Simulation of charge transport in micro and nanoscale FETs with elements having different dielectric properties

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Abstract. The hydrodynamical model is used for description of the process of charge transport in semiconductors with a high rate of reliability. It is a set of nonlinear partial differential equations with small parameters and specific conditions at the boundaries of field effect transistors (FETs), which essentially complicates the process of finding its stationary solutions. To overcome these difficulties in the case of FETs with elements having different dielectric properties, a fast pseudospectral method has been developed. This method was used for advanced numerical simulation of charge transport in DG-MOSFET.

1. Introduction

The size of semiconductor electron devices is becoming increasingly smaller, up to micro and nanoscales, which leads to the complication of both fabrication methods and structures of modern field effect transistors (FETs). Therefore, for designing such devices, one needs to develop a theoretical basis that includes new reliable mathematical models and accurate numerical methods. Indeed, an adequate description of processes taking place in the semiconductor requires accounting for energy transport effects and impact ionization, as well as dielectric, doping and geometric properties of structural elements of FETs. Since the study of such models by analytical methods can be technically impossible, methods of predictive numerical simulation are often used. However, due to small parameters and complex boundary conditions, many of today's numerical methods turn out to be not sufficiently stable, accurate and fast. The aim of our work is to develop the mathematical model and method for solving these problems. As an example, we consider the problem of charge transport in DG-MOSFET (nano-size Double Gate-Metal Oxide Semiconductor Field Effect Transistor).

2. Hydrodynamical model based on the Maximum Entropy Principle and its applications

Here we shall focus on a hydrodynamical model based on the Maximum Entropy Principle (or MEP) describing the process of charge transport in semiconductors with a high degree of reliability. This model was proposed in [1,2], and it is a set of quasilinear non-stationary partial differential equations (PDEs) written in the form of conservation laws obtained from the system of moments of the Boltzmann transport equation. While constructing this model, the MEP was used for closing the system of moments. In [3], a specific procedure was applied for deriving the dimensionless form of the MEP model and for obtaining its resolving equations. In the 2D case, these equations are:
\[
\begin{align*}
\begin{cases}
R + \text{div}(\vec{J}) = 0, & \vec{J} = \frac{2}{3} \nabla (RE) = R\vec{Q} + c_1\vec{J} + c_{12}\vec{I}, \\
(\text{RE}), + \text{div}(\vec{I}) = (\vec{J}, \vec{Q}) + cR\sigma, & \vec{I} = \frac{10}{9} \nabla (RE^2) = \frac{5}{3} R\vec{Q} + c_2\vec{J} + c_{22}\vec{I}.
\end{cases}
\end{align*}
\]

Here \( R \) is the electron density, \( E \) is the electron energy, \( \vec{J} = R\vec{u}, \ \vec{I} = R\vec{q}, \ \vec{u} = (u^{(x)}, u^{(y)}) \) is the vector of the electron velocity in a Cartesian coordinate system \((x, y)\), \( \vec{q} = (q^{(x)}, q^{(y)}) \) is the energy flux, \( \vec{Q} = \nabla \varphi = (\varphi_x, \varphi_y) \), \( \varphi = \varphi(t, x, y) \) is the electric potential satisfying the Poisson equation:

\[
\Delta \varphi = \varphi_{xx} + \varphi_{yy} = \beta (R - \rho); \quad (2)
\]

\( \rho = \rho(x, y) \) is the doping density (a given function in the interior of the semiconductor). In certain domains of semiconductor devices, the values of this function are less than in other domains by a factor of \( 10^5 - 10^{10} \). The coefficients \( c_{11}, \ldots, c_{22}, c \) of system (1) are smooth functions of the energy \( E \), detailed in [3], and \( \beta > 0 \) is a dimensionless constant (see [3]) that depends on the dielectric properties of the semiconductor and on other parameters and takes high values. Note that equations (1), (2) of the MEP model were studied both analytically and numerically in [3–5].

