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Numerical simulation of nonlinear processes in semiconductor devices with the application of the Newton's method for linearization

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Abstract. This article relates to the use of Newton's method and Scharfetter–Gummel scheme, to linearize and discretize the equations, for numerical modeling of nonlinear processes in semiconductor devices. The mathematical model of the problem represents a system of nonlinear differential equations, in the unknowns φ–electrostatic potential, n, p–the concentrations of electrons and holes, respectively. The problem is further complicated by the fact that the boundary conditions are of two types: the Dirichlet conditions and the Neumman conditions, which act on different portions of the boundary. The subproblems that were solved in this paper: linearization of nonlinear differential equations, using Newton's method; discretization of equations, using Scharfetter–Gummel scheme. The obtained systems have five diagonal and nonsymmetrical matrices. The numerical method of Bi–Conjugate Gradients was used to solve the systems.

Mathematics subject classification: 34C05, 58F14.
Keywords and phrases: nonlinear processes, semiconductor devices, Scharfetter-Gummel scheme, Newton's linearization.

Simulation of semiconductor devices has been and remains to be a current problem, with a wide range of application results, obtained from experiments on the simulation models.

The simulation of semiconductor devices involves several steps: the mathematical formulation of the problem, the discretization of nonlinear differential equations, the linearization of nonlinear equations, solving the algebraic systems.

The mathematical formulation of semiconductor devices is described extensively in the literature [1, 2]. The discretization steps and solving of the algebraic systems will be briefly described in this article.

1 Mathematical formulation of the semiconductor device problem, based on the Drift–Diffusion Model (DDM)

We consider one of the models of a semiconductor diode (Figure 1). A diode consists of two regions, with different types of doping: the hole area (p–type area), with a dominant concentration of holes and the electron area (n–type area), with a dominant concentration of electrons.

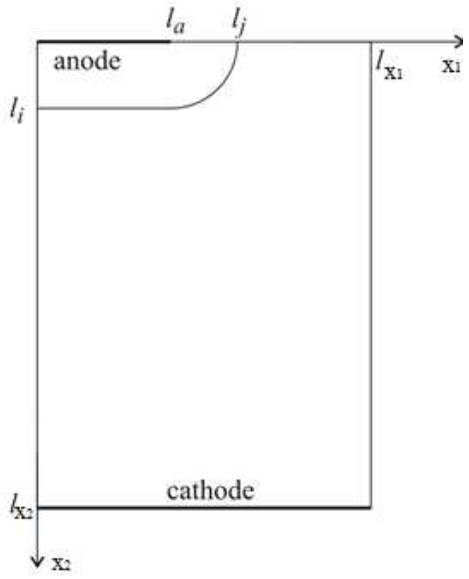

Figure 1. *Two-dimensional representation of the semiconductor diode*

The anode electrode is connected to the p–type area and the cathode is connected to the n–type area. Impurities, added to the semiconductor material, determine the type of conductivity of each area. In semiconductor physics the concentration of impurities is denoted by N. The function

$$N(x_1, x_2) = N_D^+(x_1, x_2) - N_A^-(x_1, x_2)\ m^{-3}$$

defines the profile of impurities and is expressed by the concentration of ionized donors and acceptors, denoted by N_D^+ and N_D^-, respectively. The negative value of $N(x_1, x_2)$ is determined by the dominance of boron acceptor atoms (p–type semiconductor) and a positive value is determined by the domination of phosphorus donor atoms (n–type semiconductor).

The mathematical formulation, of the semiconductor device problem, is described extensively in the literature [1–3]. One of the mathematical models is given by a set of equations with three unknown functions: φ–the electrostatic potential, n, p–the concentrations of electrons and holes, respectively. The functions φ, n, p satisfy the following system of nonlinear differential equations:

$$-\nabla \cdot (\varepsilon \nabla \varphi) = q(p - n + N); \tag{1.1}$$
$$-\nabla \cdot (J_n) = -q(R_{SRH} + R_{AUG}); \tag{1.2}$$
$$\nabla \cdot (J_p) = -q(R_{SRH} + R_{AUG}); \tag{1.3}$$
$$J_n = q\mu_n nE + qD_n \nabla n; \tag{1.4}$$
$$J_p = q\mu_p pE - qD_p \nabla p; \tag{1.5}$$
$$E = -\nabla \varphi. \tag{1.6}$$

Here E is the intensity vector of electric field, ε is the dielectric constant, q is the (positive) electron charge ($q = 1.602176565 \cdot 10^{-19}\ C$), D_n and D_p are the electron and hole coefficients of diffusion, N is the so-called doping profile, J_n and J_p are the electron and hole current densities, R_{SRH}, R_{AUG} represent the Shockley-Hall and Auger recombination rates, μ_n, μ_p are the electron and hole carrier mobilities.

Also $\varepsilon = \varepsilon_r \cdot \varepsilon_0$ is the absolute permitivity (dielectric constant), ε_r is the relative permittivity, ε_0 is the electrical constant ($\varepsilon_0 = 8.854187817 \cdot 10^{-12}\ F \cdot m^{-1}$), n and p are the concentrations of electrons and holes, n_i is the concentration of electrons and holes in its own semiconductor; $\varphi_T = k_B T/q$ is thermal voltage, k_B is constant of Boltzmann ($k_B = 1.3806488 \cdot 10^{-23} J/K$) and T is temperature (K).

