CELLULAR AUTOMATON SIMULATIONS OF PLANAR DOPED BARRIER FIELD EFFECT TRANSISTOR IN SILICON

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Abstract

We report new developments in cellular automata transport simulations and present a study of vertically grown Si ultra-short channel FET's with these new methods. The probabilistic scattering rates for the electric field have been replaced in the cellular automaton by a new deterministic scattering rule in a fully three-dimensional momentum-discretization, leading to a significant suppression of statistical errors. We have also developed a fast multigrid-solver for the Poisson equation that offers the possibility to solve the Boltzmann and Poisson equations asynchronously in a multi-processor environment.

I. Introduction

Simulation of nanostructured devices has become a crucial and strategic part of today's microelectronics [1–3]. Conventional drift–diffusion approaches [4] are no longer valid for modeling of ultra-short devices with a gate length below 100 nm because they cannot predict hot carrier effects such as velocity overshoot quantitatively. Recently, the cellular automaton (CA) approach [5] has been developed as a discrete variant of the Monte Carlo (MC) technique [6,7]. So far, several tests of its applicability to sub-μm device modeling have been carried out successfully [5–9]. We introduce a new implementation of the CA method in this paper that allows precise control and efficient suppression of statistical errors in the CA. The central point is to replace the probabilistic treatment of the electric field used in [5] by a deterministic hopping of the particles in a three dimensional and periodic k-space. Furthermore, to take advantage of the high intrinsic speed of the CA, we have adapted the multigrid method to general device geometries in order to obtain a fast and efficient Poisson solver. These new developments have been implemented in our CA device simulator to study transport in planar doped barrier field effect transistors (PDBFET) with a gate length below 50 nm. We demonstrate that this new ultra-short Si-based device yields a high transconductance and transit-time frequency.

II. New developments in the Cellular Automaton approach for device simulations

Recently [5], the full Boltzmann equation (BE) has been transformed into a CA, where the kinetic terms of the BE are replaced by hopping probabilities in such a way that the equation of motion are fulfilled on the average for an ensemble of quasi particles. In an explicit procedure, the drift term of the BE has been transformed into probabilistic field scattering rates. This corresponds to a substitution of the free flight by a random walk. For very high electric fields, this procedure leads to artificial diffusion effects on the k-space lattice. For a *periodic* momentum discretization, this statistical error can be estimated analytically as follows. The CA-scattering probability to nearest neighbor sites due to the electric field $E(R)$ at lattice site R is given by [5] $P_E = e\Delta t E(R)/(\hbar\Delta k)$, where Δk is the lattice constant of the periodic k-space lattice, Δt the timestep, e the elementary charge and $\hbar$ the Plank constant. A particle moves in one time step with probability P_E to one of the nearest neighbor cells and remains in the cell with the probability $1-P_E$. Associated with this random walk, there is a diffusion in k-space given by $D_{art} = \Delta k^2 P_E(1-P_E)/(2\Delta t)$ which causes an artificial enhancement of the kinetic energy, the entropy and the longitudinal diffusion in real space of the system. In principle, this error can be reduced by a sufficiently small lattice constant Δk but this becomes impractical in a three dimensional momentum space.

We now show that it is possible to transform the drift term of the BE into a new *deterministic*

scattering rule of the CA that completely suppresses this statistical error. The main point is to replace the probabilistic scattering rate by a discrete free flight. We derive this scattering rule by calculating the number of time steps N a particle needs to change its momentum by an amount equal to the lattice constant Δk in k-space. To illustrate the procedure, we restrict ourselves to one dimension; the generalization to more dimensions is straightforward. Integration of the semiclassical equation of motion $\dot{k} = eE(r(t))/\hbar$ gives

$$\Delta k = k(t+\tau) - k(t) = \frac{e}{\hbar} \int_{t}^{t+\tau} dt' E\big(r(t')\big) \ . \tag{1}$$

Let us denote the initial time by $t = t_0$, and assume that $\tau = N\Delta t = t_N - t_0$ and set the real space position at time t_i equal to lattice vector $R(t_i)$. The discrete version of Eq. (1) reads

$$\Delta k = \sum_{i=0}^{N} \Delta t \frac{e}{\hbar} E(R(t_i)) \ , \tag{2}$$

which is a condition for N and yields a deterministic scattering rule for the electric field: A particle remains in its k-cell for N time steps and hops subsequently into its nearest neighbor cell. Consequently, this procedure confines the statistical error to one k-cell. With this procedure, only of the order of 10^3 3–D k-cells are required for a nonparabolic band structure up to 2 eV. The lattice we have chosen is a hexagonal close-packed structure where each cell has twelve nearest neighbors. The restriction to nearest neighbors transforms the drift-term of the BE into a *local* interaction on momentum cells, in complete analogy to the treatment of the real-space diffusion-term of the BE [5].

