

Lecture XVI Basics of semiconductor device modeling

In this lecture, we review the very basic facts of semiconductor device modeling. We only considered the pn-junction in the 1D case.

Part I What is given?

1. Doping profiles

In a pure or *intrinsic* sample of a semiconductor crystal there is always a non-zero *intrinsic* concentration of holes and an equal concentration of electrons, called n_i . This concentration is well documented; at room temperature

$$n_i \approx 1 \times 10^{10} \text{ cm}^{-3} \quad \text{for Si} \quad (1a)$$

$$n_i \approx 2 \times 10^6 \text{ cm}^{-3} \quad \text{for GaAs} \quad (1b)$$

$$n_i \approx 2 \times 10^{13} \text{ cm}^{-3} \quad \text{for Ge} \quad (1c)$$

Note that the common units for the pn-junction analysis are *cm* rather than *m*.

The concentration of donor atoms (leading to free electrons and the n-type semiconductor) is denoted by doping concentration $N_D(x) > 0$. The concentration of acceptor atoms (leading to free holes and the p-type semiconductor) is the doping concentration $N_A(x) > 0$. We will assume that all of those atoms are ionized and thus create either one free electron or one free hole per atom. The doping concentrations vary with the distance x along the pn-junction. The (total) impurity concentration $N_E(x)$ is given by

$$N_E(x) = N_D(x) - N_A(x) \quad (2)$$

The value of the impurity concentration is directly related to the charge density of (immovable) ions,

$$qN_E(x) \quad (3)$$

Possible values for doping concentrations in Si are in a wide range 10^{12} - 10^{19} cm^{-3} , with typical values around 10^{15} - 10^{17} cm^{-3} .

Example: As a base example we will consider a Si pn-junction shown in Fig. 1 with the total length $R = 2 \times 10^{-4} \text{ cm} = 2 \text{ } \mu\text{m}$ and with the doping profiles

$$N_D(x) = N_{D0} \left[1 - \exp\left(-\frac{x}{L}\right) \right] \quad \text{at } x > 0; \quad N_D(x) = 0 \quad \text{at } x \leq 0 \quad (4a)$$

$$N_A(x) = N_{A0} \left[1 - \exp\left(+\frac{x}{L}\right) \right] \quad \text{at } x < 0; \quad N_A(x) = 0 \quad \text{at } x \geq 0 \quad (4b)$$

$$N_{D0} = N_{A0} = 10^{16} \text{ cm}^{-3} \quad (4c)$$

These profiles are shown in Fig. 1 by blue and red curves, respectively. Note that the donor concentration only exists in the n-side and the acceptor concentration only exists in the p-side. The total impurity concentration $N_E(x)$ is strictly negative in the p-side and strictly positive in the n-side. This concentration is shown by a magenta curve. The point $x=0$ may be called *the metallurgical junction*. The present pn-junction is symmetric with regard to $N_E(x)$. However, this may be not the case in general. Another parameter of interest is L in Eq. (4a), which has the sense of the thickness of a metallurgical junction. We will choose $L = 10^{-5} \text{ cm} = 0.1 \text{ } \mu\text{m}$.

Note: We will denote by N_{D0} and N_{A0} the limiting values of doping concentrations at the terminations of the junction - the *terminal concentrations*.

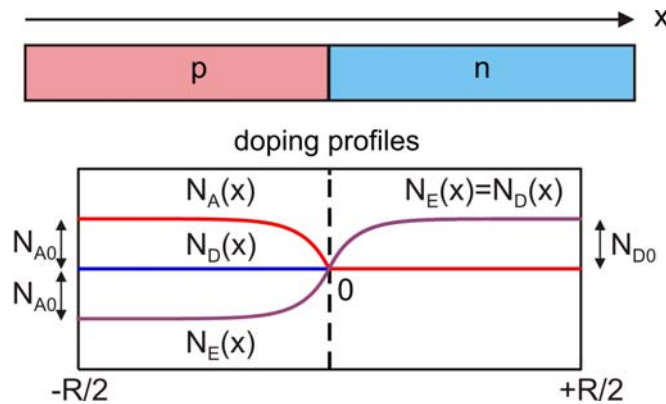


Fig. 1. Doping profiles $N_D(x)$ and $N_A(x)$, and the total impurity concentration $N_E(x)$ predicted by Eqs. (4).

Question: We now introduce the concentrations of electrons $n(x) > 0$ and holes $p(x) > 0$ along the junction. Both are measured in cm^{-3} , similar to doping profiles. Can these concentrations be expressed through the already given doping profiles?

Answer: That would be by far the easiest solution, but it is essentially wrong. The answer is yes only far away from the central region of the junction - the so-called *depletion region*. For this example we can write for majority carriers

$$x = -R/2 \Rightarrow p(x) \equiv p_{p0} \approx N_{A0} \quad (5)$$

$$x = +R/2 \Rightarrow n(x) \equiv n_{n0} \approx N_{D0} \quad (6)$$

However, the terminal concentrations of *minority carriers*, i.e. electrons in the p-side, n_{p0} , and holes in the n-side, p_{n0} , still remain unknown. Although very small, both these values are important. We cannot find them from Eq. (1), since doping has been introduced. Eq. (1) is legitimate for intrinsic Si,

$$p(x) = n(x) = n_i \quad (7)$$

but is no longer valid for the doped material. Something else must be used to find all the concentrations at the terminations. Moreover, we cannot even tell if Eqs. (5) and (6) are the exact expressions or not. In fact, they aren't.

2. Semiconductor equations

a. Electron and hole currents

The hole current density is equal to the number of positive carriers (holes) passing through a unit cross-section of the pn-junction from left to right in one second times the charge q of each carrier, and is measured in A/cm^2 . Similarly, the electron current density is the number of negative carriers (electrons) passing through a unit cross-section of the pn-junction from right to left in one second times the absolute charge q of each carrier.

The flow of holes and electrons is due to two reasons. The first reason is an electric field, either a built-in local electric field in the depletion region (already discussed in section 1 of Chapter 7, or an external applied electric field, or both. This situation is similar to a current in a DC circuit, where the flow of electrons is caused by an applied electric field of the DC power supply accelerating the charges up to certain constant velocities. The second and somewhat less expected reason is the sole mechanical *diffusion* of charged carriers in a semiconductor. The diffusion process is familiar to chemical and mechanical engineers, and material scientists, but to a lesser extent to electrical engineers. According

to W. Shockley (1952), the process of diffusion is a *basic one* in transistor electronics¹. In fact, the celebrated Shockley equation governing the semiconductor pn-junction is a direct derivative from the diffusion current. The electron and hole currents thus have two components each,

$$J_n = q\mu_n nE + qD_n \frac{dn}{dx} \quad (8a)$$

$$J_p = q\mu_p pE - qD_p \frac{dp}{dx} \quad (8b)$$

The first component is the conduction current in the electric field E , and the second component is the diffusion current. Here, μ_n and μ_p are the electron and hole *mobilities*, closely related to the total local conductivity of the doped specimen, $\sigma = q(\mu_n n + \mu_p p)$. When the electric potential is known, the electric field within the semiconductor material can be expressed as

$$E(x) = -\frac{d\phi}{dx} \quad (8c)$$

everywhere in the pn-junction. The diffusion constants D_n and D_p may be expressed precisely in terms of the mobilities using the Einstein relations

$$D_n = \left(\frac{kT}{q}\right)\mu_n = \mu_n V_T, \quad D_p = \left(\frac{kT}{q}\right)\mu_p = \mu_p V_T \quad (8d)$$

which were derived by A. Einstein based on very general assumptions. Here, k is the Boltzmann constant and T is the absolute temperature in K.

b. Transport equations

Now it is time to write down the system of semiconductor equations. The first two equations are the continuity equations that are again more familiar to material scientists and mechanical engineers: one equation for the holes and another equation for the electrons. In the steady-state case, one has

$$\frac{dJ_n}{dx} = +U - G_n \quad (9a)$$

$$\frac{dJ_p}{dx} = -U + G_p \quad (9b)$$

¹ W. Shockley, "Transistor electronics: imperfections, unipolar and analog transistors," *Proceedings of the I. R. E.*, Nov. 1952, pp. 1293.