Connections, between diffusion coefficients D_n, D_p and mobilitie μ_n, μ_p, for electrons and holes, respectively, are given by Einstein relations:

$$D_n/\mu_n = (k_B T)/q = \varphi_T,\ D_p/\varphi_p = (k_B T)/q = \varphi_T \qquad (1.7)$$

Any diode is made of silicon. The input parameters of the problem have the following values: $n_i = 1.46 \cdot 10^{16}\ m^{-3},\ \mu_n = 0.08\ m^2/(V \cdot s),\ \mu_p = 0.02\ m^2/(V \cdot s)$, $\varepsilon_r = 11.8,\ \varphi_T = 0.026V$ at room temperature $T = 300K$.

The functions R_{SRH} and R_{AUG} are defined by the following formulas:

$$R_{SRH}(n,p) = \frac{(pn - n_i^2)}{((\tau_p(n+n_i) + \tau_n(p+n_i))}, \qquad (1.8)$$
$$R_{SRH}(n,p) = (pn - n_i^2)(C_n n + C_p p)$$

here τ_n and τ_p signify the times of existence of the carriers ($\tau_n = \tau_p = 0.1 \cdot 10^{-6}\ s$); C_n and C_p are Auger coefficients ($C_n = 1.1 \cdot 10^{-42}\ m^6 s^{-1}$, $C_p = 0.3 \cdot 10^{-42} m^6 s^{-1}$, at $T = 300K$). The function N, in the field of search for the solution, is represented by the Gaussian function G:

$$N = N_{Dn} + N_{Dnmax} G(x_1, -x_2, \infty, l_{x_2}, \alpha) - N_{A_{pmax}} G(x_1, x_2, l_a, 0, \alpha) \qquad (1.9)$$

here N_{Dn} is the alloying epitaxial layer of the semiconductor, N_{Dnmax} is the alloying substrate, N_{Apmax} is the maximum value of implantation of the diffusion profile, G is the Gaussian function [5].

$G(x_1, x_2, a, b, \alpha) =$

$$= \begin{cases} exp[-((x_1-a)/\alpha)^2] \cdot exp[-((x_2-b)/\alpha)^2], & x_1 > a,\ x_2 > b \\ exp[-((x_1-a)/\alpha)^2], & x_1 > a,\ x_2 \leqslant b \\ exp[-((x_2-b)/\alpha)^2], & x_1 \leqslant a,\ x_2 > b \\ 1, & x_1 \leqslant a,\ x_2 \leqslant b \end{cases} \qquad (1.10)$$

The constants in formula (1.9), in the field of search for the solution (Figure 2), have the following values:

$$N_{D_n} = 10^{17} m^{-3},$$
$$N_{D_{nmax}} = 10^{19} m^{-3},$$
$$N_{Apmax} = 10^{19} m^{-3},$$
$$\alpha = 0.5 \cdot 10^{-6} m,$$
$$l_{x_1} = 5 \cdot 10^{-6} m,$$
$$l_{x_2} = 7 \cdot 10^{-6} m,$$
$$l_a = 2 \cdot 10^{-6} m,$$
$$l_i = l_j = 1 \cdot 10^{-6} m.$$

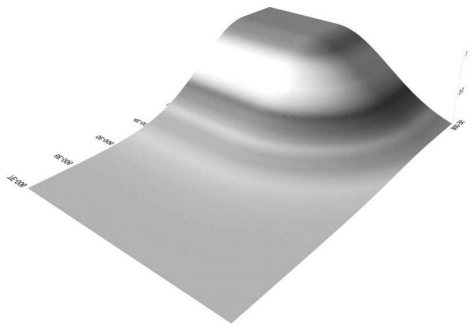

Figure 2. *The surface of the Gaussian function for* $a = 2 \cdot 10^{-6},\ b = 1 \cdot 10^{-6},\ \alpha = 2 \cdot 10^{-6}$

Boundary conditions

It is considered that the cathode is connected to ground ($V_c = 0$) and an external voltage $V_a > 0$ is applied to the anode. Then on the boundary Γ_D (thicker boundary), the functions $\varphi,\ n,\ p$ satisfy the relations:

$$\varphi(\bar{x}) = V_a + \varphi_T * ln\left((N + \sqrt{N^2 + 4n_i^2})/(2n_i)\right);$$
$$n(\overline{x}) = \left(N + \sqrt{N^2 + 4n_i^2}\right)/2; \quad p(\bar{x}) = \left(-N + \sqrt{N^2 + 4n_i^2}\right)/2,\ \bar{x} \in \Gamma_D. \quad (1.11)$$

On the Γ_N (less thickened boundary) the boundary conditions have the form of Neumann conditions:

$$\bar{n} \cdot \nabla\varphi = \partial\varphi/\partial n = 0;\ \bar{n} \cdot \bar{J}_n = 0;\ \bar{n} \cdot \bar{J}_p = 0,\ \bar{x} \in \Gamma_N, \qquad (1.12)$$

Initial conditions

In the absence of external voltage on the anode ($V_a = 0$), the solution of the problem, on the whole surface $\overline{\Omega}$, has the form of the conditions (1.11) with $V_a = 0$.

