Computational modeling of a charge transport problem in MOSFET transistor

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Abstract

We propose and describe in detail a new effective numerical algorithm for finding the stationary solutions of charge transport problem in MOSFET transistor. For mathematical description of charge transport process a hydrodynamical MEP model is used. It is worth noting that this model is a set of nonlinear PDE's with small parameters and specific boundary conditions corresponding to MOSFET. It makes the computational process much more complicated. The proposed algorithm is based on the stabilization method, the application of regularized smoothing operators and ideas of schemes without saturation.

Keywords: mathematical modeling; нydrodynamic model; MOSFET; stationary solution; nonstationary regularization; stabilization method;

1. Introduction

Mathematical modeling of semiconductor devices is of great importance for technical applications and becomes in nowadays a rapidly developing area of applied mathematics. The modern state of the art in microelectronic processing allows one to construct such small semiconductor devices that the accuracy of simplified mathematical models is inadmissible for analysis and designing of these devices. We need advanced mathematical models which describe physical phenomena in semiconductors in more detail.

Theory of semiconductor devices is based on the Boltzmann transport equation. However, a direct numerical computation of the full Boltzmann equation (e.g., by Monte Carlo methods) requires a big computational burden. In many cases an admissible accuracy can be achieved by exploiting the drift-diffusion model obtained on the basis of moment equations of the Boltzmann equation. On the other hand, the growing miniaturization of modern electronic devices needs a more accurate modeling of the energy transport in semiconductors. Therefore, we have to improve the standard drift-diffusion model by taking into account the energy of charge carriers. This goal is achieved in hydrodynamical models of charge transport in semiconductors. One of such latest models is described in [1, 2]. This model contains the Poisson equation for the electric potential φ. On Fig. 1 we give a schematic sketch of 2D Silicon MOSFET (Metal Oxide Semiconductor Field Effect Transistor) by using dimensionless parameters. Its typical peculiarity is the presence of a silicon oxide nanochannel.

The main goal of this work is the design, the justification, and the software development of new efficient computational algorithms for finding approximate stationary solutions of hydrodynamical models of charge transport in semiconductors as well as the calculation of electric potential for 2D silicon transistor with a silicon oxide nanochannel.
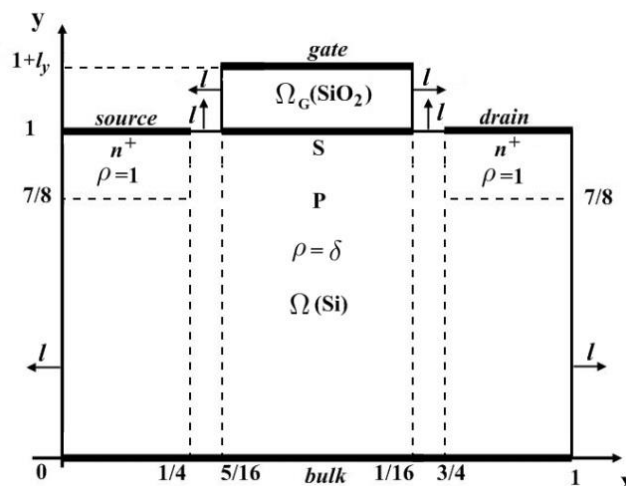

Fig. 1. Schematic view of 2D silicon transistor MOSFET.

2. Problem statement

For physical description of processes taking place in semiconductor devices we will apply the so-called hydrodynamical MEP model proposed in [1, 2]. This model is a set of quasilinear non-stationary PDE's written in the form of conservation laws obtained from a system of moments of the Boltzmann transport equation. While constructing this model the Maximum Entropy Principle (or MEP) was used for for closing the system of moments. In 2D case and dimensionless form the equations of

hydrodynamical MEP model are the following:

$$\begin{aligned}
&R_t + \operatorname{div}\mathbf{J} = 0, \\
&\mathbf{J}_t + \frac{2}{3}\nabla(RE) = R\mathbf{Q} + c_{11}\mathbf{J} + c_{12}\mathbf{I}, \\
&(RE)_t + \operatorname{div}\mathbf{I} = (\mathbf{J},\mathbf{Q}) + cR\sigma, \\
&\mathbf{I}_t + \frac{10}{9}\nabla(RE^2) = \frac{5}{3}RE\mathbf{Q} + c_{21}\mathbf{J} + c_{22}\mathbf{I}.
\end{aligned}\right\} \tag{1}$$