Here, G_n and G_p are the external electron/hole *generation* rates caused by optical light or by other means. They are vital for photodetectors and solar cells, but are negligibly small in the present case. U is the *recombination* rate of holes/electrons. When an electron and a hole recombine, the conduction electron takes the place of the hole in the semiconductor lattice; both of them disappear from the number of free carriers. We will use a general nonlinear expression here

$$U(n, p) = \frac{pn - n_i^2}{\tau_p(n + n_i) + \tau_n(p + n_i)} \quad (9c)$$

that is known as the *Shockley-Read-Hall statistics*. Here, τ_n and τ_p are the average *lifetimes* of electrons and holes in the most important diffusion region of the pn-junction. Here, the lifetime means the time before the recombination. The lifetimes depend on doping concentrations. For minority carriers in silicon, $\tau_n \sim \tau_p \leq 10^{-3}$ s. For GaAs, $\tau_n \sim \tau_p \leq 10^{-8}$ s. After we integrate over x , Eqs. (9a) and (9b) state that a change in the flow of either carrier type through two boundaries of a certain volume in the pn-junction is solely due to sources or sinks of these carriers in the given volume.

Note: One not very serious analogy of Eq. (9a) and (9b) is the difference in the number of students coming to an auditorium and leaving it per unit time; this difference (if any) is equal to the number of students who perhaps fell asleep in the auditorium and were thus transformed from the active moving carrier state to a passive state ("recombined").

c. Poisson equation

The last equation, which closes the system of semiconductor equations, is the Poisson equation for the electric potential. A varying electric potential $\phi(x)$ exists along the junction. Hence, a varying electric voltage also exists along the junction, much as a varying electric voltage exists along the path in a DC circuit with a few resistor and/or power supply elements. However, unlike discrete voltage drops across each lumped element in the DC circuits, this voltage now changes from point to point in a pn-junction - a *continuous* variation. One might think of such a behavior as that of a DC circuit with many small elements closely tightened together. Thus, the electric potential $\phi(x)$ and the related junction voltage $\phi(+R/2) - \phi(-R/2)$ corresponding to Fig. 1 are no longer governed by the KVL equations studied in Chapter 1. Instead, we must use the Poisson equations known from electrostatic physics classes. This is the last junction equation. For the electric potential $\phi(x)$, the second-order Poisson Ordinary Differential Equation (ODE) has the form

$$\frac{d^2 \phi}{dx^2} = -\frac{\rho}{\epsilon}, \quad \rho = q(p - n + N_E), \quad N_E = N_D - N_A \quad (10)$$

where ε is the dielectric constant of the semiconductor under study, and, as before, q is the electron charge and N_E is the impurity concentration. In Si, $\varepsilon = 1.05 \times 10^{-12}$ F/cm; in GaAs, $\varepsilon = 1.14 \times 10^{-12}$ F/cm. If the total charge density ρ were constant, a solution to Eq. (10) would become straightforward. Eq. (10) is named in honor of Siméon-Denis Poisson (1781-1840), a French mathematician and physicist.

d. Model of the pn-junction

This model involves three independent unknown functions: electron concentration $n(x)$, hole concentration $p(x)$, and electric potential $\phi(x)$. Hence, it must include three independent equations. They are two transport equations (9) and Poisson's equation (10). Using the definition of the currents from Eqs. (8), one can write these equations together:

$$\frac{dJ_n}{dx} = +U(n, p), \quad J_n = q\mu_n \left[-n \frac{d\phi}{dx} + V_T \frac{dn}{dx} \right] \quad (11a)$$

$$\frac{dJ_p}{dx} = -U(n, p), \quad J_p = q\mu_p \left[-p \frac{d\phi}{dx} - V_T \frac{dp}{dx} \right] \quad (11b)$$

$$\frac{d^2\phi}{dx^2} = -\frac{\rho}{\varepsilon}, \quad \rho = q(p - n + N_E) \quad (11c)$$

In Eqs (11) we again have used the notation $V_T = kT/q$ for the thermal voltage. The reason for this will become clearer in the next subsection. Eqs. (11) are the most accurate equations for the pn-junction, with no assumptions or simplifications. Eq. (11a) is the second-order ODE vs. electron concentration, $n(x)$. One can recognize this fact by substituting the expression for the current into its derivative and performing the differentiation with respect to x . Similarly, Eq. (11b) is the second-order ODE vs. hole concentration $p(x)$. Finally, Eq. (11c) is the second-order ODE for the electric potential $\phi(x)$. Thus, we have a coupled system of three second-order ODEs for three unknown functions.

Note: After hard work with the model formulation it would be fair to obtain one simple yet useful result immediately. It is given by adding Eqs. (11a) and (11b) together; this yields

$$\frac{d(J_n + J_p)}{dx} = 0 \Rightarrow J = J_n + J_p = \text{const} \quad (12)$$

for the total J current in the pn-junction.

Note: Eqs. (11) are extremely difficult to solve. The nonlinearity is the major reason, but it is not the only reason. The hidden difficulty is that two different domains exist in the pn-junction, each with a very distinct solution behavior. One is a domain near the metallurgical junction - the depletion region. Parameters are quickly changed there and the electric fields are most important in this domain. This domain is somewhat similar to a shock wave domain in gas dynamics, familiar to aerospace engineers. The other domain is away from the metallurgical junction, where the diffusion dominates. The solution changes are slower there, but they eventually accumulate in space and lead to important consequences. A blind attempt to solve Eqs. (11), for example, with the built-in ODE solvers in MATLAB, will most likely fail for this reason.