This solution can be used as an initial approximation of the system solution (1.1)–(1.6), using an iterative method, with the gradual increase of the external voltage, applied to the anode.

2 Discretization of nonlinear differential equations with the application of finite differences and the Scharfetter–Gummel scheme

In the field of problem definition (1.1) – (1.3), a grid step is inserted: h_{x_1}(horizontal step) and h_{x_2} (vertical step). Thus, a network of internal nodes is obtained, we denoted: $\Omega_h = \{(x_1^{(i)}, x_2^{(j)})$, where

$$x_1^{(i)} = (i-1) * h_{x_1},\ x_2^{(j)} = (j-1) * h_{x_2}.$$

By $\overline{\Omega} = \{(x_1^{(i)}, x_2^{(j)})\}$ we denote the set of all nodes (internal and boundary nodes $\overline{\Omega} = \Omega_h \bigcup \Omega_D \bigcup \Omega_N$), where Ω_D is the network of nodes, covering the portion of the boundary to which the anode and cathode are connected and on which the Dirichlet conditions act, Ω_N is the network of nodes, covering the remaining part of the boundary, on which the Neumann conditions act.

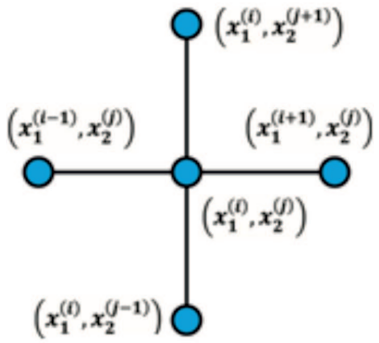

Figure 3. *Location of the internal nodes in the network*

Using the theory of finite differences, in the equations (1.1) – (1.3) we discretized electrostatic potential (φ), electron concentrations (n), hole concentrations (p) in entire nodes: $(x_1^{(i)}, x_2^{(j)})$ with $x_1^{(i)} = (i-1)h_1,\ x_2^{(j)} = (j-1)h_2$ and the densities of electron and hole currents J_n, J_p in the seminodes: $(x_1^{(i-1/2)}, x_2^{(j)})$, $(x_1^{(i+1/2)}, x_2^{(j)})$, $(x_1^{(i)}, x_2^{(j-1/2)})$, $(x_1^{(i)}, x_2^{(j+1/2)})$ with $x_1^{(i-1/2)} = (i-1/2)h_1,\ x_2^{(i+1/2)}) = (i+1/2)h_1,\ x_2^{(j-1/2)} = (j-1/2)h_2$, $x_2^{(j+1/2)} = (j+1/2)h_2$,

Applying the finite differences, the three algebraic systems are obtained, having the order $((NN-1)\times(MM-1))$, from the differential equations (1.1) – (1.3):

$$\left(\frac{2\epsilon}{h_{x_1}^2}+\frac{2\epsilon}{h_{x_2}^2}\right)\varphi_{i,j}-\frac{\epsilon}{h_{x_1}^2}\varphi_{i+1,j}-\frac{\epsilon}{h_{x_1}^2}\varphi_{i-1,j}-\frac{\epsilon}{h_{x_2}^2}\varphi_{i,j+1}-\frac{\epsilon}{h_{x_2}^2}\varphi_{i,j-1}=$$

$$=(p_{i,j}-n_{i,j}+N_{i,j}) \quad (1.13)$$

$$-\left(\frac{J_{n\ i+1/2,j}-J_{n\ i-1/2,j}}{h_{x_1}}+\frac{J_{n\ i,j+1/2}-J_{n\ i,j-1/2}}{h_{x_2}}\right)=$$

$$=-q\left(\frac{n_{i,j}p_{i,j}-n_i^2}{\tau_p\left(n_{i,j}+n_i\right)+\tau_n\left(p_{i,j}+n_i\right)}+\left(n_{i,j}p_{i,j}-n_i^2\right)\left(C_nn_{i,j}+C_pp_{i,j}\right)\right) \quad (1.14)$$

$$\left(\frac{J_{p\ i+1/2,j}-J_{p\ i-1/2,j}}{h_{x_1}}+\frac{J_{p\ i,j+1/2}-J_{p\ i,j-1/2}}{h_{x_2}}\right)=$$

$$=-q\left(\frac{n_{i,j}p_{i,j}-n_i^2}{\tau_p\left(n_{i,j}+n_i\right)+\tau_n\left(p_{i,j}+n_i\right)}+\left(n_{i,j}p_{i,j}-n_i^2\right)\left(C_nn_{i,j}+C_pp_{i,j}\right)\right). \quad (1.15)$$

