THREE-DIMENSIONAL TRANSIENT DEVICE SIMULATION WITH MINIMOS

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Abstract

Our device simulator MINIMOS has been used for the numerical analysis of three-dimensional non-planar silicon MOSFET and GaAs MESFET structures. Here we present an extension of the program for the simulation of transient effects. This version of MINIMOS has further been enhanced by a new, highly accurate current integration method.
The computational complexity of three-dimensional transient simulations is tackled by preconditioned iterative methods. We present efficient algorithms and their implementation for the solution of the large linear systems of equations on vector and parallel computers.

1 Transient Simulation

Three-dimensional transient simulation of MOSFET structures is necessary to analyze both the influence of time dependent physical quantities such as the recombination rate, and three-dimensional non-planar geometries such as the field-oxide transition. The current continuity equations are discretized in space by the Scharfetter-Gummel method and in time by the fully implicit (backward Euler) method. Time-step control is based on the functional

$$\begin{aligned} I &= \int_{\Omega} [((n^{i+1} - n^i)\ln\frac{n^{i+1}}{n^i} + (p^{i+1} - p^i)\ln\frac{p^{i+1}}{p^i} \\ &+ \frac{\epsilon}{2}(\text{grad}\,(\psi^{i+1} - \psi^i))]d\Omega \end{aligned}$$

The time-step τ_{i+1} is chosen such that

$$\frac{\tau_{i+1}}{\tau_i} = \delta \cdot I$$

remains bounded. For the solution of the device equations the decoupled (Gummel) algorithm is used. The convergence of Gummel's algorithm in the linear regime is accelerated effectively by least squares extrapolation for the update of the electric potential ψ.

Transient simulation is an important method for the analysis of physical effects such as e.g. the kinetic of deep traps in the semi-insulating substrates of GaAs MESFETs [3][4], and the simulation of the charge-pumping experiment (interface trap kinetic). The deep trap model in GaAs for the donor trap rate-equation is given by

$$\frac{\partial\left(N_T - N_T^+\right)}{\partial t} = R_n - R_p$$

in which the effective recombination rates $R_{n,p}$ are

$$\begin{aligned} R_n &= C_n N_T^+ n - e_n\left(N_T - N_T^+\right) \\ R_p &= C_p\left(N_T - N_T^+\right)p - e_p N_T^+ \end{aligned}$$

In these equations N_T denotes the total and N_T^+ the density of the electrically active deep donors. $C_{n,p}$ are capture coefficients and $e_{n,p}$ are the emission rates [3]. An equivalent formulation holds for the acceptor traps. For the simulation of the charge-pumping experiment in silicon MOSFETs we use a model for the interface trap kinetic given in [2]. Assuming the acceptor type of the interface traps with density D_T, the time dependent charge-pumping current is obtained by integration with respect to the gate-oxide surface and the time (period length T_0). The falling pulse slope is assumed to start at $t = t'$:

$$I_{CP}(t) = \frac{1}{T_0}\sigma v_{th} \int_{t'}^{t'+T_0} \int_{\Gamma_G} N_T(\tau)p(\tau)d\Gamma d\tau$$

where $N_T(t)$ is the non-equilibrium part of the trapped charge density, obtained by integration of the rate equation

$$\begin{aligned} N_T(t) = &- \int_{E_{F(t')}}^{E_{F(t)}} D_T(E)\exp\left(-\frac{\delta(t,E)}{\tau_n(E)}\right)dE \\ &- \sigma v_{th} \int_{t'}^{t} N_T(\tau)\,p(\tau)\,d\tau \end{aligned}$$

The time interval $\delta(t, E)$ is determined for a given E by the condition $E_F(t-\delta) - E = 0$. All parameters are assumed as spatial variables along the channel surface. $\tau_n(E)$ denotes the trap lifetimes which depend on the energy in the well-known way [6].
A selfconsistent transient solution of these equations enables the simulation of the charge-pumping experiment. This facilitates a proper design of this experiment and the extraction of the spatial distribution and energy density of the traps created by a hot carrier injection.

2 Current Integration

After a solution at some timestep has been found a critical step is the terminal current integration. We have implemented a new method which is based on choosing weight functions w^i for each terminal T_i and evaluating a volume integral instead of a surface integral. E.g. for the electron current on the terminal T_i we compute

$$I_n^i = \int_\Omega [\text{grad} w_n^i \cdot J_n - w_n^i R] d\Omega$$

In this formula J_n denotes the electron current density and R the recombination rate. The functions w_n^i are smooth functions on Ω. They have to suffice homogenous Dirichlet boundary conditions at all terminals $T_j \neq T_i$, non-homogenous constant Dirichlet boundary conditions at the terminal T_i and homogenous Neumann boundary conditions elsewhere. To obtain optimal weight function for e.g. the electron current on terminal T_i we minimize the functional

$$\Phi_n^i = \int_\Omega \left[\frac{n}{2}\left(\text{grad} w_n^i\right)^2 - w_n^i R\right] d\Omega$$

This choice is motivated by the experimental observation that a high degree of accuracy for terminal currents is achievable, if the gradients of the weight functions are minimized in highly doped regions of the device [5]. The variation of the functional above leads to the elliptic partial differential equation

$$\text{div}\left(n \text{grad} w_n^i\right) = R$$

which is discretized by the Scharfetter-Gummel method and solved by the standard preconditioned conjugate gradient method. For the deviation currents the Laplace equation is solved on Ω.

3 Implementations

The backward Euler time discretization in general increases the diagonal dominance of the linearized discrete carrier continuity equations, thus making preconditioned iterative methods converge quickly. Apart from the classical conjugate gradient algorithm (CG), which is used to solve the discrete Poisson and weight function equation, we use the conjugate gradient squared method (CGS) for the carrier continuity equations.
The convergence rate on one hand and the efficiency of the implementation on parallel computers on the other is determined to a large extent by the applied preconditioner. Incomplete LU factorizations have proven to be a nearly optimal choice on vector computers. We have carried out various implementations on vector supercomputers such as the Cray-2 and the Fujitsu VP200 resulting in execution speeds of more than 100 megaflops for the critical triangular solves of the ILU preconditioner. This is achieved by the hyperplane-reordering technique using list-vectors. We have investigated also several massively parallelizable preconditioners, namely truncated Neumann series and multicolor incomplete factorization preconditioners. Experiments performed on a massively parallel architecture, the Connection Machine [1], indicate that an incomplete factorization of the reduced system matrix performs best.

References

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