Here $\mathbf{J} = R\mathbf{u}$, $\mathbf{I} = R\mathbf{q}$, R is an electron density, E is the electron energy, $\mathbf{u} = \left(u^{(x)}, u^{(y)}\right)$ is the vector of electron velosity in the Cartensian system (x, y), $\mathbf{q} = \left(q^{(x)}, q^{(y)}\right)$ is the energy flux, $\sigma = \frac{2}{3}E - 1$; $\mathbf{Q} = \nabla\varphi = (\varphi_x, \varphi_y)$, $\varphi = \varphi(t, x, y)$ is the electron potential, satisfying the Poisson equation

$$\Delta\varphi = \varphi_{xx} + \varphi_{yy} = \beta(R - \rho), \ (x, y) \in \Omega, \tag{2}$$

$\rho = \rho(x, y)$ is the doping density. The coefficient c, c_{11}, c_{12}, c_{21}, c_{22} of system (1) are smooth function of the energy E (see [3]), $\beta > 0$ is a constant. Note that in [3-8] a number of different computational algorithms was proposed for finding the numerical solutions of the mathematical model (1), (2).

The hydrodynamical model (1), (2) will be used in this work for seeking the stationary solutions describing the motion of electrons in the 2D silicon transistor MOSFET. The detailed description of such a semiconductor device with electron conductivity is given in the work [3]. The schematic view of MOSFET in the dimensionless variables x, y is given in Fig. 1.

Since there is no charge transport in the nanochannel Ω_G (see fig.1) and, therefore, the electric potential $\Phi = \Phi(t, x, y)$ in the domain Ω_G satisfies the Laplace equation

$$\Delta_{x,y}\Phi = \Phi_{xx} + \Phi_{yy} = 0, \ (x, y) \in \Omega_G, \tag{3}$$

$$\rho = \rho(x, y) = \begin{cases} 1, (x, y) \in \bar{\Omega}_+, \\ \delta(=-0.001), (x, y) \in \bar{\Omega}\setminus\bar{\Omega}_+; \end{cases} \quad \Omega_+ = \left\{(x, y): \frac{7}{8} < y < 1, \left(0 < x < \frac{1}{4}\right) \cup \left(\frac{3}{4} < x < 1\right)\right\}, \quad \Omega = \{(x, y): \ 0 < x < 1, \ 0 < y < 1\},$$

$\Omega_G = \left\{(x, y): \frac{5}{16} < x < \frac{11}{16}, \ 1 < y < 1 + l_y\right\}$ is the nanochannel and l_y is the width of the nanochannel.

Following the work [4] we pose for the mathematical model (1)–(3) the boundary conditions:

$$\varphi = \begin{cases} 0 \text{ at the source: } y=1, \ 0 \le x \le \frac{1}{4}, \\ D \text{ at the drain: } y=1, \ \frac{3}{4} \le x \le 1, \\ B \text{ at the bulk: } y=0, \ 0 \le x \le 1, \end{cases} \tag{4}$$

$$\Phi = G \text{ at the gate: } y = 1 + l_y, \ \frac{5}{16} \le x \le \frac{11}{16}, \tag{5}$$

$$\begin{aligned}
&a) \ (\mathbf{l}, \nabla\varphi) = 0 \ \text{ on } \Gamma_l, \\
&b) \ (\mathbf{l}, \nabla\Phi) = 0 \ \text{ on } \Gamma_l^{(G)},
\end{aligned}\right\} \tag{6}$$

with the matching condition on S:

$$\begin{cases} \frac{1}{3}\Phi_y = \varphi_y, \\ \Phi = \varphi ; \end{cases} \tag{7}$$

where $\Gamma_l = \left\{(x, y): x = 0 \cup x = 1, \ 0 < y < 1; \ y = 1, \left(\frac{1}{4} < x \le \frac{5}{16}\right) \cup \left(\frac{11}{16} \le x < \frac{3}{4}\right)\right\}$,