3. Boundary conditions

We know from calculus that one second-order ODE needs two boundary conditions. Three second-order differential equations (19) thus need $3 \times 2 = 6$ boundary conditions. The boundary conditions may include three unknown functions and/or their derivatives. We will formulate these conditions with reference to Fig. 1.

a. Space-charge neutrality (SCN) law

The first pair of boundary conditions is given by the space-charge neutrality law in the vicinity of the pn-junction terminations. The total volume density of electric charges is the combination of four individual contributions: hole charges, electron charges, and the charges of ionized doping atoms (donors plus acceptors). Quantitatively

$$\rho = q(p - n + N_E), \quad N_E = N_D - N_A \quad (13)$$

Far away from the depletion region, the material must be electrically neutral, no matter what the doping concentrations are. This condition requires the right-hand side of Eq. (13) to be zero, i.e.

$$\rho = q(p - n + N_E) = 0 \quad \text{at} \quad x = \pm R/2 \quad (14a)$$

b. Mass-action law (carrier equilibrium)

Far away from the depletion region, where the doping profiles are constant, we should use the mass-action law, which states that the product of electron and hole concentrations is equal to the square of the intrinsic concentration of carriers in the undoped material, i.e.

$$pn = n_i^2 \quad \text{at} \quad x = \pm R/2 \quad (14b)$$

where n_i is the intrinsic concentration discussed at the beginning of this section. Eq. (14b) is the substitute for the simpler Eq. (7) in the undoped material. According to W.

Shockley (1952²), this equation is reminiscent of a mass-action law in chemistry in which the tendency of the reaction to go in one direction is proportional to the product of the concentrations of the reacting constituents. Eq. (14b) gives another pair of boundary conditions.

c. Boundary conditions for the electric potential

Two remaining boundary conditions are those for the electric potential, $\phi(x)$, across the junction. They must take into account an external *applied voltage* V . The voltage V is the open-circuit voltage of a circuit to be connected to the junction - see Fig. 2. It is also known as the *bias voltage*. Due to positive and negative ion charge layers in the depletion region, the pn-junction itself has a non-zero open-circuit voltage - the *built-in voltage* $\phi_{bi} = V_{bi}$ studied in Chapter 6.

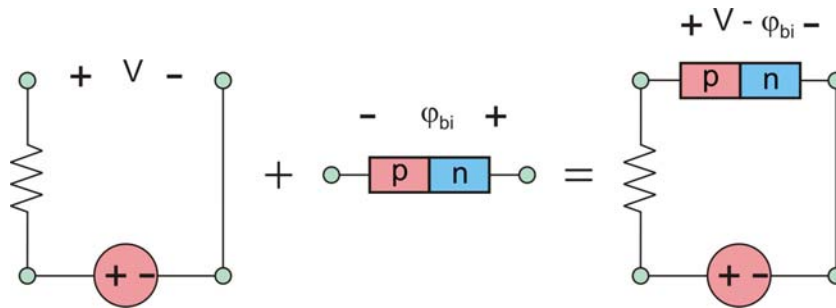


Fig. 2. The concept of voltage across the pn-junction.

Assuming positive voltage polarity on the p-side, the total junction voltage is given by the difference of two terminal potential values, $\phi(-R/2) - \phi(+R/2)$. The same voltage is also given by $V - \phi_{bi}$. Equating these two values, we have

$$\phi(-R/2) - \phi(+R/2) = V - \phi_{bi} \quad (14c)$$

which is the fifth boundary condition. The last boundary condition is trivial - the electric potential is defined to within a constant, so we may assign to it an arbitrary value at $x = +R/2$.

² W.Shockley, "Transistor electronics: imperfections, unipolar and analog transistors," *Proceedings of the I. R. E.*, Nov. 1952, p. 1299.

Question: How is the built-in voltage calculated?

Answer: We will show in the next subsection (see also Chapter 6) that (assuming that the terminal doping concentrations are much higher than the intrinsic concentration n_i) the built-in voltage of the pn-junction is given by

$$\phi_{bi} = V_T \ln \left(\frac{N_{A0} N_{D0}}{n_i^2} \right) \quad (15a)$$

when $N_D(x) = 0$ at $x \leq 0$, $N_A(x) = 0$ at $x \geq 0$. For the example from Fig. 1,

$$\phi_{bi} = V_T \ln \left(\frac{N_{D0}^2}{n_i^2} \right) \approx 0.71V \quad (15b)$$

One can see from Eq. (15a) that the built-in voltage is the sum of two logarithmic terms: one is due to acceptor concentration and another is due to donor concentration. Both donor and acceptor doping thus contribute to the built-in voltage. Therefore, Eq. (14c) may be rewritten in a more "symmetric" form:

$$\phi(-R/2) = V + V_T \ln \left(\frac{n_i}{N_{A0}} \right) \quad (16a)$$

$$\phi(+R/2) = -V_T \ln \left(\frac{n_i}{N_{D0}} \right) \quad (16b)$$

We will use these two boundary conditions instead of Eq. (14c), although this is a matter of personal preference.

Note: The boundary conditions (14a), (14b), and (16) are not unique. The number of boundary conditions must remain six, though. If it is less than six, the system of equations may have multiple solutions. If it is greater than six, a unique solution that satisfies all the boundary conditions may not exist.

Fig. 3 relates the boundary conditions formulated above to two sides of the pn-junction under study.

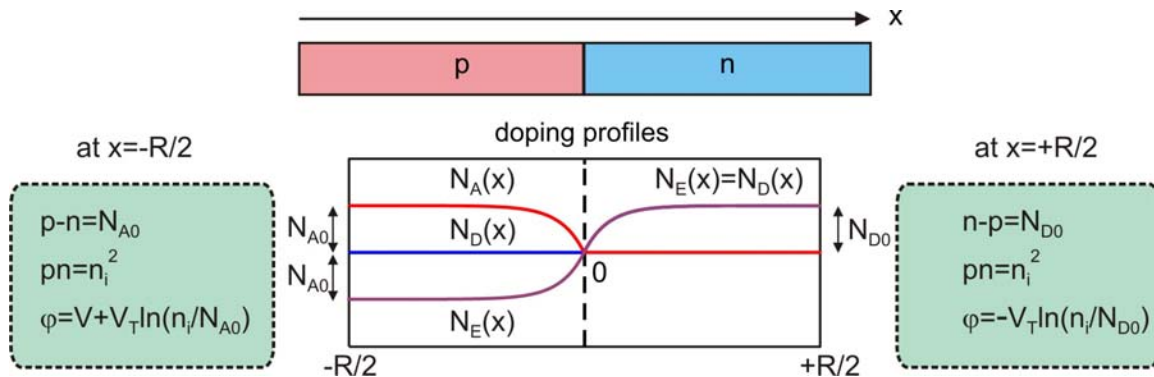


Fig. 3. The complete set of boundary conditions for the pn-junction.

Part II Exact solution for zero bias voltage

1. Analytical solution to junction equations

The result of this section

- is valid for an external bias voltage, V , equal to zero;
- is an *exact* mathematical solution to junction equations, which precisely satisfies all three Eqs. (11) and the six boundary conditions (14) to (16);
- is valid for arbitrary doping profiles.

Since there is no applied voltage, there should be no electric current through the junction. We therefore look for a solution in the form

$$J_p = 0, \quad J_n = 0 \quad \text{at} \quad -R/2 \leq x \leq R/2 \quad (17)$$

This requires that *both* the hole current and the electron current densities be equal to zero everywhere through the junction. Eq. (17) implies that the total current in the junction, which is given by the sum of the above expressions, is equal to zero, too.

