

A Comparison of Monte Carlo and Cellular Automata Approaches for Semiconductor Device Simulation

G. Zandler, A. Di Carlo, K. Kometer, P. Lugli, P. Vogl, and E. Gornik

Abstract—We present a detailed comparison of Monte Carlo and cellular automata approaches as applied to the study of nonequilibrium transport and semiconductor device simulation. We show that the novel cellular automata (CA) technique enjoys all benefits of the more traditional Monte Carlo (MC) method, while at the same time allowing considerably higher performances.

I. INTRODUCTION

DEVICE simulation has become a crucial and strategic part of today's microelectronics [1]–[3]. The Monte Carlo (MC) method [4], [5] belongs to the most sophisticated, but at the same time the most costly, of all simulators. For this reason, the MC method still remains restricted to university and laboratory research, and has not yet become a common modeling tool. It would therefore be highly desirable to develop a simulator of comparable physical content as the MC, but much faster and also capable of exploiting the potential offered by vector and parallel processors more naturally [6].

Recently, a new method has been developed which appears to meet these requisites, the cellular automata (CA) approach [7]. So far, only preliminary tests of its applicability to device modeling have been carried out. In this paper, a critical assessment of the strengths and limitations of the CA is given by presenting the first quantitative and detailed comparisons between MC and CA device simulations.

II. CELLULAR AUTOMATA AND MONTE CARLO METHODS

The MC method for the study of semiconductor transport is based on the simulation of a random walk of the classical particles subject to probability rules determined from quantum mechanics. In such a frame, Fermi's golden rule allows the calculation of energy-dependent scattering rates of carriers (electrons and holes) with phonons, impu-

rities, other carriers, etc. The momentum-dependent scattering rate $P(k(t))$ determines the mean time between collisions and leads to the possibility of stochastically generating the duration of the free flights. During such flights the carriers obey the classical equations of motion [5].

In general, the electric field is a function of position; in order to fully account for nonhomogeneous situations (and therefore to simulate semiconductor devices), the MC simulation has to be self-consistently coupled to Poisson's equation [5]. It has been shown that the MC method provides a solution of the Boltzmann equation (BE) [8].

Recently, the full BE for carrier transport in semiconductors has been transformed to a CA [7]. This constitutes an important improvement, since CA's are traditionally only used, in the context of transport, for fluid dynamics [9]–[11] or drift-diffusion simulations [12]. In general, a cellular automaton consists of a lattice with a finite number of states attached to each lattice site. The population of these states is simultaneously updated according to deterministic or nondeterministic rules in discrete time steps. Importantly, the dynamics of CA are governed by local rules, i.e., the updating of site variables involves only a small number of neighbors in each time step. For this reason, CA constitutes one of the very few algorithms for physical processes that can optimally utilize massively parallel computer technology. In addition, the locality of the dynamical rules allows an efficient and flexible treatment of complex geometries. The major characteristics of CA are the two length scale on which they operate. First, there is the discrete microworld on a lattice obeying a fictitious dynamics of pseudoparticles. The length and the time scales for this dynamics are much shorter than the physical scales. Second, there is the continuous macroscale with the physical observables, which are obtained in practice by taking averages over many cells.

In its implementation for the solution of the BE, the CA consists of a lattice in position space, each site of which has a finite number of momentum states. The nondeterministic transition rules between these states associated with collision events are determined from the quantum mechanical scattering rates (in the same way as in MC) and from the classical equations of motion. Due to the locality in position space of quantum mechanical

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G. Zandler, A. Di Carlo, K. Kometer, P. Vogl, and E. Gornik are with the Walter Schottky Institut and Physik Department, Technische Universität München, D-8046 Garching, Germany.

P. Lugli is with the Walter Schottky Institut and Physik Department, Technische Universität München, D-8046 Garching, Germany, on leave from the Dipartimento di Ingegneria Elettronica, Università di Roma "Tor Vergata," 00133 Roma, Italy.

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scattering events, which is a basic assumption underlying the BE, there is no principle problem in converting these transitions in momentum space into local CA rules. On the other hand, the drift and diffusion terms in the BE link the distribution function to its value in different position and momentum space locations, being therefore nonlocal in nature. Additionally, a single semiclassical particle trajectory cannot in general be reproduced exactly on the discretized phase space of the automata. Therefore, the kinetic terms of the BE are replaced by hopping probabilities in both position and momentum space in such a way that the equations of motion are fulfilled in average for an ensemble of pseudoparticles. By an appropriate choice of lattice constant a and time step dt , the hopping events can be restricted to transitions between nearest neighbors (or second nearest neighbors). This choice is restricted by the desired resolution in position space and by the maximum physically relevant velocity, which must be less than a/dt . This procedure results in a master equation for the state occupancies that contains only on-site transitions between different momentum states and transitions between nearest neighbors with the same momentum state. We point out that this algorithm allows an efficient treatment of electron-electron scattering kernels since the primary variables can be chosen to be the local site occupancies (rather than the particle trajectories as in MC). For a rigorous derivation and a detailed discussion of the basic algorithm, see [7].

III. SIMULATION PARAMETERS

We have carried out both CA simulations and ensemble MC calculations employing exactly the same materials parameters [13]. We have taken a two-dimensional hexagonal real space lattice and a three-dimensional k-space lattice. The 3-D k-space attached to each lattice site has been divided into 60° sectors (corresponding to the six neighbors in position space) made up of onion-like shells. Each shell represents an energy interval of typically one optical phonon energy (except the first two shells, which have a finer energy resolution). Altogether, between 20 and 30 shells have been included for each valley. We have used a parabolic three-valley model for the carrier dispersion and included optical phonon and intervalley phonon scattering as well as the interaction with ionized impurities. The time step was chosen to be 2 fs both for the CA or the MC transport equations as well as for the Poisson equation. Both the MC and the CA simulations were carried out with ensembles of 10 000 particles.