$\Gamma_l^{(G)} = \left\{ (x, y) : x = \dfrac{5}{16} \cup x = \dfrac{11}{16}, 1 < y < 1 + l_y \right\}$, $\boldsymbol{l}$ – is a unit outer normal vector, $S = \left\{ (x, y) : y = 1, \dfrac{5}{16} < x < \dfrac{11}{16} \right\}$, $D = V_D \dfrac{e}{K_B T_0}$,

$G = V_G \dfrac{e}{K_B T_0} - 10$, $B = -11 \ln 10$, V_D, V_G is the applied voltage ($V_D = 1 \div 2V$, $V_G = 0.5 \div 1.5V$), K_B is the Boltzmann constant, T_0 is the lattice temperature, and e is the electron charge.

Following [5,7] recall that the mathematical model (1)–(3) in the stationary case can be reduced to a system of elliptic quasilinear equations:

$$\Delta \sigma = \mathrm{F}^{(\sigma)}(\nabla \sigma, \nabla R, \mathbf{Q}, \sigma, R) = a_1 |\nabla \sigma|^2 + \dfrac{1}{R}(\nabla R, a_2 \nabla \sigma + a_4 \mathbf{Q}) + a_3 (\nabla \sigma, \mathbf{Q}) + a_5 |\mathbf{Q}|^2 + bc\sigma, \tag{8}$$

$$\begin{aligned} \Delta R = \mathrm{F}^{(R)}(\nabla \sigma, \nabla R, \mathbf{Q}, \sigma, R, \rho) &= b_1 R |\nabla \sigma|^2 + b_2 (\nabla \sigma, \nabla R) + \\ &+ b_3 R (\nabla \sigma, \mathbf{Q}) + b_4 (\nabla R, \mathbf{Q}) + b_5 R |\mathbf{Q}|^2 + \dfrac{\beta}{1 + \sigma}(R - \rho) R + ncR\sigma, \end{aligned} \tag{9}$$

$$\Delta \varphi = \mathrm{F}^{(\varphi)}(R, \rho) = \beta (R - \rho), \tag{10}$$

and the components of vectors $\mathbf{u}$, $\mathbf{q}$ can be obtained as follows:

$$\begin{cases} \mathbf{u} = F(E) \left\{ \mathbf{Q} - \dfrac{1 + \sigma}{R} \nabla R - F_0(E) \nabla \sigma \right\}, \\ \mathbf{q} = G(E) \left\{ -\mathbf{Q} + \dfrac{1 + \sigma}{R} \nabla R + G_0(E) \nabla \sigma \right\}. \end{cases}$$

Here $|\nabla \sigma|^2 = \sigma_x^2 + \sigma_y^2$ etc., $a_1 = -a' F(E) F_0(E) + b' G(E) G_0(E)$, $a_2 = -1 + (1 + \sigma)\{ b' G(E) - a' F(E) \}$, $a_3 = a' F(E) - b' G(E) - b F(E) F_0(E)$, $a_4 = -b(1 + \sigma) F(E)$, $a_5 = b F(E)$, $b_1 = -m' F(E) F_0(E) + n' G(E) G_0(E)$, $b_2 = (1 + \sigma)\{ n' G(E) - m' F(E) \}$, $b_3 = -\dfrac{1}{(1 + \sigma)^2} + m' F(E) - n' G(E) - n F(E) F_0(E)$, $b_4 = \dfrac{1}{1 + \sigma} + b F(E) F_0(E)$, $b_5 = n F(E)$,

$a = a(E) = \dfrac{2}{5} \dfrac{c_{21}}{1 + \sigma} - c_{11}$, $b = b(E) = \dfrac{2}{5} \dfrac{c_{22}}{1 + \sigma} - c_{12}$, $m = m(E) = \dfrac{c_{11} - a}{1 + \sigma}$, $n = n(E) = \dfrac{c_{12} - b}{1 + \sigma}$, $F(E) = -\dfrac{c_{22} - \dfrac{5}{3} E c_{12}}{det}$,

