger equation and get the equation  $u'' + 2iku' + \left[\frac{2ma^2}{\hbar^2}\left(E - U(x)\right) - k^2\right]u = 0$ on u(y).

Let's nondimensionalize the problem, so we introduce  $2mabU_0/\hbar^2 = k_0^2$  and  $Ea/(U_0b) = \varepsilon$ . The values of  $k_0$  and b/a include all physical properties of the system.

Then we have a linear differential equation with constant coefficients on u(y) in each of the domains  $y \in [-b/a, 0]$  and  $x \in [0, 1 - b/a]$ :

$$u'' + 2iku' + \left[k_0^2\left(\varepsilon + \frac{a}{b}\right) - k^2\right]u = 0 \quad \text{for} \quad y \in \left[-b/a, 0\right]$$
$$u'' + 2iku' + \left[k_0^2\varepsilon - k^2\right]u = 0 \quad \text{for} \quad y \in \left[0, 1 - b/a\right]$$

**A2** Consider a linear differential equation with constant coefficients  $\alpha$  and  $\beta$ :

$$u'' + 2i\alpha u' + (\beta - \alpha^2)u = 0.$$

Find the values of  $\lambda_{1,2}$  for which the function  $u_{1,2}(y) = e^{\lambda_{1,2}y}$  is a solution to this equation. Check that for any constants A and B, the function  $u(y) = Ae^{\lambda_1 y} + Be^{\lambda_2 y}$  is also a solution to this equation.

Now we understand how the function u(y) can be arranged and its form is completely given by two pairs of constants A and B (a pair on each segment):

$$u(y) = u_I(y) = A_1 e^{\lambda_{11}y} + B_1 e^{\lambda_{12}y} \quad \text{for} \quad y \in [-b/a, 0]$$
$$u(y) = u_{II}(y) = A_2 e^{\lambda_{21}y} + B_2 e^{\lambda_{22}y} \quad \text{for} \quad y \in [0, 1 - b/a].$$

So that u(y) can be substituted into expressions for the wave function  $\Psi(x) = e^{ikx/a}u(x/a)$ , it remains to be required that

- 1. Periodicity of u(x).
- 2. Continuity of u(x) at the point y = 0 of the gluing solutions  $u_I$  and  $u_{II}$ .
- 3. Continuity of u'(x) at the point y = 0 of the gluing solutions of  $u_I$  and  $u_{II}$ .
- 4. Continuity of  $\Psi'(x)$  at the points  $x = -b + a \cdot n$ .
- A3 Write a system of equations for the coefficients  $A_1$ ,  $A_2$ ,  $B_1$  and  $B_2$  corresponding to the requirements on the functions  $u_I(x)$  and  $u_I I(x)$ , in matrix form

$$M\begin{pmatrix}A_1\\A_2\\B_1\\B_2\end{pmatrix} = \begin{pmatrix}M_{11} & M_{12} & M_{13} & M_{14}\\M_{21} & M_{22} & M_{23} & M_{24}\\M_{31} & M_{32} & M_{33} & M_{34}\\M_{41} & M_{42} & M_{43} & M_{44}\end{pmatrix}\begin{pmatrix}A_1\\A_2\\B_1\\B_2\end{pmatrix} = 0.$$

Write the coefficients of the matrix  $M_{ij}$  by  $\lambda_{11}$ ,  $\lambda_{12}$ ,  $\lambda_{21}$ ,  $\lambda_{22}$ , a, and b.

The system of equations for the constants  $A_{1,2}$ ,  $B_{1,2}$  considered above has a non-trivial solution (a solution other than  $A_1 = A_2 = B_1 = B_1 = B_2 = 0$ ) only if det M = 0.