For systems (1.14), (1.15), applying the Scharfetter–Gummel scheme [6,7,9], the following nonlinear algebraic system are obtained, the number of equations coincides with the number of internal nodes $((NN-1)*(MM-1))$:

$$\left(\left(\mu_n\varphi_\tau B\left(\frac{\varphi_{i,j}-\varphi_{i+1,j}}{\varphi_\tau}\right)+\mu_n\varphi_\tau B\left(\frac{\varphi_{i,j}-\varphi_{i-1,j}}{\varphi_\tau}\right)\right)\Big/h_{x1,i}^2+\right.$$

$$\left.+\left(\mu_n\varphi_\tau B\left(\frac{\varphi_{i,j}-\varphi_{i,j+1}}{\varphi_\tau}\right)+\mu_n\varphi_\tau B\left(\frac{\varphi_{i,j}-\varphi_{i,j-1}}{\varphi_\tau}\right)\right)\Big/h_{x2,j}^2\right)*n_{i,j}-$$

$$-\left(\left(\mu_n\varphi_\tau B\left(\frac{\varphi_{i,j}-\varphi_{i+1,j}}{\varphi_\tau}\right)\right)/h_{x1,i}^2\right)*n_{i+1,j}-$$

$$-\left(\left(\mu_n\varphi_\tau B\left(\frac{\varphi_{i,j}-\varphi_{i-1,j}}{\varphi_\tau}\right)\right)/h_{x1,i}^2\right)*$$

$$*n_{i-1,j}-\left(\left(\mu_n\varphi_\tau B\left(\frac{\varphi_{i,j}-\varphi_{i,j+1}}{\varphi_\tau}\right)\right)/h_{x2,j}^2\right)*n_{i,j+1}-$$

$$-\left(\left(\mu_n\varphi_\tau B\left(\frac{\varphi_{i,j}-\varphi_{i,j-1}}{\varphi_\tau}\right)\right)/h_{x2,j}^2\right)*n_{i,j-1}=$$

$$=-q\left(\left(\frac{n_{i,j}p_{i,j}-n_i^2}{\tau_pn_{i,j}+n_i}\right)+\tau_n(p_{i,j}+n_i)+\left(n_{i,j}p_{i,j}-n_i^2\right)\left(C_nn_{i,j}+C_pp_{i,j}\right)\right) \quad (1.16)$$

$$\left(\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i+1,j}-\varphi_{i,j}}{\varphi_\tau}\right)+\mu_p\varphi_\tau B\left(\frac{\varphi_{i-1,j}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h_{x1,i}^2+\right.$$

$$+\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i,j+1}-\varphi_{i,j}}{\varphi_\tau}\right)+\mu_p\varphi_\tau B\left(\frac{\varphi_{i,j-1}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x2,j}\Bigg)*p_{i,j}-$$

$$-\Bigg(\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i+1,j}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x1,i}\Bigg)*p_{i+1,j}-$$

$$-\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i-1,j}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x1,i}\Bigg)*$$

$$*p_{i-1,j}-\Bigg(\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i,j+1}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x2,j}\Bigg)*p_{i,j+1}-$$

$$-\Bigg(\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i,j-1}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x2,j}\Bigg)*p_{i,j-1}=$$

$$=-q\Bigg(\left(\frac{n_{i,j}p_{i,j}-n_i^2}{\tau_p n_{i,j}+n_i}\right)+\tau_n(p_{i,j}+n_i)+(n_{i,j}p_{i,j}-n_i^2)(C_n n_{i,j}+C_p p_{i,j})\Bigg) \quad (1.17)$$

where $B(x)=\dfrac{x}{e^x-1}$ is the function of Bernoulli.

3 Linearization of differential equations using the Newton's method

Denote by $\varphi^{(ex)}(x_1,x_2)$ the exact solution of the system (1.13), with $\varphi^{(old)}(x_1,x_2)$–the system solution, calculated at the previous iteration, $\varphi^{(new)}(x_1,x_2)$–the solution calculated at the current iteration and $\delta_\varphi(x_1,x_2)$–the error;
with $n^{(ex)}(x_1,x_2)$–the exact solution of the system (1.16), $n^{(old)}(x_1,x_2)$–the system solution calculated at the previous iteration, $n^{(new)}(x_1,x_2)$–the system solution calculated at the current iteration, and $\delta_n(x_1,x_2)$–the error;
with $p^{(ex)}(x_1,x_2)$–the exact solution of the system (1.17), $p^{(old)}(x_1,x_2)$–the system solution calculated at the previous iteration, $p^{(new)}(x_1,x_2)$–the system solution calculated at the current iteration and $\delta_p(x_1,x_2)$–the error. Then we have the following expressions:

$$\varphi^{(new)}(x_1,x_2)=\varphi^{(old)}(x_1,x_2)+\delta_\varphi(x_1,x_2) \quad (1.18)$$
$$n^{(new)}(x_1,x_2)=n^{(old)}(x_1,x_2)+\delta_n(x_1,x_2) \quad (1.19)$$
$$p^{(new)}(x_1,x_2)=p^{(old)}(x_1,x_2)+\delta_p(x_1,x_2) \quad (1.20)$$

