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NUMERICAL ANALYSIS OF TRANSPORT PHENOMENA IN SEMICONDUCTOR DEVICES AND STRUCTURES.

3. MODELING OF MIS STRUCTURES

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A universal algorithm for multidimensional numerical analysis of unipolar semiconductor devices is studied.

The theoretical study of unipolar semiconductor devices is at the present time most often carried out employing numerical models based on the solution of the equations of continuity for holes and electrons and Poisson's equation for the electrostatic potential [1].

It is sufficient to cite only some works on the multidimensional analysis of MOS transistors with short channels. Thus in [2, 3] the mechanisms of avalanche breakdown were studied; in [4] the effect of the spread in a number of the electrophysical parameters (channel length, impurity concentration in the substrate, depth of the p–n junction, etc.) on one of the basic parameters – the threshold voltage – was studied; in [5, 6] the effect of adjoining was studied, etc. Naturally, the importance of such studies increases with the transition to the submicron technology for fabricating integrated circuits because of the complexity of the experimental development of such circuits.

One of the basic difficulties standing in the way of the assimilation of numerical experiments in practice is the lack of efficient and reliable universal algorithms for the multidimensional numerical analysis of unipolar semiconductor devices. Thus the most efficient algorithms and programs [7, 8], based on Mock's method [9], do not permit carrying out a rigorous calculation of devices in prebreakdown operating states [3] and taking into account the mechanisms of surface recombination [10]. This is linked with the fact that in Mock's method [9] it is assumed that there is no recombination-generation term in the equation of continuity. Algorithms which do not have this drawback either make use of additional physical assumptions [11] or they require supercomputers [12] or they require dense grids in the neighborhood of the insulator–semiconductor interface [13]. The latter circumstance, naturally, places the problem of selecting a grid at the forefront [14].

In this work we propose a universal algorithm for the multidimensional numerical analysis of the static states of unipolar semiconductor devices, based on the method of [1] and not having the above-mentioned drawbacks. The efficiency of the algorithm is illustrated for the

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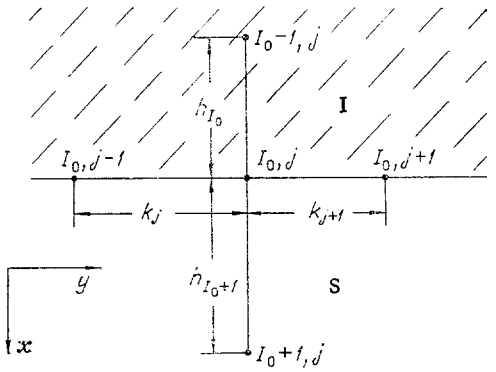

Fig. 1. Grid at the insulator (I) and semiconductor (S) interface.

example of a two-dimensional numerical analysis of an n-channel MOS transistor using a coarse spatial grid.

In the stationary state the problem under study consists of solving the fundamental system of equations from the physics of semiconductor devices [1] with the boundary conditions, formulated very completely in [13]. In the case when Boltzmann's statistics are valid the Poisson equation for unipolar semiconductor devices is usually written in the form (for the semiconductor and insulator, respectively)

$$\varepsilon_s \nabla^2 \psi = q\,[n_i \exp\,[(\psi - \Phi_n)/\varphi_T] - n_i \exp\,[(\Phi_p - \psi)/\varphi_T] - N_i + N_a], \qquad (1)$$

$$\varepsilon_i \nabla^2 \psi = -\rho_i .$$

The most important conditions for the algorithm are the conditions at the insulator–semiconductor interface [13, 15]:

$$J_{px} = qR_S(p,\ n,\ \psi) = -J_{nx}, \qquad (2)$$

$$J_{px} + J_{nx} = J_{Tx} = 0,$$

where the model of surface recombination has, as an example, the form [16] $R_S = A(pn - n_i^2)$, while

$$\varepsilon_s (\partial\psi/\partial x)_s - \varepsilon_i (\partial\psi/\partial x)_i = \sigma_{sur}, \qquad (3)$$

$$\sigma_{sur} = qD_{St}(\psi_{sur} - \psi^0)/\varphi_T,$$

which for accuracy we supplement with

$$(\partial\psi/\partial y)_s = (\partial\psi/\partial y)_i . \qquad (4)$$

Equations (3) and (4) follow from the Gauss–Ostrogradskii theorem for the interface of two media oriented parallel to the y axis. The algorithm can be easily extended to the general case, when the interface is not parallel to the y axis.