Moreover, if we require the equality det M = 0 to be satisfied, we are restricted in choosing the values of  $\lambda_{11}$ ,  $\lambda_{12}$ ,  $\lambda_{21}$ ,  $\lambda_{22}$  when a and b are fixed. Recall that  $\lambda_{ij}$  are expressed through the physical parameter of the system  $k_0$  and the chosen values of quasimomentum k and energy E. That is, the equation det M = 0 restricts the choice of k and E. In other words, for a particular quasimomentum k the energy E cannot be any, but only some from a restricted set.

Thus, we can search for all pairs of values of energy E and quasimomentum k that we are interested in, to us and check for which of them the equation det M = 0 is satisfied. This problem is computationally challenging but conceptually trivial, so we will solve it using a computer. We will consider a particular pair (k, E) as a solution of the quantum mechanical problem if the equality det M = 0 is satisfied for some  $\varepsilon_0$ :  $|\det M| < \varepsilon_0$ .

Exactly this algorithm is implemented in the program energy.py. The results are presented graphically as a plot  $\varepsilon = Ea/(U_0b)$  of k, which is also called the energy spectrum. The meaning of this graph is as follows: for each value of the quasimomentum k the values of the energy E are given, which are solutions of to the Schrödinger equation, The graph is derived only for  $k \in [0, \pi]$ , since it is symmetric with respect to k = 0 and  $k = \pi$ .



Figure 2. An example of the spectrum of  $\varepsilon$  vs. k with small (indistinguishable in the chosen scale) band gaps on the left and with large band gaps on the right (highlighted in red).

For different model parameters  $k_0$  and b/a the energy spectrum (E, k) changes. On the left graph we see that for any energy  $E > -U_0 a/b$  there is a corresponding state, i.e. the value of the quasimomentum k. On the right graph, however, we see that there are segments of energy E to which no stationary quantum states correspond, i.e. there are forbidden regions of energy E which are called band gaps.

To demonstrate the importance of band gaps for semiconductors, let us consider how the electrons are distributed among the states we have found. Recall that no two electrons can be in the same state because of the Pauli exclusion principle.

First, instead of a crystal, we consider a "box" of length L such that no electron can be outside the box (i.e., the wave function  $\Psi(x)$  converges to 0 at the boundaries of the box). Inside the box, we have the Schrödinger equation

$$-\frac{\hbar^2}{2m}\Psi'' = E\Psi,$$

whose solutions are de Broglie waves  $\Psi(x) = e^{ikx/a}$ .

A5 Show that the de Broglie wave  $\Psi(x) = e^{ikx/a}$  has the energy  $E = \frac{\hbar^2 k^2}{2ma^2}$ .

At the box boundaries, the wave functions must go to 0, i.e., we fit de Broglie wave functions of the following form:

$$\Psi(x) = \frac{e^{ikx/a} - e^{-ikx/a}}{2i} = \sin\frac{kx}{a}, \quad \text{where} \quad \sin\frac{kL}{a} = 0$$

so  $k = \pi na/L$  where n is a natural number. If there are N electrons in the box at zero temperature (i.e., we find their collective lowest energy state), then they occupy the first N lowest energy states. Accordingly, the Fermi energy  $E_F$  is the energy of the highest level occupied by the set of electrons at zero temperature. Since that electrons have spin, two different states with opposite spin direction and the same values of k and E correspond to one pair (k, E).

A6 | Express 
$$E_F$$
 in terms of  $L$ ,  $N$ ,  $m$ , and  $\hbar$ .

For a similar consideration of the collective behavior of electrons in the considered crystal lattice, let us place the lattice in a box, i.e., we will also require that the wave function to be zero at the boundaries of the box. The wave functions obtained by means of Bloch's theorem  $e^{ikx/a}u(x/a)$  allow us to easily satisfy this requirement (if we choose constants so that  $u^*(0) = u(0)$  and  $u^*(L) = u(L)$ , where \* is the complex conjugation operation):

$$\Psi(x) = u(x/a)e^{ikx/a} + u^*(x/a)e^{-ikx/a} \quad \Rightarrow \quad \Psi(0) = 0, \\ \Psi(L) = 2iu(L/a)\sin(kx/a)$$

when  $k = a\pi n/L$ , where n is natural.