Substituting (1.18) – (1.20) in the systems (1.13), (1.16), (1.17), respectively and using Gummel technique [5], the three linear algebraic systems are obtained, having the order $((NN-1)\times(MM-1))$, from differential equation (1.1) – (1.3), separate from the other two, in the unknowns $\delta_\varphi(x_1,x_2),\delta_n(x_1,x_2),\delta_p(x_1,x_2)$, respectively:

$$\left(\frac{2\epsilon}{h^2_{x_1}}+\frac{2\epsilon}{h^2_{x_2}}\right)\delta_{\varphi,i,j}-\frac{\epsilon}{h^2_{x_1}}\delta_{\varphi,i+1,j}-\frac{\epsilon}{h^2_{x_1}}\delta_{\varphi,i-1,j}-\frac{\epsilon}{h^2_{x_2}}\delta_{\varphi,i,j+1}-\frac{\epsilon}{h^2_{x_2}}\delta_{\varphi,i,j-1}=$$
$$=-\left(\frac{2\epsilon}{h^2_{x_1}}+\frac{2\epsilon}{h^2_{x_2}}\right)\varphi^{(old)}_{i,j}+\frac{\epsilon}{h^2_{x_1}}\varphi^{(old)}_{i+1,j}+\frac{\epsilon}{h^2_{x_1}}\varphi^{(old)}_{i-1,j}+\frac{\epsilon}{h^2_{x_2}}\varphi^{(old)}_{i,j+1}+\frac{\epsilon}{h^2_{x_2}}\varphi^{(old)}_{i,j-1}+$$
$$+q*(p^{(old)}_{i,j}-n^{(old)}_{i,j}+N_{i,j}) \quad (1.21)$$

$$\left(\left(\mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} - \varphi_{i+1,j}^{(old)}}{\varphi_\tau} \right) + \mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} - \varphi_{i-1,j}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x1,i}^2 + \right.$$

$$\left. + \left(\mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} - \varphi_{i,j+1}^{(old)}}{\varphi_\tau} \right) + \mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} - \varphi_{i,j-1}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x2,j}^2 \right) * \delta_{n\ i,j} -$$

$$- \left(\left(\mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} - \varphi_{i+1,j}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x1,i}^2 \right) * \delta_{n\ i+1,j} -$$

$$- \left(\left(\mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} - \varphi_{i-1,j}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x1,i}^2 \right) * \delta_{n\ i-1,j} -$$

$$- \left(\left(\mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} - \varphi_{i,j+1}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x2,j}^2 \right) * \delta_{n\ i,j+1} -$$

$$- \left(\left(\mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} - \varphi_{i,j-1}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x2,j}^2 \right) * \delta_{n\ i,j-1} =$$

$$= - \left(\left(\mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} - \varphi_{i+1,j}^{(old)}}{\varphi_\tau} \right) + \mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} - \varphi_{i-1,j}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x1,i}^2 + \right.$$

$$\left. + \left(\mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} - \varphi_{i,j+1}^{(old)}}{\varphi_\tau} \right) + \mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} - \varphi_{i,j-1}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x2,j}^2 \right) * n_{i,j}^{(old)} -$$

$$- \left(\left(\mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} - \varphi_{i+1,j}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x1,i}^2 \right) * n_{i+1,j}^{(old)} +$$

$$+ \left(\left(\mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} + \varphi_{i-1,j}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x1,i}^2 \right) * n_{i-1,j}^{(old)} -$$

$$- \left(\left(\mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} + \varphi_{i,j+1}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x2,j}^2 \right) * n_{i,j+1}^{(old)} -$$

$$- \left(\left(\mu_n \varphi_\tau B \left(\frac{\varphi_{i,j}^{(old)} + \varphi_{i,j-1}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x2,j}^2 \right) * n_{i,j-1}^{(old)} - q \left(\frac{n_{i,j}^{(old)} p_{i,j}^{(old)} - n_i^2}{\tau_p n_{i,j}^{(old)} + n_i} + \right.$$

$$\left. + \tau_n \left(p_{i,j}^{(old)} + n_i \right) + \left(n_{i,j}^{(old)} p_{i,j}^{(old)} - n_i^2 \right) \left(C_n n_{i,j}^{(old)} + C_p p_{i,j}^{(old)} \right) \right. \qquad (1.22)$$

$$\left(\left(\mu_p \varphi_\tau B \left(\frac{\varphi_{i+1,j}^{(old)} - \varphi_{i,j}^{(old)}}{\varphi_\tau} \right) + \mu_p \varphi_\tau B \left(\frac{\varphi_{i-1,j}^{(old)} - \varphi_{i,j}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x1,i}^2 + \right.$$

$$\left. + \left(\mu_p \varphi_\tau B \left(\frac{\varphi_{i,j+1}^{(old)} - \varphi_{i,j}^{(old)}}{\varphi_\tau} \right) + \mu_p \varphi_\tau B \left(\frac{\varphi_{i,j-1}^{(old)} - \varphi_{i,j}^{(old)}}{\varphi_\tau} \right) \right) \Big/ h_{x2,j}^2 \right) * \delta_{p\ i,j} -$$

$$-\left(\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i+1,j}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x1,i}\right)*\delta_{p\ i+1,j}-\left(\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i-1,j}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x1,i}\right)*$$

$$*\delta_{p\ i-1,j}-\left(\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i,j+1}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x2,j}\right)*\delta_{p\ i,j+1}-$$

$$-\left(\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i,j-1}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x2,j}\right)*\delta_{p\ i,j-1}=$$