Note: Eq. (17) is closely related to the physical principle of *thermal equilibrium*. Thermal equilibrium implies no net fluxes of any kind, including the net electric current, J , which must be zero. Since the last condition is the pn-junction at no bias voltage, we conclude that the unbiased junction is at thermal equilibrium. This principle of statistical mechanics says that each process and its opposite occur equally frequently, so that the flow of holes from the p-region to the n-region (if any), followed by recombination, must be exactly balanced by a reverse process. Thus, at thermal equilibrium, we must employ not only $J = J_p + J_n = 0$, but also $J_p = 0$, $J_n = 0$. If this were not the case, we would have electrons and holes moving in the same direction somewhere in a pn-junction - a rather strange result.

Substituting Eq. (17) into Eqs. (11a), (11b) and taking into account the definition of recombination rate Eq. (9c) yields

$$U(n, p) = 0 \Rightarrow pn = n_i^2 \quad \text{at} \quad -R/2 \leq x \leq R/2 \quad (19)$$

One can see that mass-action law is imposed not only as the terminal boundary condition, but also everywhere in the junction. The next step is to consider the expressions for the currents themselves; from Eqs. (11a) and (11b)

$$-n \frac{d\phi}{dx} + V_T \frac{dn}{dx} = 0 \Rightarrow n(x) = C_n \exp\left(\frac{+\phi(x)}{V_T}\right) \quad (20a)$$

$$-p \frac{d\phi}{dx} - V_T \frac{dp}{dx} = 0 \Rightarrow p(x) = C_p \exp\left(\frac{-\phi(x)}{V_T}\right) \quad (20b)$$

where C_p and C_n are two arbitrary integration constants. These constants may be cast in the form

$$n(x) = n_i \exp\left(\frac{\phi(x) - \phi_n}{V_T}\right) \quad \text{at} \quad -R/2 \leq x \leq R/2 \quad (21a)$$

$$p(x) = n_i \exp\left(\frac{\phi_p - \phi(x)}{V_T}\right) \quad \text{at} \quad -R/2 \leq x \leq R/2 \quad (21b)$$

where ϕ_n and ϕ_p are two alternative (normalization) constants. We will call these constants by a remarkable name - *Fermi potentials*.

Note: Eqs. (21) are none other than the Boltzmann statistics for electron and hole concentrations, which we first introduced in Chapter 6. In particular, Eq. (21a) for the electrons exactly coincides with the Boltzmann relation in plasma physics. In terms of the electric potentials, the Boltzmann statistics relate particle concentration not to the physical position, but rather, to the value of the potential at that position. Eq. (21b) in particular states that there are more hole carriers in a domain where ϕ is low (in the domain of low potential) and less holes in a domain where ϕ is high (the potential barrier). Alternatively, the concentration $p(x)$ may be related to the hole energy, E_i , in the corresponding electric field, since $\phi = -qE_i$.

Thus, the Boltzmann statistics is inherently included in the pn-junction equations, and does not have to be introduced separately.

Next, substitution of Eqs. (21) into Eq. (19) gives

$$\phi_p = \phi_n \quad (22)$$

Eqs. (11a) and (11b) are thus satisfied in full, and so are two boundary conditions (14b). Boundary conditions (14a) (space-charge neutrality conditions) yield

$$n - p = n - \frac{n_i^2}{n} = N_E = -N_{A0} \quad \text{at} \quad x = -R/2 \quad (23a)$$

$$n - p = n - \frac{n_i^2}{n} = N_E = +N_{D0} \quad \text{at} \quad x = +R/2 \quad (23a)$$

A solution of two quadratic equations in n gives

$$n = \frac{1}{2} \left[\sqrt{(N_{A0})^2 + 4n_i^2} - N_{A0} \right] \approx \frac{n_i^2}{N_{A0}}, \quad p \approx N_{A0} \quad \text{at} \quad x = -R/2 \quad (24a)$$

$$n = \frac{1}{2} \left[\sqrt{(N_{D0})^2 + 4n_i^2} + N_{D0} \right] \approx N_{D0}, \quad p \approx \frac{n_i^2}{N_{D0}} \quad \text{at} \quad x = +R/2 \quad (24b)$$

Here, we made the usual assumption that the terminal doping concentrations are much larger than the intrinsic concentration, $N_{A0}, N_{D0} \gg n_i$. This assumption corresponds to physical reality and in no way affects the accuracy of the solution itself. It may be avoided when necessary; the structure of the solution will not change.

Now, we require that the solution given by Eqs. (21) is consistent with terminal values from Eqs. (24). This gives

$$\exp\left(\frac{\varphi_p - \varphi(x)}{V_T}\right) = \frac{N_{A0}}{n_i} \quad \text{at } x = -R/2 \quad (25a)$$

$$\exp\left(\frac{\varphi(x) - \varphi_n}{V_T}\right) = \frac{N_{D0}}{n_i} \quad \text{at } x = +R/2 \quad (25a)$$

It follows from these two equations that

$$\varphi(-R/2) - \varphi(+R/2) = -\varphi_{bi} \quad \text{where } \varphi_{bi} = V_T \ln\left(\frac{N_{A0}N_{D0}}{n_i^2}\right) \quad (26)$$

Thus, we have not only satisfied the remaining boundary condition (14c) at $V = 0$ but also *derived* the value of the built-in potential, which was introduced in the previous subsection. We can also satisfy Eqs. (16) at $V = 0$ by letting

$$\varphi_p = \varphi_n = 0 \quad (27)$$

2. Numerical solution for the electric potential

The last step in the solution is to find the electric potential that satisfies the Poisson equation (10) when the carrier concentrations are given by Eqs. (21) and the boundary conditions are those of Eqs. (16). Analytical solutions exist for abrupt doping profiles and some other profiles. For more realistic doping profiles, this step requires a numerical solution to the Poisson equation with the boundary conditions Eqs. (16).

The numerical solution may be obtained in a number of ways. In particular, the standard MATLAB package has a number of powerful ODE solvers, which could handle the present problem. However, one intuitive way is an iterative solution. This solution starts with a certain initial guess for the potential and continues until the residual error becomes reasonably small. An example that follows illustrates the iterative solution.

Example: We will now obtain a solution for the base example shown in Fig. 1 and described in subsection 1 at zero bias voltage $V = 0$ and for arbitrary doping profiles. We need to find the potential in Eqs. (21) solving the Poisson equation. An initial guess is given by a potential $\varphi_s(x)$. The initial guess (which also satisfies the required boundary conditions!) is obtained if, rather than using the Poisson equation, we use a much simpler space-charge neutrality model,

$$\rho = q(p - n + N_E) = 0 \text{ at any } x \quad (27)$$

instead. We substitute Eqs. (21) with $\varphi(x) = \varphi_s(x)$ into that model and solve for $\varphi_s(x)$. This is, indeed, a wrong solution, since Eq. (27) is valid only at terminations, not for any x . However, it is an acceptable initial guess, and it satisfies the required boundary conditions. Next, we integrate two times in the Poisson's equation and rewrite it in the following integral form

$$\varphi(x) = F(x) + C_1 + (x + R/2)C_2 \quad (28a)$$

$$F(x) = \int_{-R/2}^x dx' \int_{-R/2}^{x'} dx'' \left[-\frac{q}{\epsilon} (p(\varphi(x'')) - n\varphi(x'') + N_E(x'')) \right] \quad (28b)$$