In the case of silicon, a one-dimensional crystal of length L contains L/a atoms, with each atom corresponding to 4 electrons from the outer orbitals, i.e., eventually 4L/a electrons are in the upper levels and so the estimate for the position of the Fermi level is:

$$E_F = \frac{2\pi^2\hbar^2}{ma^2}, \quad \varepsilon_F = \frac{4\pi^2}{k_0^2}$$



The Fermi level position for certain parameters of a one-dimensional problem.

**A7** Use the program energy.py to obtain the dependence of the band gap  $E_g$ , where the Fermi level is located, on the parameter  $k_0$  at b/a = 0.1. Consider a = 0.5 nm, electron mass  $m = 9.1 \cdot 10^{-31}$  kg, Planck constant  $\hbar = 1.05 \cdot 10^{-34}$  J · s, elementary charge  $e = 1.60 \cdot 10^{-19}$  C. Fill in the table.txt table and use the program bandgap.py to draw a graph of this relationship. In table.txt table, the separator between columns is tab.

**A8** What  $k_0$  corresponds to the forbidden zone of silicon  $E_{\rm Si} = 1.12$  eV? Do all further calculations for this  $k_0$ .

If the temperature of the electrons is different from zero, the energy boundary is slightly "blurred" and a some of the electrons with energy  $E < E_F$  appear in states with energy  $E > E_F$ . Formally, this is described as follows: if there are g different states with the same energy E, then

$$F(g, E) = \frac{g}{e^{\frac{E-E_F}{k_{\mathrm{B}}T}} + 1}$$

of which on average will be filled with electrons, where  $k_{\rm B} = 1.38 \cdot 10^{23} \text{ J/K}$  is the Boltzmann constant. As you can see at  $T \to 0$  all states with  $E < E_F$  are completely filled and all states with  $E > E_F$  are free.

The state of electrons in a semiconductor at finite temperature is usually described in this form:

- 1. We first consider the electron gas at zero temperature: it completely occupies all levels with  $E < E_F$ .
- 2. The heating of the electron gas is equivalent to the appearance of excitations: electrons that have moved from the lower band (valence band) to the upper band (conduction band).
- 3. Such an electron transition is equivalent to adding one electron to the conduction band and adding a hole (i.e., "no" electrons) to the valence band.

We will use this approach. To do this, we need to find an approximation for the conduction band edge  $E(k) = E_c + \alpha k^2$  and the valence band edge  $E(k) = E_v - \beta k^2$ . You can find the values  $\varepsilon_c$ ,  $\varepsilon_v$ ,  $\tilde{\alpha} = \alpha a/(U_0 b)$ ,  $\tilde{\beta} = \beta a/(U_0 b)$  in the output of energy.py.

**A9** Use the program energy.py to find the values of  $E_c - E_F$ ,  $E_F - E_v$ ,  $\alpha$ , and  $\beta$ . Check for yourself that  $E_c - E_v = E_{\rm Si}$ . Also find the values of  $(E_c - E_F)/k_{\rm B}T$  and  $(E_F - E_v)/k_{\rm B}T$  for T = 300 K.

Use the program energy.py to find the values of  $E_c - E_F$ ,  $E_F - E_v$ ,  $\alpha$ , and  $\beta$ . Check for yourself that  $E_c - E_v = E_{\rm Si}$ . Also find the values of  $(E_c - E_F)/k_{\rm B}T$  and  $(E_F - E_v)/k_{\rm B}T$  for T = 300 K.Earlier we obtained that, because of the "box" in which we placed the crystal, the states with any value of the quasimomentum k in the interval  $[-\pi, \pi]$  are admissible, but only a discrete set of quasimomentums  $k \in [0, \pi]$  differ from each other by  $\Delta k = \pi a/L$ . In result  $g = \frac{2}{\Delta k} \left| \frac{dE}{dk} \right|^{-1} \Delta E$  of different states (with different values of quasi-momentum and spin) correspond to the domain  $[E, E + \Delta E]$ .