$$=-\left(\left(\mu_p\varphi_\tau B\left(\frac{\varphi^{(old)}_{i+1,j}-\varphi^{(old)}_{i,j}}{\varphi_\tau}\right)+\mu_p\varphi_\tau B\left(\frac{\varphi^{(old)}_{i-1,j}-\varphi^{(old)}_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x1,i}+\right.$$

$$\left.+\left(\mu_p\varphi_\tau B\left(\frac{\varphi^{(old)}_{i,j+1}-\varphi^{(old)}_{i,j}}{\varphi_\tau}\right)+\mu_p\varphi_\tau B\left(\frac{\varphi^{(old)}_{i,j-1}-\varphi^{(old)}_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x2,j}\right)*p^{(old)}_{i,j}+$$

$$+\left(\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i+1,j}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x1,i}\right)*p^{(old)}_{i+1,j}+\left(\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i-1,j}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x1,i}\right)*$$

$$*p^{(old)}_{i-1,j}+\left(\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i,j+1}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x2,j}\right)*p^{(old)}_{i,j+1}+$$

$$+\left(\left(\mu_p\varphi_\tau B\left(\frac{\varphi_{i,j-1}-\varphi_{i,j}}{\varphi_\tau}\right)\right)\Big/h^2_{x2,j}\right)*p^{(old)}_{i,j-1}-q*\tag{1.23}$$

$$*\left(\frac{n_{i,j}p^{(old)}_{i,j}-n_i^2}{\tau_p\left(n^{(old)}_{i,j}+n_i\right)+\tau_n\left(p^{(old)}_{i,j}+n_i\right)}+\left(n^{(old)}_{i,j}p^{(old)}_{i,j}-n_i^2\right)\left(C_nn^{(old)}_{i,j}+C_pp^{(old)}_{i,j}\right)\right)$$

where $B(x)=\dfrac{x}{e^x-1}$ is the function of Bernoulli.

When we solve the systems (1.21)–(1.23) we can use the numerical methods, applicable to systems with asymmetric matrices (Simple Iteration Method, Bi-Conjugate Gradient Method) [4, 8] or to systems with predominant diagonal matrices (Gauss-Seidel Method, Super Relaxation Method) [4].

Based on the solutions of the systems (1.21)–(1.23), the new values of the unknown functions are recalculated, according to the relations (1.18)–(1.20).

In the nodes on the boundary, the values of the electrostatic potential, at the current iteration $\varphi^{(k+1)}$, are approximated according to the boundary conditions (1.11), (1.12), based on the system:

$$\begin{cases}\varphi^{(new)}_{1,j}=\varphi^{(new)}_{2,j}, & \text{i=1, j=1..MM+1}\\ \varphi^{(new)}_{NN+1,j}=\varphi^{(new)}_{NN,j}, & \text{i=NN+1, j=1..MM+1}\\ \varphi^{(new)}_{i,1}=\varphi^{(new)}_{i,2}, & \text{i=1..NN+1, j=1, } x^{(i)}_1>l_a\end{cases}$$

Similarey, to the electrostatic potential, we calculat the boundary values of the concentrations of electron and hole $n^{(new)}$, $p^{(new)}$, at the current iteration.

The values of the unknown functions are recalculated, under the conditions of the thermodynamic equilibrium, with $V_a\neq 0$, increased iteratively. Then the internal cycles are resumed, to solve the three algebraic systems.

The iterative process lasts as long as the calculations remain stable, with the gradual increase in voltage, applied to the anode.

4 Numerical results with graphic representation

Solving the system (1.1)–(1.3), with the boundary conditions (1.11)–(1.12) was done by writing a program in the Matlab. The obtained results were represented in Figure 4 – Figure 6. The initial numerical solutions, for the systems (1.13)–(1.15), are represented in Figure 4. The recalculated values of the unknown functions, under the conditions of thermodynamic equilibrium $V_a \neq 0$, are represented in Figure 5. The graph in Figure 6 illustrates the distribution of the functions φ, n and p, when applying, from outside to anode, the voltage $V_a = 2.0\ V$ and with a concentration of impurities $N \approx 10^{19}\ m^{-3}$.