We shall study Poisson's equation (1) with the boundary conditions (3) and (4). To obtain a finite-difference analog of (1) at the insulator–semiconductor interface (Fig. 1), just as in [17], except that there the case $\sigma_{sur} = 0$ was considered, the expansion $\psi_{I_0-1,j}$ and $\psi_{I_0+1,j}$ in a uniform medium in a Taylor series, including also the second derivatives, was used. The latter terms are eliminated by using Poisson's equation in the semiconductor (for $\psi_{I_0+1,j}$) and in the insulator (for $\psi_{I_0-1,j}$), (3), and the properties of continuity (conservation) of the tangential components of the electric field (4). Mathematically, this approach for approximating the boundary conditions is more accurate than the approaches usually used (the expansion includes only the first derivatives of ψ) [18]. From the physical viewpoint, which should be specially emphasized, it includes all equations [including also (4)] characterizing the electric properties of the interface of the two media. It may therefore be expected that the approximation of Poisson's equation at the insulator–semiconductor interface will have a higher degree of stability. This should alleviate the problem of selecting the spatial grid in this region.

As a result, the finite-difference analogs of Poisson's equation assume the form

$$A_{i,j}\psi_{i-1,j} + B_{i,j}\psi_{i+1,j} + D_{i,j}\psi_{i,j-1} + E_{i,j}\psi_{i,j+1} + C_{i,j}\psi_{i,j} = F_{i,j}, \tag{5}$$

where

$$\begin{gathered} A_{i,j} = h_{i+1}\delta_{i,j};\ B_{i,j} = h_i;\ C_{i,j} = -[h_{i+1}\delta_{i,j}(1 + h_i r_{i,j}/\varepsilon_i) + h_i + S_i W_{i,j}]; \\ W_{i,j} = h_{i+1}h_i/(k_j k_{j+1});\ S_i = h_{i+1} + h_i\delta_{i,j}; \\ l_{i,j} = h_{i+1}h_i/(k_j + k_{j+1});\ D_{i,j} = l_{i,j}S_i/k_j,\ E_{i,j} = l_{i,j}S_i/k_{j+1}; \\ f_{i,j} = q[n_i \exp[(\psi_{i,j} - \Phi_{ni,j})/\varphi_T] - n_i \exp[(\Phi_{pi,j} - \psi_{i,j})/\varphi_T] - N_{i\,i,j} + N_{ai,j}]/\varepsilon_s. \end{gathered} \tag{6}$$

Here $\delta_{i,j}$, $r_{i,j}$, and $F_{i,j}$ are given by

$$\begin{gathered} \delta_{i,j} = \varepsilon_i/\varepsilon_s,\ r_{i,j} = D_{Si}q/\varphi_T, \\ F_{i,j} = 0{,}5h_{i+1}^2 h_i[f_{i,j} - 2(r_{i,j}\psi_{i,j}^0 - 0{,}5h_i\rho_{i\,i,j})/(h_{i+1}\varepsilon_s)] \end{gathered} \tag{7}$$

for the insulator–semiconductor interface ($i = I_0$); by

$$\delta_{i,j} = 1,\ r_{i,j} = 0,\quad F_{i,j} = 0{,}5f_{i,j}h_i h_{i+1}(h_i + h_{i+1}) \tag{8}$$

for the semiconductor; and by

$$\delta_{i,j} = 1,\ r_{i,j} = 0,\ F_{i,j} = 0{,}5\rho_{i\,i,j}h_i h_{i+1}(h_i + h_{i+1})/\varepsilon_i \tag{9}$$

for the insulator.

The boundary conditions at other boundaries, because of their linearity, are taken into account by changing the corresponding coefficients in (5). Thus, in the course of the solution of (5), the boundary conditions are satisfied automatically [19]. This method can be called the implicit treatment of the boundary conditions and is preferable to the explicit method [20], especially for nonlinear boundary-value problems, because of its absolute stability to roundoff errors which arise in the computational process.

In what follows Eqs. (5)-(9) are quasilinearized with respect to $\delta\psi$ using the Boltzmann statistics, as done in Gummel's method [21]. This leads to the matrix equation

$$A_\psi \delta\psi = -F_\psi(\psi,\ n,\ p). \tag{10}$$

The derivation of the elements A_ψ, F_ψ from Eqs. (5)-(9) does not present any difficulties and is omitted in this work. We note that the described method for taking into account the boundary conditions can be used together with the approach proposed in [22] to the finite-difference approximation of Poisson's equation.