Substituting the approximation for the E(k) edges of the valence band and conduction bands we get

$$g_c(\Delta E, k) = \frac{L\Delta E}{\pi a \alpha k}, \quad g_v(\Delta E, k) = \frac{L\Delta E}{\pi a \beta k}$$

Thus the total number of states filled in the conduction band:

$$n = \sum_{E \ge E_c} F(g(\Delta E, k), E) = \sum_{E \ge E_c} \frac{g_c(\Delta E, k)}{e^{\frac{E - E_F}{k_B T}} + 1} \simeq \sum_{E \ge E_c} g_c e^{\frac{E_F - E}{k_B T}} \simeq$$
$$\simeq \int_{E_c}^{+\infty} \frac{L}{\pi a \alpha k} e^{\frac{E_F - E}{k_B T}} dE = \frac{2L}{\pi a} e^{\frac{E_F - E_c}{k_B T}} \int_{0}^{\infty} e^{-\frac{\alpha k^2}{k_B T}} dk = \frac{L}{a} e^{\frac{E_F - E_c}{k_B T}} \sqrt{\frac{k_B T}{\pi \alpha}}.$$

This number n is the number of electrons involved in the transfer processes.

A10 Show that the total number p of NOT-filled states in the valence band is

$$p = \frac{L}{a} e^{\frac{E_v - E_F}{k_{\rm B}T}} \sqrt{\frac{k_B T}{\pi \beta}}.$$

This number p is the number of holes involved in the transfer processes. Show that  $p \cdot n$  does not depend on the position of the Fermi level  $E_F$ . Find the value of  $n_i = \sqrt{p \cdot n} \cdot a/L$  for silicon at temperature T = 300 K.

A11 What should the Fermi level  $E_F$  be so that the crystal is electrically neutral, i.e., the number of holes p is equal to the number of electrons n?

As we can see, the number of objects involved in the transfer processes depends significantly on the temperature; the edges of the conduction band  $E_c$  and the valence band  $E_v$ ; and the position of the Fermi level.

Of these three parameters, the position of the Fermi level turns out to be the most interesting, since it can be controlled by impurities:

- By replacing a silicon atom Si in the crystal lattice with an aluminum atom Al, we practically do not change the type of potential U(x)m but the number of electrons on the outer shells has decreased by one. That is, the value of p n has increased by one.
- By replacing a silicon atom Si with phosphorus atom P we practically do not change the form of the potential U(x), but we increase the number of electrons on the outer shells by one. That is, the value of p n has decreased by one.



A qualitative picture of charges inside a p-type semiconductor.

Large white circles represent Si atoms, large red circles represent Al atoms, small red circles represent electrons, and small blue circles represent holes. Blue corresponds to a positive charge, and red corresponds to a negative charge.

The arrows in the green area illustrate the mechanism of hole conduction: a valence electron from an atom without a hole can "jump" to a neighboring atom if there is a hole there. We consider this process to be the movement of a hole.

Doped silicon in terms of charges then consists of 4 components:

- 1. Electrically neutral silicon atoms
- 2. Impurity atoms that are charged  $\pm e$  so that their electron shells become the same as those of silicon.
- 3. Free electrons with negative charge.
- 4. Positively charged holes that «sit» on the atoms.

The semiconductor as a whole is electrically neutral.

A12 What fraction c of silicon Si atoms must be replaced by aluminum Al to increase the ratio of holes to electrons p/n to  $q = 10^6$  with respect to pure silicon? Consider the temperature to be 300 K.

