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Analysis of the transient response of MIS circuits using pseudo-wavelet approach

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ABSTRACT

This paper deals with the possibilities offered by the wavelet transform used in the analysis of the transient response of MIS circuits. This approach has certain advantages over the classical finite element or finite difference-based algorithms when applied to drift-diffusion (Roosbroeck's) model.

1. INTRODUCTION

The transient response of MIS circuits is determined by the transient response of the concentration of carriers in MIS structures, for example in the channel of the MIS transistors.

At the most fundamental level the flow of the charge carriers is described by transport equations derived from quantum mechanics, semiclassical or classic models. The common feature of these equations is the employment of a phase space density function $f(x,v,t)$ of the spatial variable $x \in \Omega$, velocity variable $v \in \mathbb{R}^3$, and the time variable $t \in (0,\infty)$.

A widely used transport equation is the Boltzmann equation:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f - \nabla U \cdot \nabla_v f = (\mathcal{C})_c$$

(1)

where $U(x,t)$ is the electrostatic potential:

$$\Delta U = \int f dv - C$$

(2)

$C$ is the doping profile and the term $(\mathcal{C})_c$ is the collision operator.

The simulations by solving the Boltzmann equation are known to be very time-consuming, so they cannot be employed for fast circuit simulations.

A frequently employed method to make the Boltzmann equation more tractable was found to be the 'moment method' approach.

By this method the hydrodynamic model is derived which in turn is reduced to drift-diffusion equations, e.g. van Roosbroeck model which consist of:

Poisson's equation:

$$\varepsilon \Delta U = \rho$$

(3)

continuity equation for electrons:

$$\frac{\partial n}{\partial t} = \frac{1}{q} \text{div} J_n - R(n,p)$$

(4)

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continuity equation for holes:

\[ \frac{\partial p}{\partial t} = \frac{1}{q} \text{div} J_p + R(n, p) \]  

(5)

where \( J_n \) is the electron current density:

\[ J_n = q\mu_n (U_T \nabla n - n \nabla U) \]  

(6)

\( J_p \) is the hole current density:

\[ J_p = q\mu_p (U_T \nabla p + p \nabla U) \]  

(7)

\( \rho \) is the charge concentration:

\[ \rho = q(n - p - C) \]  

(8)

\[ R(n, p, x) \] is the net generation-recombination rate, \( \mu_n = \mu_n(n, \nabla U, C, x) \) and \( \mu_p = \mu_p(p, \nabla U, C, x) \) are the mobilities of electrons and holes, respectively, \( C = C(x) \) is the doping profile, \( U_T \) is the thermal voltage, \( \varepsilon(x) \) is the electric permittivity and \( q \) is the elementary charge.

That drift-diffusion model constitutes up to now the core of state-of-the-art semiconductor device simulation programs. In conclusion, the mathematical description of the transient process in MIS circuits is based on the nonlinear partial differential equations for electrons and holes, which are coupled together through the Poisson equation. The crucial element in realisation of the algorithm is effectiveness of this coupling.

2. SOME NOTES ON POISSON EQUATION

The potential distribution is described using the equation:

\[ \frac{d^2 u}{dx^2} = \frac{Q(u, x)}{\varepsilon}, \]

where:

\[ Q(u, x) = Q(u) + qN(x); \]

\[ N(x) = N_0 + N_1(x); \]

\[ Q(u) = -q(a_1 \exp(-au) - a_2 \exp(au)); \]

\[ N_0 = (a_1 - a_2); \]

\( u \) is the potential, \( Q \) – the charge density, \( \varepsilon \) - the dielectric susceptibility, \( q \) - the elementary charge; \( a_1, a_2 \) – are dependent on doping \( N \), \( \alpha = q/kT \), \( k \) – is the Boltzmann constant [qV/K], \( T \) is the temperature in Kelvin. Introducing the following variables in potential units: \( A_1 = \frac{qa_1}{\varepsilon} l^2 \); \( A_2 = \frac{qa_2}{\varepsilon} l^2 \) and the dimensionless variable \( y = x/l \) we can rewrite (1) in a somewhat different form.
\[
\frac{d^2 u}{dy^2} - \Omega(u)u = \hat{N}(y);
\]
\[
\Omega(u) = \frac{\hat{Q}(u)}{u},
\]
\[
\lim_{u \to 0} [\Omega(u)] = \alpha(A_1 + A_2) \begin{cases} < 0 \text{ when } q < 0 \\ > 0 \text{ when } q > 0 \end{cases}
\]

Equation (14) is thus the Helmholtz equation, where the boundary problem is unambiguously solvable for \( q > 0 \) (where an electron charge is the elementary charge), and cannot be solved unambiguously for \( q < 0 \) (where a pozyton charge is an elementary charge). The function \( \Omega(u) \) is presented in diagram 1.