For the equations of continuity (Eqs. (2) and (3) from [1]) the quasilinearization with fixed ψ of their discrete analogs with respect to δn and δp is used taking into account the nonlinearity of the problem (with respect to the boundary conditions and R_n and R_p). A formulation of the Sharfetter–Gummel type [1] is used in the finite-difference approximation of the continuity equations. The boundary conditions [including also (2)] are also quasilinearized, after which, as done previously, the coefficients of the Jacobi matrices A_n and A_p are changed:

$$A_n \delta n = -F_n(n,\ p,\ \psi), \tag{11}$$

$$A_p \delta p = -F_p(n,\ p,\ \psi). \tag{12}$$

Equations (11) and (12) are the discrete quasilinearized analogs of the equations of continuity for which the boundary conditions are satisfied automatically.

The solution algorithm, implementing the generalized two-step VRS method [1] in a basis [1] of the basic variables ψ, n, and p which is convenient for practical implementation has the following form: 1) the initial approximation for ψ, n, and p over the structure of the device over corresponding regions is given; 2) Poisson's equation is solved for ψ using Newton's method with fixed Q_n, Q_p: a) m = 1, where m is the number of Newtonian iterations

(step 2); b) the quasilinearized (using Boltzmann statistics, i.e., with fixed Q_n, Q_p) finite-difference analog (10) of Poisson's equations (5)-(9) is solved for $\delta\psi^m$; c) the new values of $\psi^{m+1} = \psi^m + \delta\psi^m$, the concentrations $n^{m+1} = n^m \exp(\delta\psi^m)$, $p^{m+1} = p^m \exp(-\delta\psi^m)$, the diagonal elements of Jacobi's matrix $A\psi^{m+1}$, and the discrepancies $F\psi^{m+1}$, $m = m + 1$ are found; d) the substeps b and c of step 2 are repeated a fixed number of times or in accordance with the criterion $|\delta\psi^m|_{max}/|\delta\psi^{m+1}|_{max} \geq K$ (where $K \simeq 10$); 3) the equations of continuity with fixed ψ are solved simultaneously by the method of vector relaxation of systems (VRS): a) $\ell = 1$, where ℓ is the number of VRS iterations* with simultaneous solution of the equations of continuity, Sec. 3; b) the finite-difference quasilinearized analogs of the continuity equations (11) and (12) are solved for δn^ℓ, δp^ℓ, in which the values of ψ are used, and for $\ell = 1$, n and p from step 2, also; c) the new values of $n^{\ell+1} = n^\ell + \delta n^\ell$, $p^{\ell+1} = p^\ell + \delta p^\ell$, as well as of $An^{\ell+1}$, $Ap^{\ell+1}$, $Fn^{\ell+1}$, $Fp^{\ell+1}$, $\ell = \ell + 1$ are found; d) the substeps b and c from step 3 are repeated either a fixed number of times (usually twice) or until the required convergence is obtained; 4) steps 2 and 3 of the two-step algorithm are continued until the required accuracy is achieved.

We shall examine the results obtained for a test example. The described universal algorithm of multidimensional analysis of unipolar semiconductor devices was initially implemented in the COSMOS program for the two-dimensional model of MIS transistors and then embedded in the universal program PNAIIL [23] with only the process for selecting the initial approximation being simplified.

In the COSMOS program one of the variants of the general procedure described in [24] was used as the initial approximation. To simplify the algorithm it was assumed that quasi-equilibrium was absent only for electrons in the substrate for the region $x < x_j$ (for an n-channel transistor, Fig. 2). The simplified equation of continuity $\nabla^2\Phi_n = R_n/\mu_n n$ in this region was solved sequentially with the quasilinearized Poisson equation for the entire device. Thus the initial approximation was selected by a method of Gummel type, since at each full iteration only the quasilinear Poisson equation was solved [21]. After the starting algorithm converged, the main algorithm continued to step 3. The solution was then conducted according to the universal algorithm described above. We note that special efforts are made in selecting the starting approximation to satisfy at the outset the boundary conditions at the interface of the two media. Chebyshev's cyclical method was used to solve all systems of linear equations [25]. The traditional normalization of the variables was used in implementing the algorithm [1].

The structure of the MOS transistor analyzed is shown in Fig. 2. The surface concentrations of the test device are as follows: for the source $N_i^{max} = 0.12 \cdot 10^{27}$, substrate $N_a = 0.12 \cdot 10^{22}$, drain $N_g^{max} = 0.12 \cdot 10^{27}$ $1/m^3$, and the dimensions are $XL_D = 5$, $YL_D = 20$, $x_j = 1.5$, $\ell_{co} \sim 12$, $\ell_g \sim 14$, $t_{ox} = 0.1$ μm.