## T11. Charge carriers in semiconductor

The charge carriers in semiconductors are electrons (*n* from «negative» with charge -e) and holes (*p* from «positive» with charge e), whose chaotic thermal motion is slightly distorted by external fields. The elementary charge  $e = 1.60 \cdot 10^{-19}$  C. To describe the transfer processes, the carrier mobility  $\mu$  is introduced, which determines the dependence of its average velocity v on the applied external electric field  $\mathcal{E}$ :

$$|v| = \mu |\mathcal{E}|.$$

The mobility depends on the temperature and the concentration of defects in the crystal lattice. Thus the volume concentration of electrons n (units  $1/m^3$ ) and the volume concentration of holes p (units  $1/m^3$ ) in a semiconductor with impurities, depend on the temperature and the change in Fermi energy  $\Delta E_F$ , which characterizes the influence of impurities, as follows:

$$n = n_i \sqrt{\frac{T}{T_0}} e^{\frac{\Delta E_F}{k_{\rm B}T}}, \quad p = n_i \sqrt{\frac{T}{T_0}} e^{-\frac{\Delta E_F}{k_{\rm B}T}}.$$

For silicon,  $n_i = 1.1 \cdot 10^{10} \text{ cm}^{-3}$  and  $T_0 = 300 \text{ K}$ .

A1 Find the charge dq flowing in time dt through the area S perpendicular to the field. Using Ohm's law  $R = U/I = \rho l/S$ , express the resistivity  $\rho$  of a semiconductor through  $\mu_n$ ,  $\mu_p$ , n, and p.

Semiconductors are often doped, i.e. impurities  $(|\Delta E_F| \gg k_B T)$  are added to them so that some carriers can be neglected relative to others. A doped semiconductor is called by the letter of the dominant carrier: p – Si for silicon which has significantly more holes than electrons and n – Si for silicon which has significantly more electrons than holes. Impurities that shift the Fermi level so that there are more electrons than holes are called donors and their concentration is denoted by  $N_D$ . Conversely, impurities that increase the concentration of holes are called acceptors and are denoted by  $N_A$ . In this case, the condition of electroneutrality is satisfied

$$n - N_D = p - N_A,$$

which, if the condition  $e^{|\Delta E_F|/k_B T} \gg 1$  leads to the expression  $p = N_A - N_D$  in the *p* doped semiconductor and to the expression  $n = N_D - N_A$  in the *n* doped semiconductor.

Thus, in p – Si and n – Si the sign of the charge of the charge carriers is different, hence the Hall voltage  $V_H$  will have a different sign. Consider a rectangular sample of a doped semiconductor with thickness W = 0.50 mm and cross-sectional area  $A = 2.5 \cdot 10^{-3}$  cm<sup>2</sup> be in a magnetic field  $B = 1.0 \cdot 10^{-4}$  T and a current I = 1.0 mA flowing through it.



A2 Which charge carrier is dominant in the sample if the measured voltage is  $V_H = +1.25$  mV? What is the charge carrier concentration in the sample?

<b>A3</b>	A measurement of $V_H = +1.25$ mV was made in winter at a temperature of $T = 290$ K in a
	laboratory with poor thermoregulation. What value of $V'_{H}$ would be measured with the same
	setup in the summer, when the temperature in the lab reaches $T = 305$ K?

#### June, 2025

# T12. PN junction physics

The charge carriers in semiconductors are electrons (*n* from "negative" with charge -e) and holes (*p* from "positive" with charge e), whose chaotic thermal motion is slightly distorted by external fields. The elementary charge  $e = 1.60 \cdot 10^{-19}$  C. To describe the transfer processes, the carrier mobility  $\mu$  is introduced, which determines the dependence of its average velocity v on the applied external electric field  $\mathcal{E}$ :

$$|v| = \mu |\mathcal{E}|.$$

The mobility depends on the temperature and the concentration of defects in the crystal lattice. In this case, the volume concentration of electrons n (dimension  $1/m^3$ ) and the volume concentration of holes p (dimension  $1/m^3$ ) under conditions of thermodynamic equilibrium are related to each other by the relation  $np = n_i^2$ , where  $n_i$  is the concentration of carriers of both types in a semiconductor without impurities.