To satisfy the boundary conditions, the integration constants are chosen in the form $C_1 = \varphi_s(x = -R/2)$ and $C_2 = (-C_1 - F(x = R/2) + \varphi_s(R/2))/R$. We solve Eqs. (28) iteratively, i.e. finding the next approximation using the previous one

$$\varphi_n(x) = F(\varphi_{n-1}) + C_1 + (x + R/2)C_2(\varphi_{n-1}) \quad (29a)$$

Then we find the relative error of the iterative solution $\|\varphi_n(x) - \varphi_{n-1}(x)\|/\|\varphi_n(x)\|$ at a given step and compare it to a predefined value of, say, 1%. If the error is higher, we condition the next iteration using a Jacobi iteration process:

$$\varphi_n(x) = J\varphi_n(x) + (1 - J)\varphi_{n-1}(x), \quad J \ll 1 \quad (29b)$$

and continue the process for $n+1$. This iteration process converges quite well if J is small. Fig. 4 shows the solution for the example from Fig. 1. A Si pn-junction is considered with the total length $R = 2 \times 10^{-4}$ cm and with the doping profiles from Eqs. (4). The plots give the doping profiles, the concentration profiles, the electric potential, charge density ρ , and the electric field through the specimen, including the depletion region where there is a significant electric field. The initial guess for the solution is shown by dashed green curves. The solution is generated by the MATLAB script `pn_junction1.m` in this section.

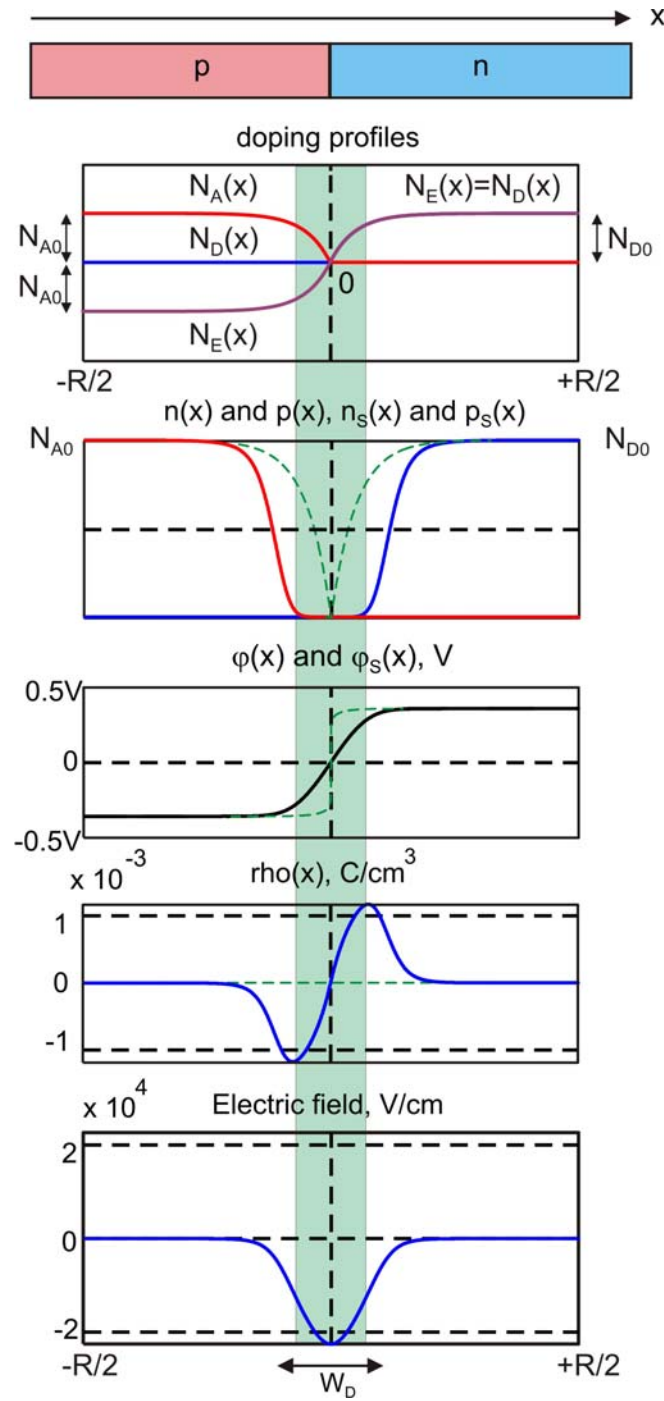


Fig. 4. Doping profiles, concentration profiles, electric potential ϕ , charge density ρ , and electric field E through the specimen including the depletion region where there is a significant electric field. An exact solution for a symmetric Si pn-junction with $N_{A0} = N_{D0} = 10^{16} \text{ cm}^{-3}$ and total length $R = 2 \times 10^{-4} \text{ cm}$ at zero bias voltage is given. The initial guess - the approximate solution $n_s(x)$, $p_s(x)$, $\phi_s(x)$ at space-charge neutrality is shown by dashed green curves. A green rectangle shows the width of the depletion region - see the next section.

Part III Approximate solutions

1. General solution to pn-junction equations

In the following subsections we shall discuss a general solution to the pn-junction equations, for any applied bias voltage. Knowledge of quasi-Fermi potentials is quite useful in establishing the form of the general solution. In this subsection, we will introduce the quasi-Fermi potentials only from the formal point of view, as certain useful new variables for the pn-junction equations. The physical meaning of these potentials will be briefly discussed at the end of this section.

a. Quasi-Fermi potentials - a key to general solution

Let us go back to the solution for the zero bias voltage performed in Part II. We have found that the exact solution at zero bias voltage has the form of Eqs. (21) of the previous section. We rewrite the equations here for convenience

$$n(x) = n_i \exp\left(\frac{\varphi(x) - \varphi_n}{V_T}\right) \quad \text{at} \quad -R/2 \leq x \leq R/2 \quad (1a)$$

$$p(x) = n_i \exp\left(\frac{\varphi_p - \varphi(x)}{V_T}\right) \quad \text{at} \quad -R/2 \leq x \leq R/2 \quad (1b)$$

Eqs. (1) relate the concentrations $n(x), p(x)$ to the electric potential. Thus, only one independent variable remains out of three: $\varphi(x)$. Two integration constants that have been obtained here, φ_n and φ_p , were called Fermi potentials.

In a general case of non-zero bias voltages, either positive or negative, the currents J_n and J_p are no longer zero³. Eqs. (1) are thus no longer valid. However, by analogy with Eqs. (1), we still may seek an *exact* solution to the pn-junction equations in the form

$$n(x) = n_i \exp\left(\frac{\varphi(x) - \varphi_n(x)}{V_T}\right) \quad \text{at} \quad -R/2 \leq x \leq R/2 \quad (2a)$$

$$p(x) = n_i \exp\left(\frac{\varphi_p(x) - \varphi(x)}{V_T}\right) \quad \text{at} \quad -R/2 \leq x \leq R/2 \quad (2b)$$

where the two constants now become two unknown functions, $\varphi_n(x)$ and $\varphi_p(x)$. Eqs. (2) are equivalent to a *change in variables* in the semiconductor equations. Now, instead

³ A very small but finite reverse current may still flow in the pn-junction at negative applied voltages.

of two unknown concentrations and the electric potential, we may use $\varphi_n(x)$, $\varphi_p(x)$, and the electric potential as *three* required independent variables, i.e.

$$n(x), p(x), \varphi(x) \Rightarrow \varphi_n(x), \varphi_p(x), \varphi(x) \quad (3)$$

The functions $\varphi_n(x)$ and $\varphi_p(x)$ are called *quasi-Fermi potentials* or *imrefs*, according to Enrico Fermi himself. As the name implies, these functions hold a significant physical meaning and are not just new variables introduced solely for our mathematical convenience. This meaning will be briefly discussed at the end of this Part.