In the test example described, illustrating the quality of the algorithm on coarse grids, for simplicity it is assumed that $\rho_i = DSt = 0$, $RS(p, n, \psi) = qA(pn - 1)$, $R = R_n = R_p$ and are fixed with the help of the Schockley–Reed–Hall model (formula (6) from [1]).

The results of the calculation of the electrostatic potential and the density of mobile carriers n and p at the interface, obtained for different biases, are presented in Fig. 3. The main feature of the given structure is the overlapping of the regions of the drain and sink by the gate ($\ell_g > \ell_{co}$). This largely determines the behavior of the basic variables ψ, n, and p. Figure 3b (curves 1 and 2) illustrates the formation of inversion layers ($n >> N_a$) for a structure with smooth p–n junctions of the drain and sink. It is evident from Fig. 3b, c (curves 1 and 2) that the mass-action law ($pn = n_i^2$) is obeyed in these cases ($V_c = 0$ V) quite accurately. Figure 3a, b (curves 3) show the mutual effect of both the gate and the drain on the physical processes in the structure of the applied voltage. A peculiarity here is the presence of a surge in the basic variables ψ and n at the surface of the drain, caused by the smoothness of the p–n junction of the drain and overlapping of the gate. As can be seen (Fig. 3b, c, curves 3), in this case the mass action law is not obeyed, which is not unexpected here (Fig. 7 of [13]).

*There is a misprint in [1] in step 3 of the generalized two-step VRS method. The phrase "where ℓ is the number of the VRS iteration for subsystem II" should be replaced by "where ℓ is the number of VRS iteration for subsystem I."

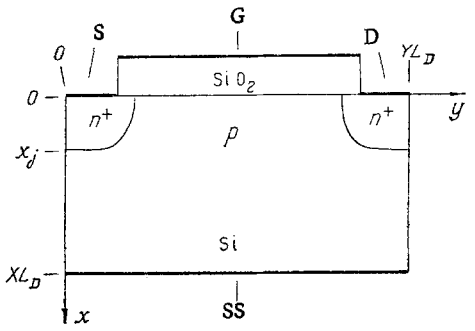

Fig. 2. Structure of the device being analyzed: S) source; G) gate; D) drain; SS) substrate.

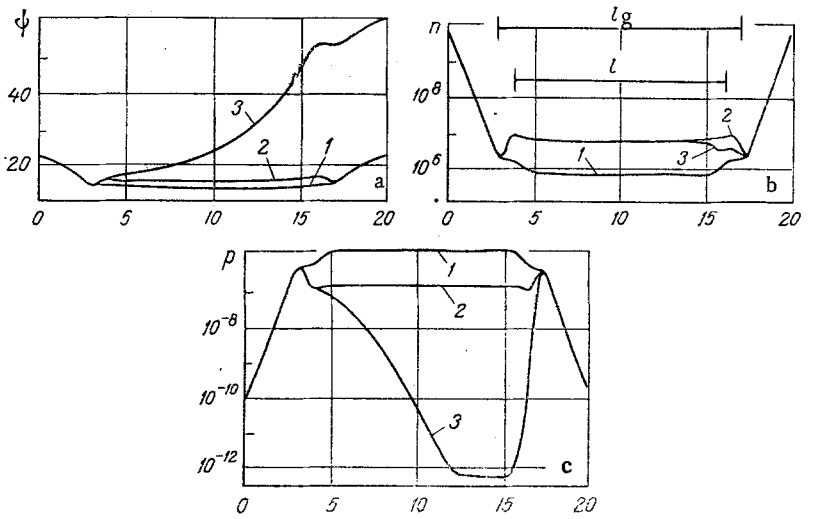

Fig. 3. Distribution of the basic variables at the $Si-SiO_2$ interface (x = 0 μm): a) electrostatic potential (ψ in normalized units φ_T = 0.0258 V); b) electron density; c) hole density (n and p in normalized units $n_i = 1.5 \cdot 10^{16}$ m^{-3}); 1) V_g = 1 V, V_D = 0 V; 2) V_g = 3 V, V_D = 0 V; 3) V_g = 3 V, V_D = 1 V ($V_s = V_{ss}$ = 0 V in all cases).