$G(E) = -\dfrac{c_{21} - \dfrac{5}{3} E c_{11}}{det}$, $F_0(E) = 1 - \dfrac{\dfrac{5}{3} E c_{12}}{c_{22} - \dfrac{5}{3} E c_{12}}$, $G_0(E) = 1 - \dfrac{\dfrac{5}{3} E c_{11}}{c_{21} - \dfrac{5}{3} E c_{11}}$, $det = c_{11} c_{22} - c_{21} c_{12}$, $a' = \dfrac{da}{d\sigma} = \dfrac{3}{2} \dfrac{da}{dE}$ etc.

Thus, in the stationary case the initial mathematical model (1), (2) can be reduced to a system of three Poisson equations (8)-(10). To complete the formulation of a problem we should pose for functions σ, R the boundary conditions:

$$\begin{aligned} R &= \begin{cases} 1 \text{ at the } y = 1, \ \left(0 \le x \le \dfrac{1}{4} \right) \cup \left(\dfrac{3}{4} \le x \le 1 \right), \\ 0 \text{ at the } y = 0, \ 0 \le x \le 1; \end{cases} \\ \sigma &= \begin{cases} 0 \text{ at the } y = 1, \ \left(0 \le x \le \dfrac{1}{4} \right) \cup \left(\dfrac{3}{4} \le x \le 1 \right), \\ 0 \text{ at the } y = 0, \ 0 \le x \le 1; \end{cases} \\ & \quad (\boldsymbol{l}, \nabla \sigma) = (\boldsymbol{l}, \nabla R) = 0 \text{ on } \Gamma_l, \\ & \quad \sigma_y = 0, \ R_y = R\varphi_y / (1 + \sigma) \text{ on } S. \end{aligned} \tag{11}$$

The boundary conditions (11) are posed in view of the recommendations from [4– 5].

In [9] we have reduced the boundary problem (2)-(7) for finding the electric potential in the domain $\Omega \cup \Omega_G$ to that of finding the potential φ only within the domain Ω with the boundary condition on S: $\varphi(x, 1) + 3l_y \varphi_y(x, 1) = G$, $(x, y) \in S$. Moreover, we have obtained the null and the first approximations for finding the potential $\Phi(x, y)$ in the domain Ω_G. The null approximation is defined in the following way: $\Phi(x, y) = 3l_y \varphi_y(x, 1) \left(\dfrac{y - 1}{l_y} - 1 \right) + G = \dfrac{y - 1}{l_y}(G - \varphi(x, 1)) + \varphi(x, 1)$.

3. Computational algorithm for the regularized problem

For finding numerical solution of three Poisson equations (8)-(10) we will apply the ideas of the computational algorithm described in [5,7,10] and based on the stabilization method [11], the method of lines [12], the principles of non-saturating schemes and usage of non-stationary regularizations. For the technology proposed in [7] we can apply one of the two nonstationary regularizations: the parabolic or Sobolev's one.

After the application of parabolic regularization to equation (8-10) we get the relations

$$\sigma_t = \Delta\sigma - F^{(\sigma)}(\nabla\sigma, \nabla R, \mathbf{Q}, \sigma, R), \ \sigma = \sigma(t,x,y), \ t > 0, \ (x,y) \in \Omega,$$

$$R_t = \Delta R - F^{(R)}(\nabla\sigma, \nabla R, \mathbf{Q}, \sigma, R, \rho), \ R = R(t,x,y), \ t > 0, \ (x,y) \in \Omega,$$

$$\varphi_t = \Delta\varphi - f(x,y), \ \varphi = \varphi(t,x,y), \ t > 0, \ (x,y) \in \Omega.$$