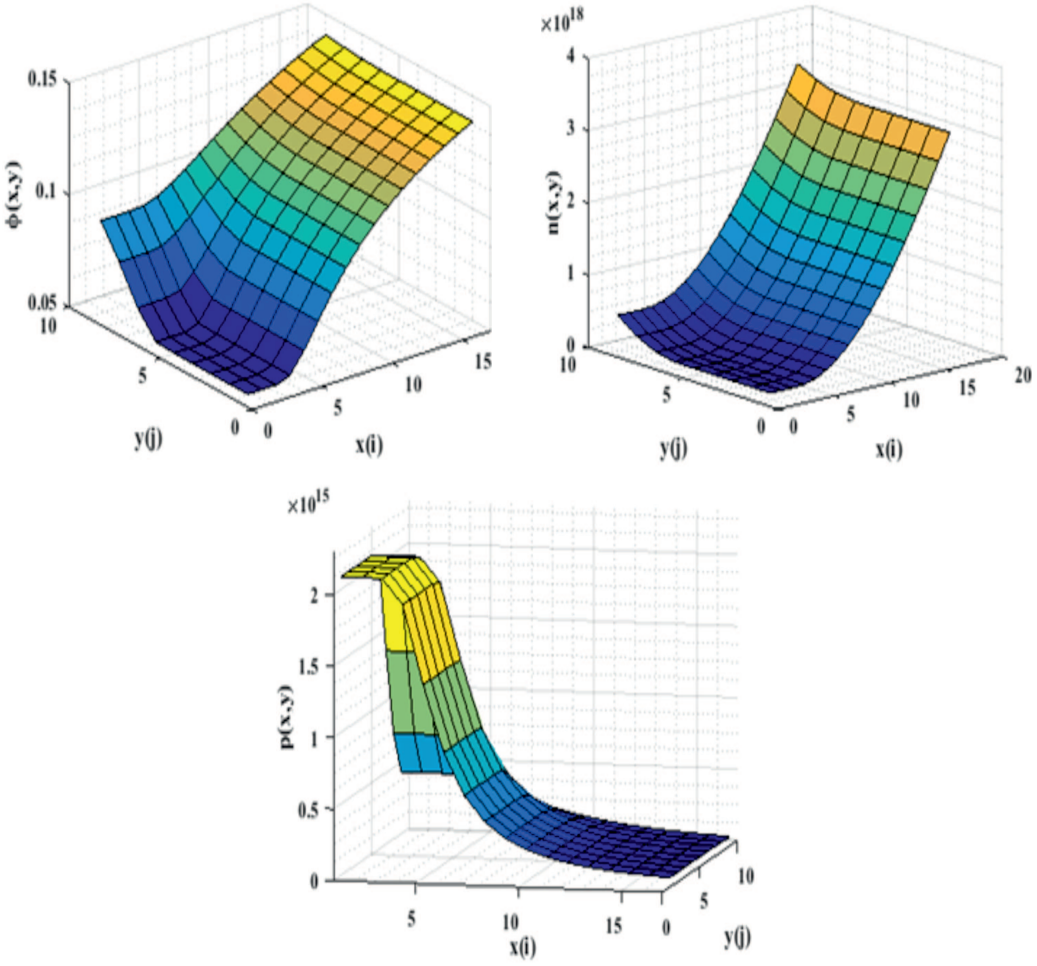

Figure 4. *Distribution of the potential φ, the concentrations of electrons n and holes p, when applying to anode voltage $V_a = 0$ and the concentration of impurities $N_{Dn} = 10^{17}\ m^{-3}$, $N_{Dn_{max}} = 10^{19}\ m^{-3}$, $N_{Ap_{max}} = 10^{19}\ m^{-3}$*