Note: One remarkable result may be seen right away. We substitute Eqs. (2) into the expressions for the electric current in pn-junction and, after differentiation, obtain

$$J_n = q\mu_n \left[-n \frac{d\varphi}{dx} + V_T \frac{dn}{dx} \right] = -q\mu_n n(x) \frac{d\varphi_n(x)}{dx} \quad (4a)$$

$$J_p = q\mu_p \left[-p \frac{d\varphi}{dx} - V_T \frac{dp}{dx} \right] = -q\mu_p p(x) \frac{d\varphi_p(x)}{dx} \quad (4b)$$

When the quasi-Fermi potentials are exactly constant, as they are in the case for the zero bias voltage, the electron and hole currents, and hence, the total current through the pn-junction, are exactly zero. When the quasi-Fermi potentials vary with distance, slowly or quickly, an electric current will flow. This is a short, yet impressive, demonstration of their significance.

b. Boundary conditions

The boundary conditions are given by Eqs. (14) of Part II - see Fig. 3 of Part II. We will rewrite them here in a more convenient form, keeping in mind the quasi-Fermi potentials. We need to check boundary conditions for $n(x)$ and $p(x)$ first. Those boundary conditions are the space-charge neutrality law (14a) and the mass-action law (14b) from Part II. The simultaneous use of these two laws leads to

$$n - p = n - \frac{n_i^2}{n} = N_E = -N_{A0} \quad \text{at} \quad x = -R/2 \quad (5a)$$

$$n - p = n - \frac{n_i^2}{n} = N_E = +N_{D0} \quad \text{at} \quad x = +R/2 \quad (5b)$$

These equations appear to be identical with Eqs. (23) of Part II for the terminal concentrations at the zero bias voltage. This is no wonder, since the boundary condition

for the electric potential is not yet involved. The solution to Eqs. (5) is also identical to the corresponding result for the zero bias voltage Eqs. (24) of Part II, i.e.

$$n \approx \frac{n_i^2}{N_{A0}}, \quad p \approx N_{A0} \quad \text{at} \quad x = -R/2 \quad (6a)$$

$$n \approx N_{D0}, \quad p \approx \frac{n_i^2}{N_{D0}} \quad \text{at} \quad x = +R/2 \quad (6b)$$

under the assumption that the terminal doping concentrations are much larger than the intrinsic concentration, $N_A^{p0}, N_D^{n0} \gg n_i$. Eqs. (6) are necessary and sufficient boundary conditions for the concentrations.

Note: For the drill example of this section, the ratio $n_i / N_{D0} = n_i / N_{A0} \approx 10^{-6}$. The relative error of Eqs. (6) has the same small magnitude. Therefore, we may consider Eqs. (6) and other similar expressions that follow as exact equalities.

Now, we are in position to establish the boundary conditions for the quasi-Fermi potentials. We plug Eqs. (2) into Eqs. (6) and obtain

$$\exp\left(\frac{\varphi(x) - \varphi_n(x)}{V_T}\right) = \frac{n_i}{N_{A0}}, \quad \exp\left(\frac{\varphi_p(x) - \varphi(x)}{V_T}\right) = \frac{N_{A0}}{n_i} \quad \text{at} \quad x = -R/2 \quad (7a)$$

$$\exp\left(\frac{\varphi(x) - \varphi_n(x)}{V_T}\right) = \frac{N_{D0}}{n_i}, \quad \exp\left(\frac{\varphi_p(x) - \varphi(x)}{V_T}\right) = \frac{n_i}{N_{D0}} \quad \text{at} \quad x = +R/2 \quad (7b)$$

Taking the natural log of both sides in every expression in Eqs. (7) and performing multiplication (when necessary) gives an elegant result

$$\varphi_n = \varphi_p, \quad \varphi_p = \varphi - V_T \ln\left(\frac{n_i}{N_{A0}}\right) \quad \text{at} \quad x = -R/2 \quad (8a)$$

$$\varphi_n = \varphi_p, \quad \varphi_p = \varphi + V_T \ln\left(\frac{n_i}{N_{D0}}\right) \quad \text{at} \quad x = +R/2 \quad (8b)$$

The boundary values of the electric potential are known from Eqs. (16) of Part II. We can use these equations and obtain the boundary conditions for the quasi-Fermi potentials in the form

$$\varphi_n = \varphi_p = V \quad \text{at} \quad x = -R/2 \quad (9a)$$

$$\varphi_n = \varphi_p = 0 \quad \text{at} \quad x = +R/2 \quad (9b)$$

Note: What could be simpler than boundary conditions given by Eqs. (9)? This is one more advantage of the quasi-Fermi potentials.

Note: After the change in variables $n(x), p(x), \varphi(x) \Rightarrow \varphi_n(x), \varphi_p(x), \varphi(x)$ is made, the boundary conditions (6) are to be replaced by Eqs. (9). The boundary conditions for the potential remain Eqs. (16) of Part II. After that, we may apply a general numerical method and solve the full semiconductor equations, either for a pn-junction or for a bipolar-junction transistor.

c. Behavior of quasi-Fermi potentials through the junction

With the boundary conditions given by Eqs. (9) in mind, we can establish a qualitative behavior of the quasi-Fermi potentials through the pn-junction. Fig. 5 shows the result at a certain positive bias voltage. The potentials in Fig. 5 must satisfy Eqs. (9), which they clearly do. Furthermore, according to Eqs. (4), the derivative of the quasi-Fermi potential $\varphi_n(x)$ at the end of the p-side determines the terminal current of minority carriers (electrons), J_n , on that side. Similarly, the derivative of the quasi-Fermi potential $\varphi_p(x)$ at the end of the n-side determines the terminal current of minority carriers (holes), J_p , on the n-side. These derivatives must be fairly large, perhaps significantly larger than shown in the figure, to compensate for small concentrations of minority carriers.