After the application of Sobolev's regularization to equation (8-10) we get the relations

$$\sigma_t - \Delta\sigma_t = \Delta\sigma - F^{(\sigma)}(\nabla\sigma, \nabla R, \mathbf{Q}, \sigma, R), \ \sigma = \sigma(t,x,y), \ t > 0, \ (x,y) \in \Omega,$$

$$R_t - \Delta R_t = \Delta R - F^{(R)}(\nabla\sigma, \nabla R, \mathbf{Q}, \sigma, R, \rho), \ R = R(t,x,y), \ t > 0, \ (x,y) \in \Omega,$$

$$\varphi_t - \Delta\varphi_t = \Delta\varphi - f(x,y), \ \varphi = \varphi(t,x,y), \ t > 0, \ (x,y) \in \Omega.$$

For numerical calculations we should define initial data $\sigma_0 = \sigma(0,x,y)$, $R_0 = R(0,x,y)$, $\varphi_0 = \varphi(0,x,y)$.

Its main idea is to approximate in the regularized equations the time derivative by a diference relation and the x derivative by an interpolation polynomial with interpolation nodes at zeros of the Chebyshev polynomial [11]:

$$P(x,\varphi) = \frac{1}{N}\sum_{i=1}^{N}(-1)^{i-1}\frac{\sin x_i}{\cos x - \cos x_i}\cos(Nx) \cdot \varphi_i(t,y), \ 0 \le x \le \pi,$$

$$\left. \begin{array}{l} x = x_j = \dfrac{2j-1}{2N}\pi, \ j = \overline{1,N}, \\ \varphi(t,x_j,y) = \varphi_j(t,y). \end{array} \right\}$$

As the result, the original problem for the equations of the MEP model is reduced to a boundary value problem for a second-order ODE system. The solution of this problem is written in the form of a cubic interpolation C^2 spline [13]. Then, we get the three point scheme [14]

$$\left\{I_N - \frac{h_y^2}{6}B_r\right\}\hat{U}_{k-1} - 2\left\{I_N + \frac{h_y^2}{3}B_r\right\}\hat{U}_k + \left\{I_N - \frac{h_y^2}{6}B_r\right\}\hat{U}_{k+1} = \frac{h_y^2}{6}\left\{F_{k-1} + 4F_k + F_{k+1}\right\}, \ k = \overline{1,K-1}. \tag{12}$$

with the boundary conditions

$$\hat{U}_1 = A_0\hat{U}_0 + L_0, \hat{U}_K = A_K\hat{U}_{K-1} + L_K. \tag{13}$$

Here $\hat{U}$ is the vector of values of the unknown in the nodes of the interpolation function, N is the number of these nodes, I_N is the unit matrix of order N, h_y is the mesh width of spline-interpolation; the elements of the matrices A_0 and A_K and the components of the vectors L_0 and L_K are determined from the boundary conditions at $y = 0$ and $y = 1$, and concrete expressions for the elements of the matrix B_r and the components of the vector F are written down in [10].

Thus, the solution of the regularized equation at each time layer can be found from (12) and (13) by the matrix sweep method. Then, using the idea of the stabilization method, we pass from the previous to the next layer until the stationary solution is found.

At each time layer in the process of stabilization we should step by step solve three boundary value problems for the regularized Poisson equations (8)–(10).

In computations we met some difficulties. Under the usage of the stabilization method there appeared a jump growth of the unknowns caused by nonlinearity of the problem. Namely, the norm of solution became very big that led to the buffer overflow

and the program stop until stabilization. To overcome this difficulty we used nonlinear iterations. The main idea of the algorithm based on nonlinear iterations is the calculation of parameters and variables of the problem by formulas assigned for a next time layer whereas we stay at the present time layer. To clarify this we use nonlinear iterations for a modification of the scheme (12), (13). In this case the scheme (12), (13) should be reduced to the form

$$\left\{I_N - \frac{h_y^2}{6} B_k^{[l-1]}\right\} \hat{U}_{k-1}^{[l]} - 2\left\{I_N + \frac{h_y^2}{3} B_k^{[l-1]}\right\} \hat{U}_k^{[l]} + \left\{I_N - \frac{h_y^2}{6} B_k^{[l-1]}\right\} \hat{U}_{k+1}^{[l]} =$$

$$= \frac{h_y^2}{6}\left\{F_{k-1}^{[l-1]} + 4F_k^{[l-1]} + F_{k+1}^{[l-1]}\right\}, \ k = \overline{1, K-1}, l = \overline{1, N_t},$$