Below, the FETs containing several domains \( \Omega_q, \ q = 1, \ldots, Q \) with different dielectric properties are considered (in this case \( \beta \) is the piecewise constant, \( \beta = \beta_q \) in \( \Omega_q \)); \( \Sigma_q \) is the border separating adjacent domains \( \Omega_q \) and \( \Omega_{q+1} \). The domain of FET is \( \Lambda = \bigcup \Omega_q \). In each \( \Omega_q \), the boundary conditions for the electric potential should be imposed. They include the following:

1) **Voltage conditions**, i.e. \( \varphi = B \) on a source of a device, \( \varphi = G \) on a gate and \( \varphi = D \) on a drain.

2) **Matching conditions** on \( \Sigma_q \), which are:

\[
\varphi|_{\Sigma_q} = \varphi|_{\Sigma_q}, \quad \frac{\partial \varphi}{\partial \mathbf{n}_q}|_{\Sigma_q} = \mu_q \frac{\partial \varphi}{\partial \mathbf{n}_q}|_{\Sigma_q},
\]

(3)

3) **Free-slip conditions** at all other points of a boundary of \( \Lambda \). They are \( (\alpha, \nabla \varphi) = 0 \).

Here \( \varphi|_{\Sigma_q}, \varphi|_{\Sigma_q} \) are the values of \( \varphi \) as its argument goes to \( \Sigma_q \) from \( \Omega_q \) and from \( \Omega_{q+1} \); \( \alpha, n_q \) are the vectors of outward normal to \( \Lambda \) and to \( \Sigma_q \). The following parameters are dimensionless:

\[
B = \ln \left( \frac{N^+}{N_i} \right), \quad D \equiv \frac{e}{K_BT_0} V_D + B, \quad G \equiv \frac{e}{K_BT_0} V - 10 + B; \quad \mu_q = \frac{\beta_q}{\beta_{q+1}}, \quad \beta_q = \frac{e^2 L N^+}{\kappa_q K_BT_0}
\]

(4)

and \( V_D, V^\pm, e, L, N^+, \kappa_q, K_B, T_0, N_i \) are dimensional parameters described in table 1.

Following [3–5], we recall that equations (1), (2) in the stationary case can be reduced to a system of nonlinear PDEs of the elliptic type:

\[
\Delta \sigma = a_1 |\nabla \sigma|^2 + a_2 (\nabla \sigma, \vec{X}) + a_3 (\nabla \sigma, \vec{Q}) + a_4 (\vec{X}, \vec{Q}) + a_5 |\vec{Q}|^2 + bc \sigma,
\]

\[
\Delta \chi = - |\vec{X}|^2 + b_1 |\nabla \sigma|^2 + b_2 (\nabla \sigma, \vec{X}) + b_3 (\nabla \sigma, \vec{Q}) + b_4 (\vec{X}, \vec{Q}) + b_5 |\vec{Q}|^2 + \frac{\beta}{1 + \sigma} (e^x - \rho) + nc \sigma,
\]

(5)

(6)

\[
(1/\beta) \Delta \varphi = (e^x - \rho)
\]

(7)

and the components of the vectors \( \vec{u}, \vec{q} \) can be obtained as follows:

\[
\vec{u} = F(E) (\vec{Q} - (1 + \sigma)\vec{X} - F_0(E)\nabla \sigma), \quad \vec{q} = G(E) (-\vec{Q} + (1 + \sigma)\vec{X} + G_0(E)\nabla \sigma).
\]

(8)
Here \( \tilde{Q} = (\varphi_x + D - B, \varphi_y)^T \), \( \tilde{X} = \nabla \chi \), \( \chi = \ln R \), \( |\nabla \sigma|^2 = \sigma_x^2 + \sigma_y^2 \), \( \sigma = 2E / 3 - 1 \) etc., and the coefficients \( a_i - a_9 \), \( b_i - b_9 \), \( n, F_0, G_0 \) are nonlinear functions of \( E \) of a certain form (see [3]).