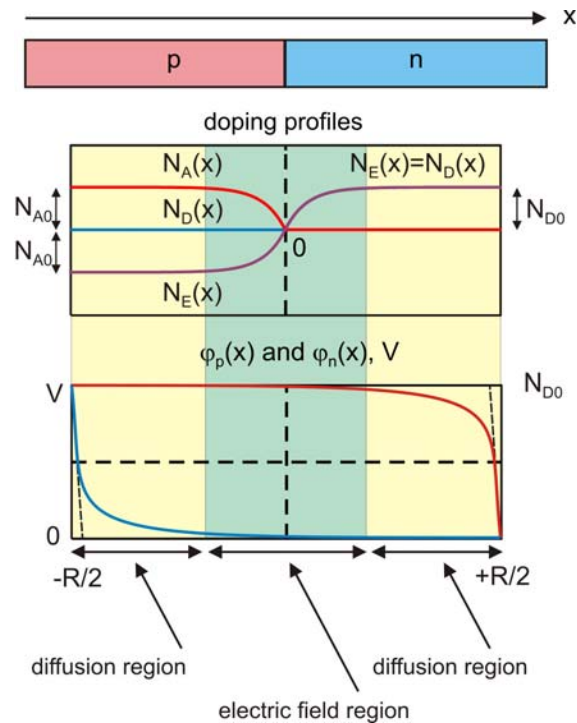


Fig. 5. Qualitative behavior of $\varphi_n(x)$ (blue curve) and $\varphi_p(x)$ (red curve) through the pn-junction for a positive bias voltage.

d. Electric field region and its approximation

Looking at Fig. 5 we can immediately recognize one very useful approximation for the electric field region $-R_E/2 < x < R_E/2$, namely

$$\varphi_n = 0, \quad \varphi_p = V = \text{const} \quad (10)$$

In other words, the quasi-Fermi potentials are approximately constant in the region. This allows us to reduce the general solution given by Eqs. (5) to

$$n(x) = n_i \exp\left(\frac{\varphi(x)}{V_T}\right) \quad \text{at} \quad -R_E/2 \leq x \leq R_E/2 \quad (11a)$$

$$p(x) = n_i \exp\left(\frac{V - \varphi(x)}{V_T}\right) \quad \text{at} \quad -R_E/2 \leq x \leq R_E/2 \quad (11b)$$

Also, we have the Poisson equation for the electric potential,

$$\frac{d^2 \varphi}{dx^2} = -\frac{\rho}{\varepsilon}, \quad \rho = q(p - n + N_E) \quad (12)$$

augmented with the corresponding boundary conditions from Eqs. (16) of Part II, which we rewrite here for convenience:

$$\varphi = V + V_T \ln\left(\frac{n_i}{N_{A0}}\right) \quad \text{at} \quad x = -R_E/2 \quad (13a)$$

$$\varphi = -V_T \ln\left(\frac{n_i}{N_{D0}}\right) \quad \text{at} \quad x = +R_E/2 \quad (13b)$$

Eqs. (11)-(13) give the conventional pn-junction approximation for the electric field region. According to Chawla and Gummel⁴, this approximation is excellent for reverse (or negative) bias voltages and does not cause any serious error in calculating the junction capacitance of the pn-junction at forward bias voltages.

However, according to the same authors, this approximation "loses validity insofar as the calculation of current is concerned". Both electron and hole currents appear to be exactly zero from the formal point of view, which is indeed wrong. Since we will find the electric current separately, from the approximation for the diffusion region, this drawback of the electric field region model is of lesser concern.

⁴ B. R. Chawla and H. K. Gummel, "Transition region capacitance of diffused p-n junction," *IEEE Trans. on Electron Devices*, vol. ED-18, no. 3, March 1971.

Note: For the electric field region, it makes sense to extend the computational domain from $-R_E/2 < x < R_E/2$ to $-R/2 < x < R/2$ since the electric field is zero outside the region and the solution accuracy will not change. In this case, we do not need to worry about the specific value of R_E .

Note: Multiplying Eqs. (11a) and (11b), we can see that the mass-action law at equilibrium - Eq. (11b) - is now transformed to

$$pn = n_i^2 \exp\left(\frac{V}{V_T}\right) \quad (14)$$

within the electric field region. Physically, Eq. (14) means that the individual concentrations $n(x)$ and $p(x)$ increase in the vicinity of the depletion region as the bias voltage increases: the potential barrier is lowered and more carriers can penetrate the depletion region. Eq. (17) will be critical in establishing inner boundary conditions for the diffusion layer.

Question: Why do we need the approximation of the electric field region (and of the diffusion region)?

Answer: It is worthwhile for one simple reason. We may obtain the general solution for the pn-junction as a *combination of two separate solutions*, one for the electric field region and another for the diffusion region. The two separate solutions are simpler than one solution of three simultaneous equations. It appears that in the electric field region we solve only *one* (Poisson) equation. In the diffusion region, we solve only *two* (diffusion) equations. Moreover, a solution to each of the diffusion equations is obtained analytically. Therefore, we will never need to solve three simultaneous nonlinear partial differential equations and perhaps lose the sense of the problem behind heavy mathematical calculations.

2. Solution to the electric field region

We will now solve the approximation of the electric field region given in the previous subsection, using Eqs. (11)-(13). This approximation, though not exact, holds for both negative and positive values of the applied bias voltage. The solution is very similar to the solution for the zero bias voltage. The Poisson equation is solved again, and the transport equations are again ignored. There are two differences, however. First, the non-zero bias voltage appears in boundary conditions (13) of Part II for the voltage. Second, after the solution is obtained, we should substitute the non-zero voltage value into the expressions for concentrations Eqs. (11).

Example: We will now obtain a solution for the base example shown in Fig. 1 of Part II at arbitrary values of bias voltage in the range $-5V < V < 0.8V$ and for arbitrary doping profiles. The iterative numerical method described in Part II for zero bias voltage is again used here. The difference is in the initial guess $\varphi_s(x)$, in the boundary conditions, which now include the bias voltage, and in the expressions for concentrations, which satisfy Eq. (14), but not the mass-action law. The initial guess also satisfies Eq. (14) instead of the mass-action law, the SCN model, and the boundary conditions Eqs. (13). The expression for the initial guess is given by equations similar to those in Part II

$$n_s(x) = \frac{1}{2} \left[\sqrt{(N_E(x))^2 + 4n_i^2 \exp\left(\frac{V}{V_T}\right)} + N_E(x) \right] \quad (15a)$$

$$p_s(x) = n_s(x) - N_E(x) \quad (15b)$$

$$\varphi_s(x) = V_T \ln \frac{n_s(x)}{n_i} \quad (15c)$$

Since the electric potential across the junction $\varphi(x)$ hardly changes at larger positive bias voltages, it makes sense to use the charge density, $\rho(x)$, to control the convergence of the iteration process. The relative convergence error is less than 1% when $\|\rho_n(x) - \rho_{n-1}(x)\| / \|\rho_n(x)\| \leq 0.01J$. The weight factor J is now 0.0001; up to 30,000 iterations may be required to obtain an accurate solution.

Fig. 6 shows the corresponding results generated by the MATLAB script `pn_junction2.m` in this section. This figure gives concentrations, electric potential, charge density, and the electric field for the example of this section found using the approximation for the electric field region Eqs. (11)-(13). Five different curves correspond to five different bias voltages of $V = -1.0, -0.5, +0.0, +0.5, +0.7$ V.