(14)

where the components of the vector $F_k^{[l-1]}$ and the elements of the matrix $B_k^{[l-1]}$ are calculated at the $(l-1)$-th nonlinear iteration; N_t is the number of nonlinear iterations at each time layer. The elements of the matrix $B_k^{[0]}$ and the components of the vector $F_k^{[0]}$ are taken from the previous time layer. At the l-th nonlinear iteration we compute the values of the components of the vector $\hat{U}_k^{[l]}, k = \overline{1, K-1}$ according to (14). Then, using these values we calculate the elements of the matrices $B_k^{[l]}$ and the components of the vector $F_k^{[l]}$. After that the program passes to the $(l+1)$-th nonlinear iteration. For $l = N_t$ it we pass to the next time layer.

4. Results of computations

To get an approximate solution for a desired set of parameters of the problem we set initial data in different ways. That is, we first set original initial data, for instance, such as $\sigma(0, x, y) = 0$, $R(0, x, y) = 1$, $\varphi(0, x, y) = 0$.

After setting the initial data we start iterations of the stabilization method in which using the variables computed at the previous and present time layers we calculate the right-hand sides $F^{(\sigma)}$, $F^{(R)}$, $F^{(\varphi)}$ and solve the equations for σ, R and φ respectively. These iterations work until the solution is stabilized, i.e., until the norm of the difference between the solutions at the next and previous time layers is close to zero.

Simulation program was created on the basis of the Object Pascal information processing language in the Delphii6 environment.

These programs include:

1. Setting of parameters of the numerical algorithm, parametrs of the original problem, initial data for the original unknowns.
2. Storage of physical parameters which are necessary for computations.
3. Regularization choice (Sobolev's and parabolic regularizations).

Computations were performed for different values of parameters.

The graphs for the electron energy E and the electric potential φ are given on Fig. 2.
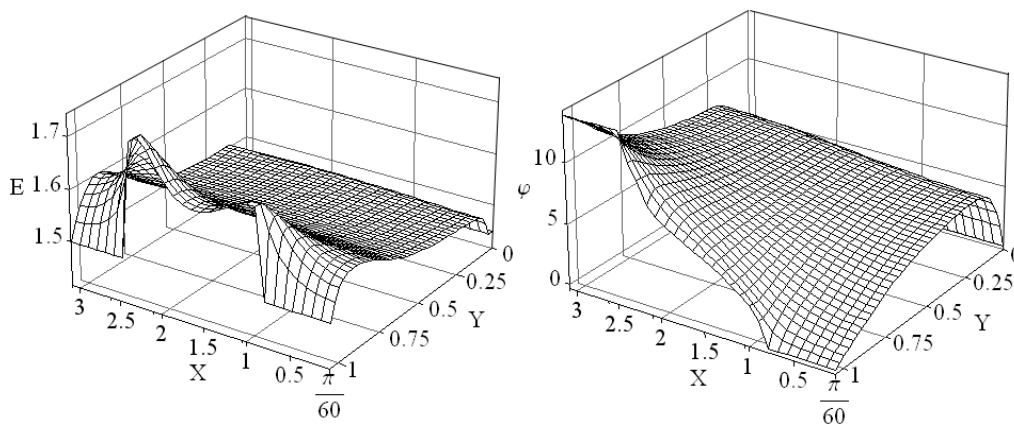

Fig. 2. Approximate solution for the electron energy and electric potential in dimensionless variables.

5. Conclusion

In this paper for finding solutions of the problem on charge transport in MOSFET we proposed numerical algorithm using interpolation polynomials, spline approximations and the matrix sweep method. We hope that the obtained results stimulate a further development and improvement of numerical algorithms for problems of physics of semiconductors (this will be useful for the construction of real devices) and the proposed methods will be adopted for finding numerical solutions of various applied problems outside semiconductor subjects.

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