We impose the conditions at the boundaries \( \partial \Lambda, S_q \) for functions \( \chi, \sigma \) as follows:

1) the dimensionless electron density \( R \) on \( \partial \Lambda \) is equal to unity, therefore \( \chi_{\partial \Lambda} = 0 \),

2) the dimensionless electron energy \( E \) on \( \partial \Lambda \) is equal to 3/2. On the borders \( S_q \), the normal derivative of \( E \) is equal to zero, then \( \sigma_{\partial \Lambda} = 0 \) (see [3]),

3) charge carriers don’t flow through \( S_q \), therefore \( (\tilde{u}, n_q) = 0 \) and the first of equations (8) yields

\[
\frac{\partial \chi}{\partial n_q}_{\partial \Lambda} = \frac{(\varphi_x + D - B)n_{q_x} + \varphi_x n_{q_x}}{1 + \sigma}, \quad n_q = (n_{q_x}, n_{q_y}).
\]

3. Pseudospectral numerical method for finding distributions of \( \varphi, \sigma, \chi \) in FET

Below we shall assume that \( \Lambda \) is a rectangular domain and \( \Omega_q \) are its rectangular subdomains, i.e. \( S_q \) are parallel to the \( x \) or \( y \) axis. Without loss of generality, let them be parallel to the \( x \) axis. Since it can be easily checked by (4) that for real devices \( 1 / \beta \sim 10^{-4} \sim 10^{-8} \), then (5) – (7) is a nonlinear coupled system with a small parameter at the highest order derivatives of \( \varphi \). To solve it, we shall design a highly accurate and stable algorithm based on an iterative stabilization technique and interpolation polynomials with Chebyshev nodes; see [4]. It is briefly described here by the example of a test boundary value problem

\[
\Delta \varphi = f(x, y, \varphi), \quad \Lambda = [0, \pi] \times [0, \pi],
\]

where \( \varphi \) satisfies Neumann or Dirichlet conditions on \( \partial \Lambda \) that are the free-slip or the voltage conditions (see above). After a linear change of variables, the domain \( \Lambda \) can be fit to any given rectangular domain. Introducing the additional time variable \( t \), we derive the evolution equation:

\[
\varphi_t = \Delta \varphi - f(x, y), \quad \varphi = \varphi(x, y, t), \quad t > 0.
\]

For (10), we take just the same boundary conditions and add the initial data to them at \( t = 0 \). We seek a solution to (9) as the limit of solutions to (10) as \( t \to \infty \). Introducing a grid with respect to the time variable \( t \) with the step \( \tau \) and the nodes \( t_n = n\tau \), \( n = 1, 2, \ldots \), denoting \( \varphi^{(n)} = \varphi^{(n)}(x) = \varphi(x, y, t_n) \) and approximating the derivative \( \varphi_t \) by the difference quotient \( \varphi^{(n)} - \varphi^{(n-1)} \), \( \tau \), one obtains the formula:

\[
\varphi^{(n)} - \tau \Delta \varphi^{(n)} = \varphi^{(n-1)} - \tau f(x, y, \varphi^{(n-1)}) = \tilde{f}(x, y, \varphi^{(n-1)}).
\]

In accordance with [4], if Neumann conditions are imposed at the boundary \( x = 0, \pi \), then the solution to (11) on the segment \( x \in [0, \pi] \) is approximated by the following interpolation polynomial obtained from the polynomial with Chebyshev nodes by a simple transformation of a variable:

\[
\mathcal{P}_1(x, \varphi^{(n)}) = \frac{1}{N} \sum_{j=1}^{N} (-1)^{j-1} \sin \frac{x_j \cos(Nx)}{\cos x - \cos x_j} \varphi^{(n)}(y) + f_1(x, y), \quad x_j = \frac{2j - 1}{2N} \pi, \quad j = 1, \ldots, N. \]

If at \( x = 0, \pi \) Dirichlet conditions are imposed, then the following approximation of \( \varphi \) is applied:

\[
\mathcal{P}_2(x, \varphi^{(n)}) = \frac{1}{N+1} \sum_{j=1}^{N} (-1)^{j-1} \sin x_j \sin(N+1)x \varphi^{(n)}(y) + f_2(x, y), \quad x_j = \frac{\pi j}{N+1}, \quad j = 1, \ldots, N.
\]
where \( x_j \) are the interpolation nodes, \( \varphi_j^{(n)}(y) = \varphi_j^{(n)}(x_j, y) \) and \( f_{1,2} \) are the functions of a simple form satisfying the given boundary conditions. Denoting by \( \mu \) one of the derivatives \( \mu \in \{x, xx\} \) and setting \( \varphi_j^{(n)}(y))_\mu = \varphi_j^{(n)}(x_j, y) \), one forms the vectors: \( \Phi(y) = (\varphi_j^{(n)}(y))_N \), \( \Phi_\mu(y) = ((\varphi_j^{(n)}(y))_\mu)_N \), \( \tilde{F}(y) = \tilde{f}(x_j, y, \varphi_j^{(n+1)}) \). Using l’Hôpital rule for each of (12), (13), one can find the limit expressions of its first order and second order derivatives as \( x \to x_j \), which are linear combinations of \( \varphi_j^{(n)}(y) \) for each \( i \). Collecting the coefficients of these combinations into matrices \( A \) and \( B \), one can finally obtain the pseudospectral matrix approximations of the derivatives:

\[
\Phi_x(y) = A\Phi(y), \quad \Phi_{xx}(y) = B\Phi(y).
\]

Substituting (12) or (13) into (11) and using (14), one obtains the system of second-order equations

\[
\Phi''(y) = B\Phi(y) + \tilde{F}(y)/\tau,
\]

where a dash means differentiation with respect to \( y \), \( \tau = (I_N - B)/\tau \) with \( I_N \) being the identity matrix of size \( N \). It is worth noting that the matrices \( B \) are symmetric in both cases of Neumann and Dirichlet conditions (see [4]), which allows one to use stable and fast methods for inverting \( B \). Approximations (12), (13) provide high accuracy only if \( \varphi \) has a high order of smoothness, therefore (3) means that the formulas similar to (12), (13) cannot be applied along the \( y \) axis. Thus, for approximating \( \Phi(y) \) an interpolation cubic \( C^2 \)-spline is used (see [3,4]). Using the continuity of spline derivatives, one obtains the following difference schemes in each \( \Omega_q \), \( q = 1, ..., Q \) from (15):

\[
\left\{ I - \frac{h^2}{6} B \right\} \bar{R}_m^{\pm} - 2\left\{ I + \frac{h^2}{3} B \right\} \bar{R}_m^{\pm} + \left\{ I - \frac{h^2}{6} B \right\} \bar{R}_{m+1}^{\pm} = \frac{h^2}{6} \left\{ \mathcal{F}_m^{\pm} + 4\mathcal{F}_m + \mathcal{F}_{m+1} \right\},
\]

where \( \bar{R}_m^{\pm} = \Phi(y_m) \) in \( \Omega_q \) and \( \tilde{F}_m = \Phi(y_m) \) \( y_m = mh_q, \quad m = 0, ..., M_q, \quad M_q h_q = \pi \). The schemes (16) should be supplemented with the conditions at the boundary of \( \Lambda \) described in the first section and with matching conditions (3). To solve (16), we propose to use a matrix Thomas algorithm, which requires \( O(N^3) \sum_{q=1}^{Q} 8M_q \). It is worth noting that a similar algorithm was used in [5] for simulation of charge transport in a single domain of MOSFET. Here, it is significantly modified in order to perform the computations for an arbitrary number of subdomains \( \Omega_q \) with different conditions (voltage or free-slip) at their boundaries. To this end, the following new methods were developed.

Firstly, the method of coordination of interpolation nodes \( x_j \) of (12), (13) was designed for the case when subdomains have different types of conditions at the boundaries \( x = 0, \pi \). The idea is to approximate the values of \( \varphi_j^{(n)}(y) \) in the nodes \( x_j \) of (12) using the linear combination of its values in four nearby nodes of (13). Thus, the space grid of (13) becomes common for all subdomains and (14) remains valid, but the expressions for elements of \( A \) and \( B \) become much more cumbersome.

Secondly, the Thomas algorithm has been significantly changed in order to correctly specify its sweep coefficients on the borders \( S_q \). The forward and backward sweeps of our algorithm have \( Q \) stages (each stage corresponds to a subdomain). On the current stage of forward sweep, the coefficients are resolved using the coefficients from the previous stage and the matching conditions. Similarly, the solution on the current stage of backward sweep is obtained using the solution from the previous one.
Finally, all these methods have been implemented using the Object Pascal environment in a programm package for solving the problems with an arbitrary number of subdomains $Q$, arbitrary geometrical and physical parameters, and boundary conditions.