Importantly, we found that the new implementation of the CA does not require more computer time per iteration than our earlier two–dimensional implementation [5] even though it is significantly more accurate.

III. Multigrid-solver for the Poisson equation

An important component of self consistent device simulations is an efficient solver for the Poisson equation (PE). For a sub-micron device with high doping such as a Si MOSFET, for example, we find that the solution of the PE dominates the total computer time and constitutes a bottleneck of the overall simulation if we employ the standard SOR (successive over–relaxation) algorithm. We have therefore developed an iterative multigrid PE solver to provide an efficient coupling to the CA.

The basic idea of the multigrid approach [10,11] is to improve an approximate solution of the PE on many length scales simultaneously. Indeed, the major deficiency of the SOR is to reduce errors only on the length scale of the smallest grid. The SOR method tends to reduce local errors within a few iterations but often shows "critical slowing down" for the global, long-wavelength errors. In contrast, the multigrid method shows the same rapid convergence on all wavelengths.

We have implemented the multigrid method for general device geometries with irregular two-dimensional grids, allowing for any type of electrostatic boundary condition. For rectangular grids, we use a "zebra"-type line relaxation scheme along both x- and y-directions[11]. When the ratio of the grid spacing in x- and y-direction lies in the range $0.85 \leq \Delta_x/\Delta_y \leq 1$, we employ instead a checkerboard point relaxation method [11].

We find this multigrid solver to be 5 to 10 times faster than the SOR and consequently to provide a significant speed-up. The gain in computer time is the larger the more complex the boundary conditions are. This algorithm thus eliminates the bottleneck posed to the simulation by the PE and offers the attractive possibility to solve the CA and the PE concurrently in an asynchronous way since both methods

are iterative and require comparable computer time per iteration. We are currently developing decoupling schemes for the solution of BE and PE in the time-domain and in the space domain by slicing.

IV. Transport simulations of PDBFETs

In order to test the present new CA, detailed calculations of Si-PDBFET's [12] have been carried out. This transistor is a vertically grown variant of a Si-MOSFET that contains a δ-p^+-layer in the intrinsic region between the contacts instead of a homogeneous p-buffer (Fig. 1 (a)). Typical gate lengths that can be achieved are 50 nm or smaller. Consequently, one may expect a high transconductance and other short-channel effects in such a device. In the present simulations, we used a gate length of 50 nm and have varied the thickness of the p^+-layer from 5 to 20 nm. We found that a doping concentration of the δ-layer up to $5x10^{18}cm^{-3}$ guarantees that no free holes are present to deteriorate the device performance.