If there is spatial inhomogeneity in the distribution of charge carriers in a semiconducting sample, diffusion currents with corresponding volume densities flow in addition to conduction currents:

$$j_{Dp} = -eD_p \frac{dp}{dx}, \quad j_{Dn} = eD_n \frac{dn}{dx}.$$

And from Einstein's relation  $D = \mu k_{\rm B} T/e$ , so the total current density inside the semiconductor is

$$j = \mu_p \left[ \mathcal{E}ep - k_{\rm B}T \frac{dp}{dx} \right] + \mu_n \left[ \mathcal{E}en + k_{\rm B}T \frac{dn}{dx} \right].$$
<sup>(1)</sup>

Let us denote  $\mu_p/\mu_n = \alpha$ , for silicon we will consider this value to be 3.1 and independent of impurities. The concentration of impurity-donors increasing the number of electrons will be called  $N_D$  and the concentration of impurity-acceptors increasing the number of holes will be called  $N_A$ .

We will consider a one-dimensional problem, for inhomogeneously doped silicon at temperature T = 300 K, then  $n_i = 1.1 \cdot 10^{10}$  cm<sup>-3</sup>.

- 1. In the region x < 0 a p-silicon is created with  $N_A = N_p \gg n_i$ ,  $N_D = 0$ .
- 2. In the region x > 0 an n-silicon is created with  $N_D = N_n \gg n_i$ ,  $N_A = 0$ .

We will also assume that all processes are stationary, i.e., charge does not accumulate anywhere and therefore dj/dx = 0. The electric potential is denoted by the letter  $\varphi$ . For nondimensionalization, let's work in terms of relative concentrations  $u = p/n_i$ ,  $v = n/n_i$ . The relative permittivity of a semiconductor is  $\varepsilon$ .

### Part A. Equilibrium in PN junction

First, let us consider an equilibrium PN junction with no current flowing. In such a case, holes and electrons are in thermodynamic equilibrium at every point, i.e. v = 1/u.

A1 Substitute j = 0 and v = 1/u into the equation (1) and get the relationship between  $\varphi'$ , u', and u.

A2 Integrate the equation obtained in A1 and find the potential difference  $V_{bi} = \varphi(+\infty) - \varphi(-\infty)$  of the electric field at the pn junction. Express the answer in terms of  $N_p$ ,  $N_n$ ,  $n_i$ 

**A3** Write down Gauss' theorem and express  $\varphi'$  by u and  $N_D - N_A$ . Get the differential equation for  $\Psi$  where  $\Psi = \ln u$  as

$$L^2 \Psi'' = 2\sinh\Psi - \frac{N_A - N_D}{n_i} \tag{2}$$

We have obtained a nonlinear differential equation on  $\Psi$  and will solve it numerically. To set the initial conditions, we consider the behavior of  $\Psi$  away from the pn junction, where  $\Psi = \operatorname{asinh} \frac{N_A - N_D}{2n_i} + \delta \Psi$  and  $|\delta \Psi| \ll |\Psi|$ .

A4 Find the analytic expression for  $\delta \Psi$  of the previous equation in regions far from the pn junction.

A5 Find the analytic expression for  $\Psi$  for the domain, where  $n_i |2 \sinh \Psi| \ll |N_A - N_D|$ .

A6 Use the program pn-junction.py to solve equation (2) numerically for  $N_p = 2 \cdot 10^5$ ,  $N_n = 10^5$ . Collect some data and plot a graph  $\Psi(0)/\ln(N_nN_p)$  vs.  $\ln N_n/N_p$ .