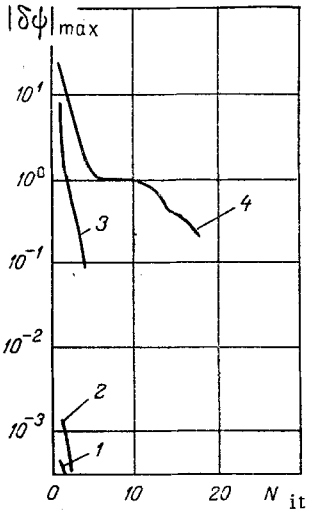

Fig. 4. Convergence of the algorithm developed for the device under study (ℓ = 1, m = 1, $\delta\psi$ in normalized units φ_T = 0.0258 V); 1) V_g = 1 V, V_D = 0 V; 2) V_g = 3 V, V_D = 0 V; 3) V_g = 1 V, V_D = 1 V; 4) V_g = 3 V, V_D = 1 V ($V_s = V_{ss}$ = 0 V in all cases).

The numerical analysis was carried out for a grid which is uniform along the y axis and quasiuniform along the x axis with 33 × 29 nodes in the semiconductor. The step along x in the oxide was chosen to be uniform (the number of points was equal to 10). In the semiconductor the step was chosen to be quasiuniform along the x axis (18 equidistant points were chosen in the region $0 \leq x \leq x_j$). Thus the spatial grid is quite coarse for the structure described with a long channel. The construction of such grids, naturally, does not require any special qualifications of the user.

Figure 4 illustrates the convergence of the algorithm developed, deliberately obtained for the slowest case m = 1, ℓ = 1 (algorithm of Gummel type) and illustrating its high efficiency and reliability on a coarse grid. We note that as the channel becomes shorter, as a rule, the convergence of the algorithm accelerates. For small biases of the gate and drain its convergence is of the quadratic type, which also indicates the quite high quality of the initial approximation obtained and is in agreement with the computer experiments for a bipolar transistor [26].

NOTATION

ψ, electrostatic potential; n and p, electron and hole densities; N_d and N_a, densities of donors and acceptors; R, excess of the recombination rate over the generation rate for holes (R_p) and electrons (R_n); R_S, the rate of surface recombination; ρ_i, space-charge density in the insulator; J_{nx}, J_{px}, J_{Tx}, x components of the electron current density, the hole current density, and the total current density; q, electron charge; ε_s, ε_i, dielectric constants of the semiconductor and insulator; n_i, intrinsic density; Φ_n, Φ_p, Fermi quasilevels of electrons and holes; φ_T, temperature potential (equal to 0.258 V at T = 300°K); B_s, B_i, values of B in the semiconductor and insulator; $B_{i,j}$, value of the variable B at a node of the spatial grid labeled by the indices i and j; Q_n, Q_p, variables equal to $n_i \exp(-\Phi_n/\varphi_T)$ and $n_i \exp(+\Phi_p/\varphi_T)$, respectively (in [1] their normalized values are used); μ_n, electron mobility; V_s, V_g, V_D, V_{ss}, voltages (potentials), applied to the contacts of the source, gate (more accurately $V_g = V_g - \varphi_{ms}$, where φ_{ms} is the difference in the work functions of the metal and semiconductor), drain, and substrate; ℓ_g, length of the gate; ℓ_{co}, length of the channel (the minimum distance between metallurgical boundaries of the p–n junctions of the drain and source); t_{ox}, thickness of the subgate oxide; XL_D, YL_D, geometrical dimensions of the device along the x and y axes; x_j, depth of the p–n junctions of the source and drain; $|\delta\psi^m|_{max}$, maximum value of $\{|\delta\psi_{i,j}|\}$ at the m-th Newton iteration (all nodes of the spatial grid are examined).

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AN INVERSE LAPLACE TRANSFORMATION FOR SOLVING HEAT-CONDUCTION PROBLEMS WITH DISCONTINUOUS BOUNDARY CONDITIONS OF THE SECOND KIND

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An inverse Laplace transformation is found for a class of functions encountered in heat-conduction problems with discontinuous boundary conditions.

In the solution of multidimensional axisymmetric nonstationary heat-conduction problems [1-3] for a system of two semibounded bodies with different thermophysical characteristics (TPC) in thermal contact in a plane wherein bounded (local) surface heat sources are operative with arbitrarily specified laws of heat flow density measurement in the corresponding domains, Laplace transform representations of the following form are encountered:

$$\mathrm{Lv}(s)=\mathrm{Lv}\left(s\left|\begin{matrix}p_1,\ p_2,\ p_3,\ \nu\\ k_1,\ k_2,\ k_3\end{matrix}\right.\right)=\frac{1}{s^{\nu}}\frac{1-k_1\exp\left(-p_1\sqrt{s}\right)}{1-k_2\exp\left(-p_2\sqrt{s}\right)-k_3\exp\left(-p_3\sqrt{s}\right)},\quad \nu,\ p_i>0,\ i=1,\ 2,\ 3. \tag{1}$$

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