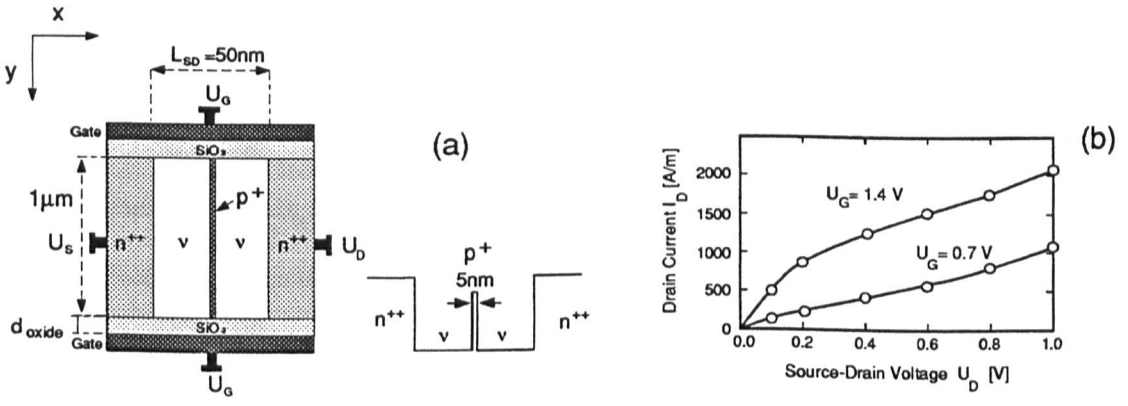

FIG 1. (a) Geometry of a vertically grown 50 nm planar-doped barrier FET. The n^{++} doping concentration is $10^{19}cm^{-3}$, the δ-buffer has a width of 5 nm and a maximum doping concentration of 5 x $10^{18}cm^{-3}$. (b) Typical calculated drain-current characteristics for two gate voltages U_G=0.7 V and 1.4 V. The high channel conductance is indicative of pronounced short channel behavior.

Fig. 1 (b) depicts the computed drain characteristics of a PDBFET with a 5nm δ-layer. The results show typical short-channel effects. In particular, the drain current does not saturate at higher drain voltages. This is due to the fact that the drain current cannot be efficiently controlled by the gate. In addition, velocity overshoot already appears at low drain voltages, as shown for a bias point at U_D=0.2 V and U_G=1.4 V in Fig. 2 (b). The corresponding longitudinal electric field is plotted in Fig 2 (a). The dashed line denotes the field in the bulk diode, which forces the electrons to remain in the n^{++} regions, whereas the full line shows the field in the inversion channel. In contrast to the continously increasing field in the inversion channel of an ultra-short MOSFET, the field in the two intrinsic regions is nearly homogeneous and has a magnitude of approximately 20 kV/cm. In the narrow p-buffer, on the other hand, there is a strongly inhomogeneous field that causes velocity overshoot of the carriers. For higher drain voltages, the field maintains its high value from the p-layer through the complete i-zone up to the n^{++} region of the drain contact. This leads to velocity overshoot nearly over the total channel length.

Our calculations predict a very high transconductance of at least 1000 mS/mm and a maximum transient time frequency of about 200 GHz. In contrast to short channel MOSFETs, where the junction fields reach values of more than 700 kV/cm, the significantly lower electric fields in the studied PDBFET's cause impact ionization to be considerable reduced.

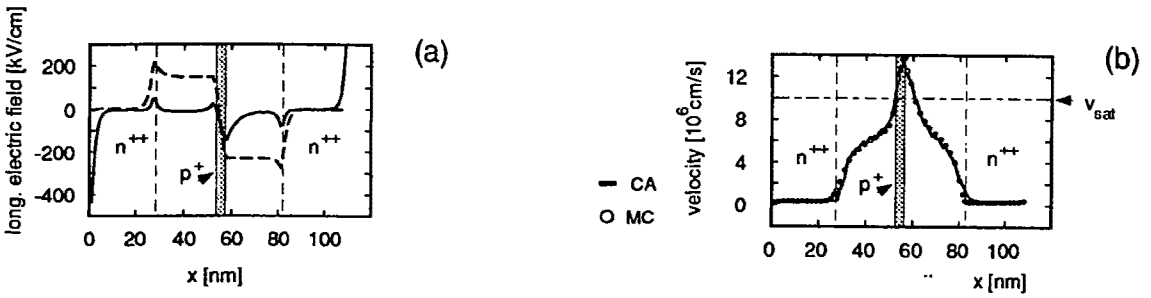

FIG 2. (a) Longitudinal electric field for a bias point at U_G=1.4 V and U_D= 0.2 V (other parameters as in Fig. 1). The field in the inversion channel (full line) is approximately constant in the intrinsic regions and exhibits a sharp maximum in the p-layer. The field in the bulk diode (dashed line) confines the electrons to the n^{++} regions. (b) Comparison of CA and ensemble Monte Carlo simulations for the vertically averaged drift velocity of the electrons. The agreement is excellent. For the chosen bias, velocity overshoot only occurs close to the p-buffer. v_{sat} denotes the saturation velocity.

V. Conclusion

We have presented new improvements in the cellular automaton approach for high field transport in semiconductors. A deterministic rule for the electric field in the CA leads to a dramatic reduction of the statstical errors in a fully three dimensional k-space discretization. In very good agreement with Monte Carlo results, we demonstrated the high speed capability of Si-PDBFET's resulting in a transconductance of 1000 mS/mm, a transit-time frequency of 200 GHz and no relevant influence of impact ionisation compared to short channel MOSFETs.

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