Due to the limited number of initial and final states in the CA, the total scattering probabilities could be stored completely in look-up tables, reducing the simulation to a sheer mapping of integer arrays onto one another. The resulting CA method can be implemented very efficiently on vector and parallel computers. On a single-vector or superscalar processor, a speedup of about a factor of 50 is obtained for the CA with respect to the MC simulations. This speed, combined with the moderate memory requirements due to the sole usage of integer arithmetic, allows

the simulation of very large ensembles, thus greatly reducing the statistical noise.

IV. RESULTS

A. Homogeneous Transport

In Fig. 1, the drift velocity (Fig. 1(a)) and the average kinetic energy (Fig. 1(b)) in homogeneous n-type GaAs are depicted as a function of the electric field at $T = 77$ K. Overall, the CA simulations can be seen to be in very good agreement with the MC data. Compared to MC, the CA results slightly overestimate the mobility and the average kinetic energy at low fields but underestimate the peak velocity near 4 kV/cm. The enhanced low-field mobility is a consequence of the coarse grained momentum space. Since the microscale of the CA has an energy resolution of typically one phonon energy and an angular resolution of only 60° , some of the small angle scatterings by ionized impurities are underestimated. Therefore, the carriers tend to be faster and also slightly hotter at low fields. The small deviation of the peak velocities, on the other hand, is a consequence of the replacement of the deterministic semiclassical trajectories by stochastic hoppings. Such a replacement only guarantees the particle trajectories to follow the equations of motion in the ensemble average. Consequently, some of the pseudoparticles gain slightly more energy from the electric field, causing those electrons to transfer to the heavy mass satellite valleys slightly more efficiently in the CA. This explains the decrease in the peak velocity. The small increase in the high-field energy is also caused by the coarse grained energy space. Since the intervalley phonon energy is smaller than the energy spacing of the CA, some of the carriers have their final state in the same energy shell of an equivalent satellite valley after emitting a phonon. This reduces the energy dissipation by this process and therefore increases the mean energy at high electric fields.

In summary, all of these deviations can be minimized by a careful design of the momentum space discretization for low temperatures, while still an even better agreement is found at room temperature even for the crude discretization used in this comparison [14].

B. Transport in *n-i-n* Structures

The stationary velocity-field and energy-field comparisons discussed above show that CA properly describes the hot-electron regime in GaAs. Next, we turn to a simple GaAs device in order to test CA simulations for inhomogeneous transport when overshoot effects are expected to play an important role. We consider a $0.25/0.4/0.25\text{-}\mu\text{m}$ n-i-n structure with an applied bias of 0.5 V across the structure. The doping concentrations are $1 \times 10^{17} \text{ cm}^{-3}$ in the n-regions and $1 \times 10^{15} \text{ cm}^{-3}$ in the i-zone. Periodic boundary conditions were applied in both simulations. Both MC and CA simulations show that the electric field varies between 10 and -25 kV/cm in the intrinsic zone (Fig. 2(c)). The high values of the electric

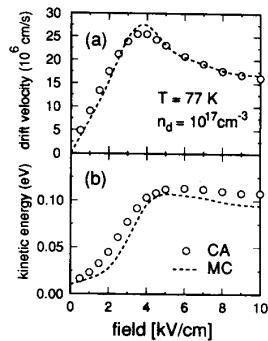


Fig. 1. (a) Stationary drift velocity and (b) average kinetic energy of n-type GaAs versus electric field. The dashed line represents MC data and the symbols are results of CA simulations.

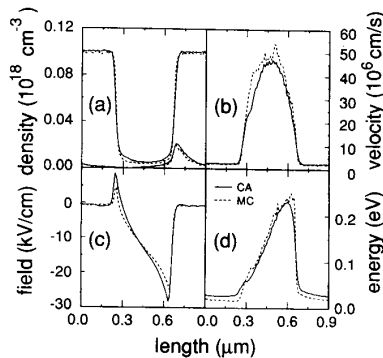


Fig. 2. Comparison of the CA results (solid lines) with MC results (dashed lines) for a GaAs n-i-n structure. (a) Electron density, (b) drift velocity, (c) electric field, and (d) kinetic energy of the electrons. The upper and lower pair of curves in (a) represent the total density of electrons and the density in the L-valleys, respectively.

field and its strong variation across the intrinsic zone lead to a marked velocity overshoot which is predicted, in very good agreement, by both methods (see Fig. 2(b)). This shows the capability of CA to describe pronounced quasi-ballistic transport. On the other hand, there is some discrepancy in the junction field between the two simulations which can be understood as follows. The enhanced carrier temperature in the low-field region of the n-zone of the CA (Fig. 2(d)), caused by the same mechanisms as in the homogeneous simulations, results in a slightly higher carrier concentration in the i-zone, as shown in Fig. 2(a).

The corresponding self-consistent field is therefore increased relative to the MC simulations. A similar good agreement as for the drift velocity is found for the average kinetic energy in the i-zone. Near the i-n interface, electron heating (see Fig. 2(d)) favors the transfer of some electrons into the L-valley, as shown in Fig. 2(a). The corresponding increase in density of L-valley electrons agrees for both methods.

V. CONCLUSIONS

We have presented a detailed comparison between MC and CA simulations of high-field charge transport in semiconductor devices. The overall agreement is remarkable and clearly shows the capabilities of the CA as a modeling tool. We are currently extending the comparison to two-dimensional simulations, which is more appropriate for field-effect transistors. Preliminary results [7] indicate a comparable agreement to the one found above.

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