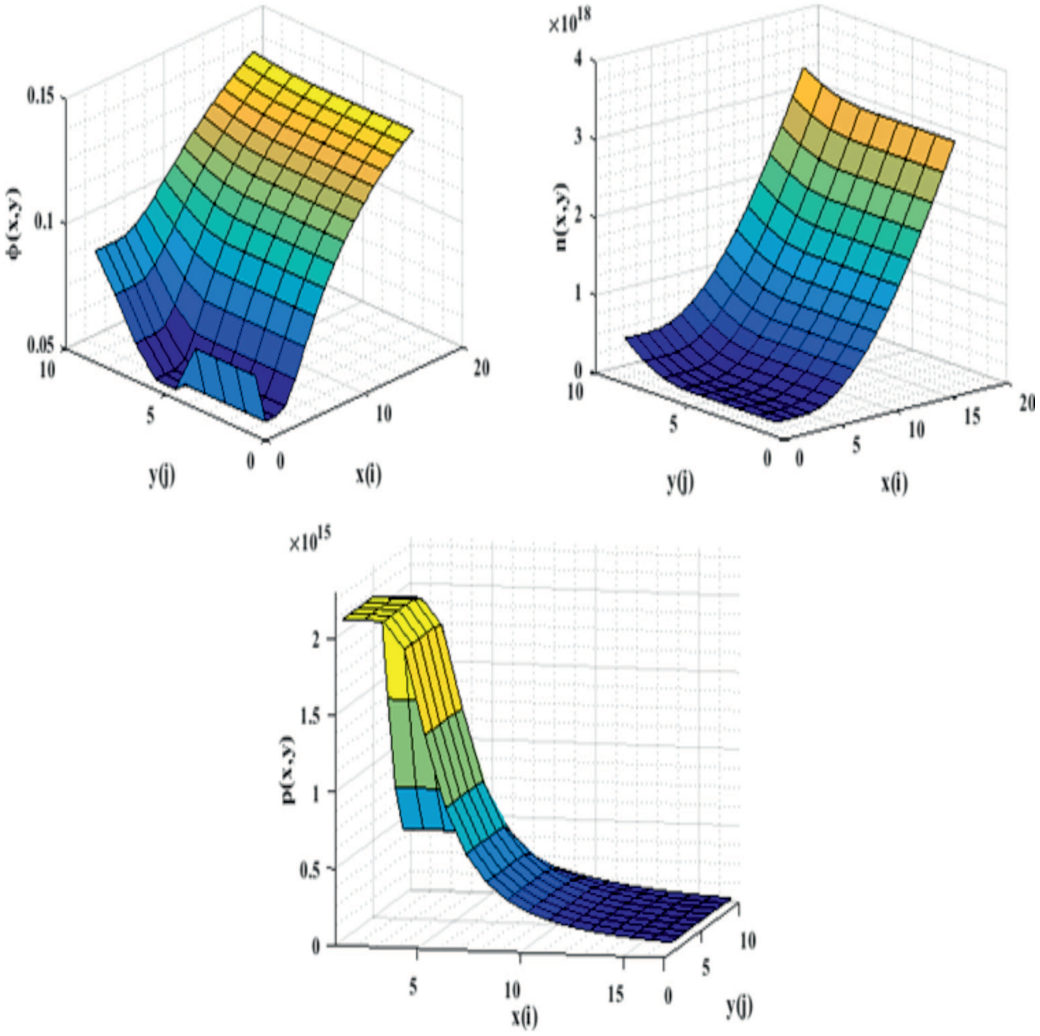

Figure 5. *Distribution of the potential φ, the concentrations of electrons n and holes p, under the conditions of thermodynamic equilibrium, when applying to anode voltage $V_a \neq 0$ and the concentration of impurities $N_{Dn} = 10^{17}\ m^{-3}$, $N_{Dn_{max}} = 10^{19}\ m^{-3}$, $N_{Ap_{max}} = 10^{19}\ m^{-3}$*

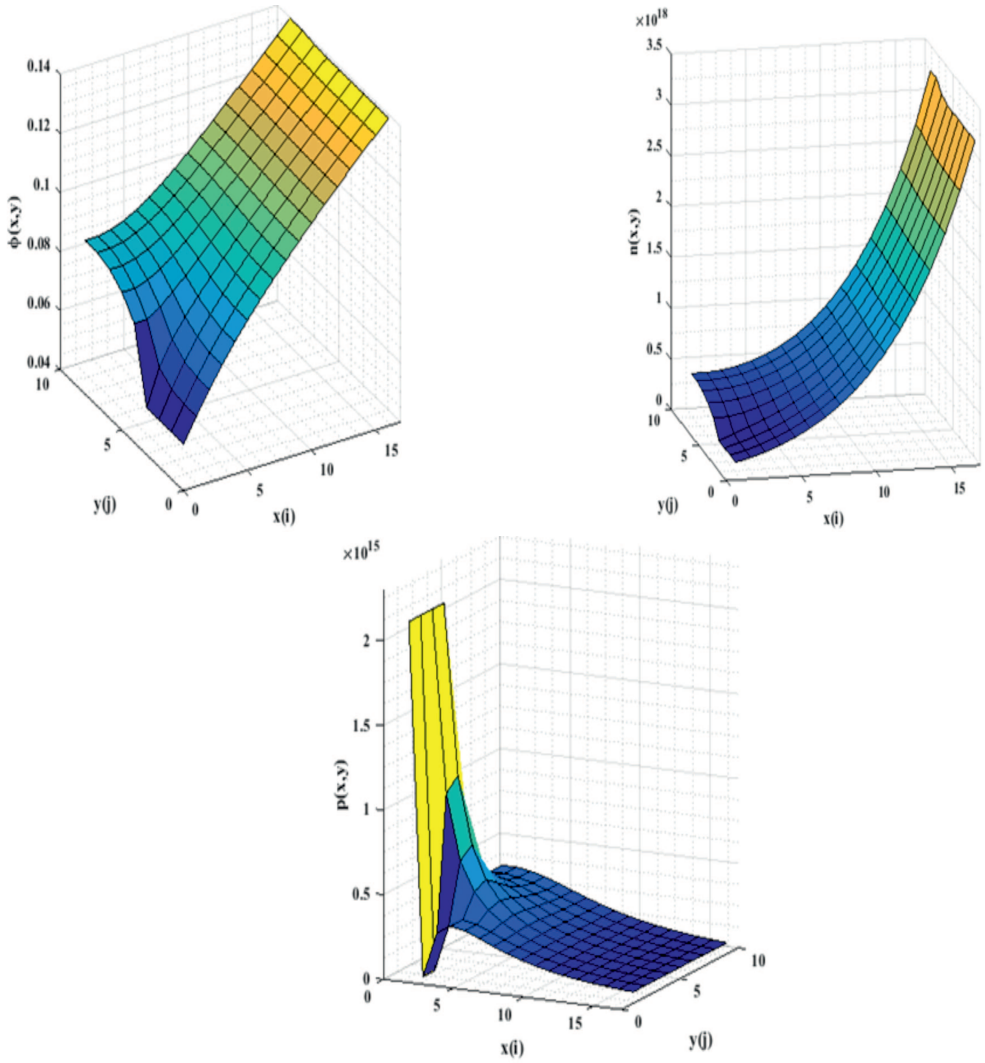

Figure 6. *Distribution of the potential φ, the concentrations of electrons n and holes p, when applying to anode voltage $V_a = 2.0\ V$ and the concentrations of impurities $N_{Dn} = 10^{17}\ m^{-3},\ N_{Dn_{max}} = 10^{19}\ m^{-3},\ N_{Ap_{max}} = 10^{19}\ m^{-3}$*

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