2.1. The conditions for applying the finite differences method

Equation (2), for a network with constant step \( h \), takes the following form:

\[
u_{i-1} - (2 + h^2 \Omega_i)u_i + u_{i+1} = h^2 \hat{N}_i,
\]

By varying (3) we get:

\[
\delta u_{i-1} - \left(2 + h^2 \Omega_i + h^2 \frac{\partial \Omega}{\partial u_i} \delta u_i \right) \delta u_i + \delta u_{i+1} = 0
\]

\[\text{Fig. 1. The dependence of } \Omega(u) \frac{P}{\varepsilon} \text{ on } u, \text{ where } q > 0\]

In order to ensure that the solution to equation (2.1) was stable under the Dirichlet border condition, that is, where \( \delta u_i = \delta u_i = 0 \), it is sufficient to have

\[
\min\left(\delta u_{i-1}, |\delta u_{i+1}|\right) < |\delta u_i|
\]

that

\[
\max\left(\delta u_{i-1}, |\delta u_{i+1}|\right) < \max\left(\delta u_{i-1}, |\delta u_{i+1}|\right)
\]

This, in turn, causes the dependence \( R = \Omega + \frac{\partial \Omega}{\partial u} u > 0 \) for each \( u \). Due to the large gradients of \( u \) in the vicinity \( y = 0 \), we can apply the 'expansion of coordinates' method to (1.1), by using the transformation
\[ y = \frac{(a + 1)^y - 1}{a} ; z = \frac{\log(a^y + 1)}{\log(a + 1)} \]  

The coefficient \((a)\) is calculated as the limit of the series presented in the following way:

\[ a_{n+1} = a_n - \frac{W_n}{W_{n+1}} \]  

Where:

\[ W_n = V_0 \left( \frac{(a_n + 1)^{\frac{1}{a}} - 1}{a_n} \right) - 0.001(U_L) \]

\[ W_{n+1} = V_0 \left( \frac{(a_n + 1)^{\frac{1}{a}} \times (a_n dz / (1 + a_n) - 1) + 1}{a_n^2} \right) \]

Equation (2) with variable "\(z\)" can be written as follows:

\[ \frac{d^2 u}{dz^2} - \log(a + 1) \frac{du}{dz} = \left[ \frac{(a + 1)^y \log(a + 1)}{a} \right]^2 \]

\[ \left[ \hat{Q}(u) + \hat{N} \left( \frac{(a + 1)^y - 1}{a} \right) \right] = Q(u, z) \]  

The dependence \(\log_{10}(dz/dy)\) on \(y\) is given in Fig. 2. 

Equation (6) can be solved on a uniform network with constant step \((dz)\) in view of the small difference in \(du/dz\) over the entire specimen investigated.

An important feature of this method is its accuracy, of evaluation according to the following formula

\[ M = \left. \frac{u_y}{x=x_l} - \frac{u_y}{x=0} \right| \varepsilon \int_0^x Q(x, u(x)) \, dx \]  

2.2. The shot method

Equation (10) is replaced by the system:

\[ \frac{du}{dy} = v ; \frac{dv}{dy} = \hat{Q}(u) + \hat{N}(y) ; \]

\[ u_y|_{y=0} = U_L ; v_y|_{y=0} = IV_0 \]  

\[ u_y|_{y=x_l} - u_y|_{x=0} = \varepsilon \int_0^x Q(x, u(x)) \, dx \]
The conditions for the stability of the shot method are examined. To this end, we create variation equations in the surrounding $[u^*(y), v^*(y)]$ fulfilling the beginning conditions

$$
\frac{d}{dy} \delta u = \delta v; \quad \frac{d}{dy} \delta v = \frac{\partial \hat{Q}}{\partial u} \delta u; \\
\delta u(0) = \varepsilon_u; \quad \delta v(0) = \varepsilon_v.
$$