#### Part B. PN junction capacitance

Inside the pn junction there is a region where  $p, n \ll N_p, N_n$ . To obtain the analytical result, we will assume that the charge density  $\rho = e(p - N_A - n + N_D)$  has the form shown in the graph below. That is

- 1. in the region  $x < -x_p$  we have equilibrium p-silicon with  $p = N_p$ ;
- 2. in the region  $-x_p < x < x_n$  we have  $N_p, N_n \gg p, n$ ;
- 3. in the region  $x > x_n$  we have equilibrium n-silicon with  $n = N_n$ .



Figure 3. Left: charge density  $\rho$  obtained from solving equation (2). Right: charge density  $\rho$  used in our model.

**B1** Find the dependences of the electric field  $\mathcal{E}(x)$  in the chosen model and draw its graph. What relation between  $x_p$ ,  $x_n$ ,  $N_p$ , and  $N_n$  must be satisfied so that the field  $\mathcal{E}$  goes to zero at the boundaries  $-x_p$  and  $x_n$  and to is continuous at the point x = 0?

If we connect the pn junction to a source of voltage U (plus to p and minus to n) and infinite internal resistance, the potential difference across at the pn junction becomes  $V_{bi} - U$ .

The capacitance of the system C is defined as C = dQ/dU, where dQ is the change in charge on each side of the pn junction (they have different signs). In our model, when voltage U is applied, the size of the spatial charge distribution region decreases from  $[-x_p, x_n]$  to  $[-x'_p, x'_n]$ . In particular, when voltage U is applied, the value of u (relative hole concentration) in the vicinity of the junction itself changes slightly, so these changes do not affect the appearance of the charge and field distributions.

**B2** Express  $x'_p$  through  $x_p$ ,  $V_{bi}$  and U. Substitute  $dQ = -SN_p dx'_p$ , where S is the area of the pn junction, into the expression for the capacitance C and find the dependence of C(U). Express the dependence C(U) in terms of S,  $N_{n,p}$ .

Thus, a pn junction can be used as a capacitor whose capacitance depends on the applied voltage - such devices are called varicaps.

# Part C. I-V characteristics of PN Junction

When an external voltage is applied, the charge carrier distribution picture changes significantly only at the edges of the pn junction, where the concentration of non-main carriers (i.e., electrons in p-silicon and holes in n-silicon) changes significantly.

In the domain  $[-x_p, x_n]$  the expression from A1 remains valid, since the current density j is a small correction relative to the other terms. We denote the recombination rate (the rate of the process of mutual annihilation of holes and electrons) by R and the formula for it follows from the consideration that the case nv = 1 must correspond to the equilibrium:

$$R = \frac{uv-1}{\tau_p(u+1) + \tau_n(v+1)} n_i$$

where  $\tau_p$  and  $\tau_n$  are the characteristic lifetimes of the corresponding particles.

C1 Suppose that due to the presence of the voltage U, the concentrations of holes and electrons have changed with respect to the equilibrium U = 0 as follows  $u \to u + \delta u$ ,  $v \to v + \delta v$ . Express the current density j through  $\delta u$ ,  $\delta v$ , their derivatives, and the field  $\mathcal{E}$ .

C2 Write the stationarity equations for  $\delta u$ ,  $\delta v$  through their values and the values of their derivatives, considering that changes in these quantities over time can only be due to currents and recombination.

C3 Transform the stationarity conditions for points where  $\mathcal{E} = 0$  and find the form of the functions  $\delta v$  and  $\delta u$  in the range  $x < -x_p$ . Take into account  $N_p, N_n \gg n_i$  and the smallness of  $\delta u, \delta v$ .

You should find that  $\delta v$  and  $\delta u$  are of the same order of magnitude, so the majority carrier density is approximately unchanged from equilibrium. Exactly the same equations can be written for the range  $x > x_n$ .

C4 Assuming that the equation from A1 is satisfied in the region  $x \in [-x_p, x_n]$ , find the constants for  $\delta u$  and  $\delta v$  for the results of C3.

C5 Obtain the I-V characteristic of the pn junction in the form j = f(U).