4. Application of the proposed method to simulation of charge transport in DG-MOSFET
A detailed description of DG-MOSFET is given in [6]. A special feature of this silicon transistor is the presence of two subdomains fabricated of silicon oxide. The dielectric properties of silicon and silicon oxide differ by three times (see table 1). The DG-MOSFET in dimensionless variables $x$ and $y$ is sketched in figure 1. Here $b = 10$ nm (0.35) is the length of gates, $l_x, l_y = 1–2$ nm (1/30–1/15) are thicknesses of silicon oxide layers, $l_x = 1.5–4.5$ nm (0.05–0.15) characterizes the distribution of $\rho$ in the domain $\Omega_2$, and $a = 4–8$ nm (2/15–4/15) is the thickness of the domain $\Omega_2$. Here the dimensionless values are given in brackets. It should be noted that there is no charge transport in silicon oxide layers $\Omega_{1,3}$ and, therefore, the electric potentials in them satisfy the Laplace equation $\Delta \varphi = 0$. Table 1 contains all physical parameters necessary to perform the simulation.

![Figure 1. Schematic sketch of a 2D silicon DG-MOSFET.](image)

| Variable | Description | Value |
|----------|-------------|-------|
| $e$ | Electron charge | $1.6 \times 10^{-19}$ C |
| $L$ | Characteristic linear size | 30 nm ($3 \times 10^{-8}$ m) |
| $N^+$ | Doping density in the domains $n^+$ | $2 \times 10^{26}$ m$^-3$ |
| $T_0$ | Temperature of lattice | 300 K |
| $K_B$ | Boltzmann constant | $1.38 \times 10^{-23}$ J / K |
| $\kappa$ (Si) | Dielectric constant of silicon | $1.03545 \times 10^{-10}$ C / Volt m |
| $\kappa$ (SiO$_2$) | Dielectric constant of SiO$_2$ | $1/3 \kappa$ (Si) |
| $N_i$ | Internal electron concentration in the domain $n_i$ | $10^{16}$ m$^-3$ |
| $V^\pm, V_D$ | Bias voltages | $0–2$ Volt |
Using the proposed algorithm, we got the distribution of (a) the electric potential (in Volts), (b) the dimensionless electron energy (see figure 2) and the current-voltage curves (see figure 3).

![Figure 2. Solutions obtained for $V_D = 2$ Volt, $V' = 0.01$ Volt, $V'' = 1.5$ Volt $\delta = 5 \times 10^{-10}$, $l_x = 0.03334$, $l_y = 0.06$, $l_z = 0.15$, $\alpha = 0.2$.](image1)

![Figure 3. Current-voltage curves for DG-MOSFET obtained for $l_y = l_y = 1$ nm, $\alpha = 4$ nm, $l_z = 3$ nm: (a) the dependence of the electrical current $J_D$ flowing through the drain on the drain voltage $V_D$ for $V'$ = 0.538 Volt; (b) the dependence of $J_D$ on the gate voltage $V''$ for $V_D = 3$ Volt.](image2)

5. Conclusions
Finally, we pay attention to an interesting fact that was discovered while drawing the current-voltage curves. Analyzing the behavior of the curve in figure 3(a), we can see that for DG-MOSFET the regimes with "blockage" are possible, i.e., when the electric current begins to flow from the drain into the device. There are other important effects that have been discovered by analyzing the solutions.

The first is a small potential well along the line $x = b - l_x$. It is caused by an extreme doping density difference on this line ($\delta = N_i / N^+ \sim 10^{-10}$; see figure 1 and table 1). This effect has been found due to the high stability of the interpolations (12), (13) and a special smoothing of doping density.

The second effect is a break of the electric potential on the lines $S_1, 2$ caused by an essential difference of dielectric properties of materials. It significantly affects all the physical processes, including the current.
The third effect is that by specifying different bias voltages on two gates, one can manipulate all
the parameters of charge transport in very wide ranges, making their profiles more or less symmetric.
The quantitative data for these manipulations can be obtained by the designed algorithm.

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