(17)

where $\varepsilon_u, \varepsilon_v$ - relate to the modules. Equation (3.2) is written in the matrix form:

$$
\frac{d}{dy} \begin{bmatrix} \delta u \\ \delta v \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ \frac{\partial \hat{Q}}{\partial u} & 0 \end{bmatrix} \begin{bmatrix} \delta u \\ \delta v \end{bmatrix},
$$

$$
\begin{bmatrix} \delta u \\ \delta v \end{bmatrix} \bigg|_{y=0} = \begin{bmatrix} \varepsilon_u \\ \varepsilon_v \end{bmatrix}.
$$

(18)

The necessary condition for stability of the trajectory $[u^*(y), v^*(y)]$ is that the real part
of the eigenvalue of the matrix are not positive. Since the eigenvalues can be expressed:

\[ \rho_{1,2} = \pm \sqrt{\frac{\partial \dot{Q}}{\partial u_{n,m}}} \]

\[ = \pm \sqrt{\alpha \left[ A_1 \exp(-au^*) + A_2 \exp(au^*) \right]} \]

in the shot method, any trajectory is unstable, if its elementary charge is an electron.

3. PSEUDOWAVELETS APPROACH

Equation (4) take the form: \( u_t = Lu + Nf(u) \), where \( L \) and \( N \) are linear differential operators and \( f(u) \) is a nonlinear function. A generic feature of the solution of such equations is that they behave in a smooth, non-oscillatory and shock-like manner. According to analysis based on the solution of the drift-diffusion model, in which the above-mentioned equations are coupled through elliptic Poisson equation, the transient response of the carriers, when pulsed from accumulation into inversion, can be divided into three periods: dielectric relaxation time, depletion time and equilibration time. During dielectric relaxation time, the surface concentration of the majority carriers sharply decreases (in some cases by about 8 orders in 1 ns). During depletion time it becomes constant and during equilibration time it slowly increases to equilibrium value.

In the approach presented the solution \( u(x,t) \) and the operators \( L \) and \( N \) were projected onto a wavelet base. The vanishing moments of the base functions are the reason for the sparsity of the representation of both the solution and operators. This sparsity makes it possible to develop fast, adaptive algorithms for applying operators to functions and for calculating the functions in the wavelet base.

These algorithms use the fact that wavelet expansions may be viewed as a localized Fourier analysis with a multi-resolution structure that adapts automatically to both the smooth and shock-like behavior of the solution. In smooth regions, few wavelet coefficients are needed, and in singular regions the large variation in the solution requires more wavelet coefficients. This approach make it possible to combine many finite-differences, (pseudo-) spectral and adaptive grid methods into a collection of efficient, generic algorithms, named adaptive pseudo-wavelet algorithms. The approach was applied to transient responses in some MIS circuits, and numerical results are presented.

The approach takes advantage of the efficient representation of functions and operators in wavelet bases, and updates the solution by implementing recently developed adaptive algorithms. These algorithms are adaptive since they update the solution using its representation in a wavelet basis, which concentrates significant coefficients near singular behavior.
We used the semigroup method to replace the nonlinear partial differential equation with a nonlinear integral equation. The transient response of the MIS circuits has both shock-like as well as smooth parts. An algorithm based on a pseudo-wavelet approach, which is automatically adaptive to both smooth and shock-like behavior of the solution, was applied to analyze this response. This approach makes it possible to combine many finite-differences, spectral and front-tracking grid methods into a collection of efficient, generic algorithms.

4. RESULTS

Changes of incremental of hole density as a function of time in cross sections placed at different distances (x) from the interface are presented in Fig. 4. At the interface and at x=0.1μm increments are negative. At x=1 μm the increments at the beginning of the transient process are negative and then, during the equilibration period, are positive.

![Graph showing the dependence of the hole charge increment on time.](image)

Fig. 4. Dependence of the hole charge increment on time.

The inversion layer buildup is presented in Fig. 5, where the move of the zero current density point as a function of time is depicted. As the gradient of the concentration of carriers in inversion layer rises, also rises the drift and diffusion components of the total current. This is very crucial when calculations are based on finite differences. Wavelets approach enable to overcome these difficulty.
5. CONCLUSIONS

The regions of stability of the finite difference algorithm for Poisson equation were determined. Approach based on combined finite-differences, spectral and front-tracking grid methods into a collection of efficient, generic algorithm was investigated. Application of the wavelet approach increase the efficiency of the algorithm, especially in the equilibration period, when coupling of the drift diffusion equations through Poisson equation is very tight.

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