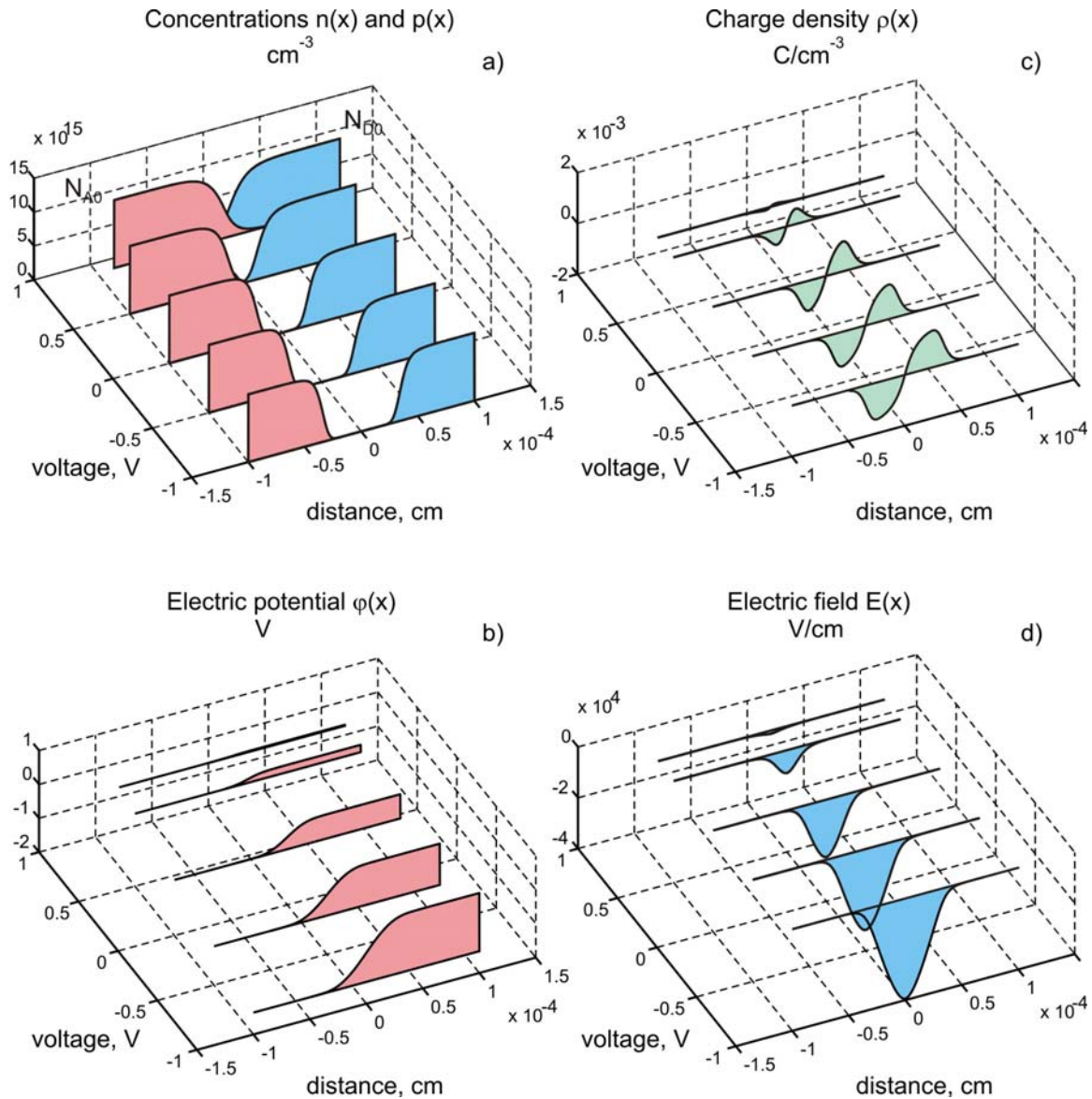


Fig. 6. Carrier concentrations, electric potential, charge density, and the electric field for the example of this section found using the approximation of the electric field region, Eqs. (14)-(16). Five different curves correspond to five bias voltages $V = -1.0, -0.5, +0.0, +0.5, +0.7$ V.

Note: Approximation of the electric field region predicts a constant offset for the concentrations once the bias voltage is equal to or exceeds the built-in voltage of the pn-junction given by Eq. (12b). This situation may be seen in Fig. 6. Although this offset hardly affects the parameters of the electric field, care should be taken with the resulting concentrations.

Note: Fig. 6a clearly demonstrates how the depletion region is filled with carriers when the bias voltage increases and reaches the built-in voltage. On the other hand, the voltage drop across the junction becomes virtually zero in Fig. 6b.

At small and, especially, negative bias voltages, the pn-junction still has positive and negative ion charge layers, as shown in Fig. 6c, and the built-in electric field in between those layers, which is shown in Fig. 6d. Furthermore, no electric current flows through the junction. This means that the pn-junction becomes a *capacitor*.

What is an advantage of the pn-junction as a capacitor? Well, as we can see from Fig. 6, the charge density in the pn-junction capacitor varies with the applied bias voltage. Therefore, the capacitance value will also change with the applied voltage. We thus obtain a variable capacitor or a *varactor*, and we can control its capacitance value electronically, by the applied bias voltage.

HW#16 Varactor diode

Dynamic capacitance

The junction (or depletion-layer) capacitance is, by definition, given by a general electrostatic expression

$$C = \frac{\Delta Q}{\Delta V} \quad (1a)$$

where Q is the total positive charge in the junction, V is the applied bias voltage, and ΔQ denotes a change in the positive charge around Q when the voltage increases from V to $V+\Delta V$. The density of positive charges, $\rho^+(x)$, in space should be used to find the total positive charge, i.e.

$$\rho^+(x) = q(p(x) - n(x) + N_E(x)) \quad \text{when} \quad p - n + N_E > 0 \quad (1b)$$

However, since $N_E(x)$ does not change with the applied voltage, only the hole concentration contributes to the change of the total positive charge, that is

$$Q = \int_{-R/2}^{R/2} \rho^+(x) dx \Rightarrow \Delta Q = \Delta \int_{-R/2}^{R/2} \rho^+(x) dx = \Delta \int_{-R/2}^{R/2} p(x) dx \quad (1c)$$

Since we know the solution for $p(x)$ for every applied voltage V , we just run the solution twice, for V and $V+\Delta V$ (ΔV is typically small, about 0.01V), find two integrals of sole hole concentrations, subtract one from another and divide the result by ΔV . The junction capacitance is then found.

Task

A MATLAB script `pn_junction3.m` constructed by you shall implement the electric field region solution and Eqs. (1) for finding the junction capacitance. The MATLAB script `pn_junction2.m` provided to you should serve as a starting point.

Approximate analytical model

The junction capacitance found from the abrupt junction model is given by

$$C = \frac{\epsilon}{W} \quad (2a)$$

where ϵ is the dielectric constant (of Si) and W is the width of the depletion layer. For nonzero bias voltages, there exists an estimate:

$$W = \sqrt{\frac{2\epsilon}{q} \frac{(N_{A0} + N_{D0})}{N_{A0}N_{D0}}} (\phi_{bi} - V) \quad (2b)$$

$$\text{where } \phi_{bi} = V_T \ln \left(\frac{N_{A0}N_{D0}}{n_i^2} \right).$$

HW exercise

The task of this exercise is to compare the approximate theory model for the junction capacitance (depletion-layer capacitance) given by Eqs. (2) with an exact numerical result obtained with your MATLAB script `pn_junction3.m`.

We shall use the parameters for the base example in Part I, choose $-5V \leq V \leq 0.6V$, and plot two curves for the capacitance (analytical one and numerical one) versus the bias voltage in that range. The units for the capacitance are nF per cm^2 .