Cellular Automata Simulation of GaAs-IMPATT-Diodes

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Abstract

A new 3-dimensional cellular automata method is presented which improves the numerical efficiency of standard Monte-Carlo codes by keeping the physical accuracy. With both methods calculated results of stationary and time-dependent bulk transport quantities of GaAs and stationary transport characteristics of a GaAs-IMPATT-diode for D-Band applications will be presented and compared in detail.

1. Introduction

The study of the microscopical transport properties of IMPATT-devices is of great importance for a successful design of mm-wave GaAs-based transit-time devices for frequencies beyond 150 GHz. The Monte-Carlo (MC) simulation of these devices offers physical insight with high accuracy, but the calculation of the avalanche processes are numerically extremely demanding, what makes a full numerical optimization impossible. To overcome this problem, a new Cellular Automata (CA) technique has been developed and applied to investigate the operation of mm-wave IMPATT-diodes.

2. Method

The CA method stochastically calculates the semi-classical movement of an ensemble of pseudo-particles like in the known MC method, but it treats the dynamics of scattering and motion on an underlying grid in wave-vector-space iteratively with constant time steps Δt (typically 1-5 fs). The structure of each conduction band valley (or valence band) is described in polar coordinates and in energy space as shown in Fig. 1. In each time step the energy, the polar and azimuthal angles of the pseudo-particles are changed by stochastically scattering into another angular cell and into another energy-level of the same or another valley (or band). These super-scattering events include the effective change of states whithin the time step Δt and include also many-scattering events with a certain probability. These probabilities are stored in "connection tables". In contrast to an earlier published CA method [1], the electric field is treated deterministically here, and the motion in real space is given by means of finite distances which are assigned to each cell when particles underlie

free flights, or by mean values assigned to a certain cell combination ($\vec{r}_{scat}$ in Fig. 1) when a particle super-scatters into another cell.

The super-scattering probabilities are calculated by a deterministic integration scheme, which allows the inclusion of generalized bandstructure, adjustable grid-sizes, and arbitrary number of valleys (or bands). Nevertheless, a non-parabolic and isotropic standard 3-valley-(band) representation is used here to describe the bandstructure of GaAs. This allows a direct comparison of the CA calculations with the results of a standard MC code. Both methods incorporate the same ionized impurity, intra- and intervalley phonon scattering, and impact ionization processes and are self-consistently coupled to a one-dimensional Poisson solver for the simulation of IMPATT-diodes. The CA method is also coupled to a one-dimensional drift-diffusion model which describes the stationary transport in the contact regions even more efficient whereas all processes in the active region are modelled by the CA method. The impact ionization rate is calculated by invoking the random-k approximation of Kane [2].

3. Results

In Fig. 2 stationary and time-dependent bulk quantities of GaAs calculated with both the CA and the MC method are presented. Fig. 2a shows the convergence of the CA method for the calculation of the autocorrelation function versus the angular mesh size. The MC result is well reproduced when 32 cells in angular space are used (leading to a necessary memory of 3.5 MByte for one connection table).

The stationary drift velocity and the longitudinal diffusivity calculated with the MC method are nicely reproduced by the CA method in all important electric field ranges (Fig. 2b, 2c). At electric fields beyond 250 kV/cm, the drift velocity and the longitudinal diffusivity increase again because impact ionization occurs which scatters carriers back into low-energy regions where scattering rates are lower.

The CA and the MC calculations also show very good agreement when non-stationary conditions are considered. As an example, the time-dependent velocity overshoot arising when thermal carriers are exposed to a sudden switch-on of an electric field is presented in Fig. 2d.

The CA method shows an at least factor of 10 higher computational speed on a HP 735 RISC workstation compared to efficient standard MC methods. At high electric fields or high temperatures (these are typical conditions in transit-time devices like IMPATT-diodes), the CA technique is about 40 times faster than MC codes because the increase of scattering rates at high energies increases the numerical effort in MC codes more than in the CA technique.

With the MC and the CA method, the Read-type GaAs-IMPATT-diode of Fig. 3 has been simulated. The investigated structure has theoretically been proposed for application at oscillation frequencies higher than 150 GHz and was experimentally realized and characterized in [3]. The diode shows an extremely short injection region of only a few 10 nm and a short drift region of approx. 130 nm. As can be seen in Fig. 3a, the electric field strengh reaches 1 MV/cm in the injection region. Consequently, the electron and hole average energies reach maximum values of more than one eV near the end of the $p^+ - i$ resp. $i - n^+$ injection regions. Related to the peak structure of the carrier energy, the generation rate also shows maximum values at the end of the injection region. This behaviour leads to a drastic *dead space* effect, that is a low ionization rate of electrons in the $p^+ - i$ and of holes in the $i - n^+$ regions, respectively. As discussed above, one finds velocity overshoot of electrons and holes in

the injection region (Fig. 3d) where the transport is dominated by impact ionization scattering processes. As shown in Fig. 3a-d, the results of the CA method are in very good agreement with those of the MC method for all physical quantities.

The typical cpu time to simulate 100 picoseconds of IMPATT-operation on a HP 735 RISC workstation is one hour when 2 fs time steps and 20.000 pseudoparticles are used in the active region.

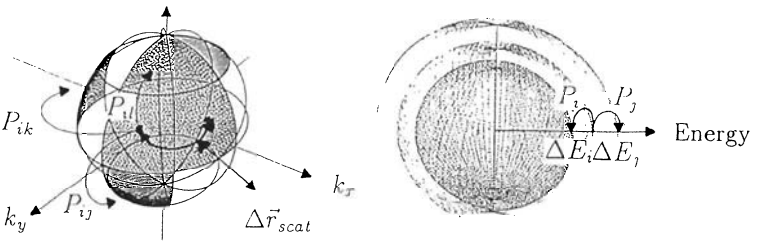

Figure 1: Discretization and super-scattering probabilities (P) in the CA method

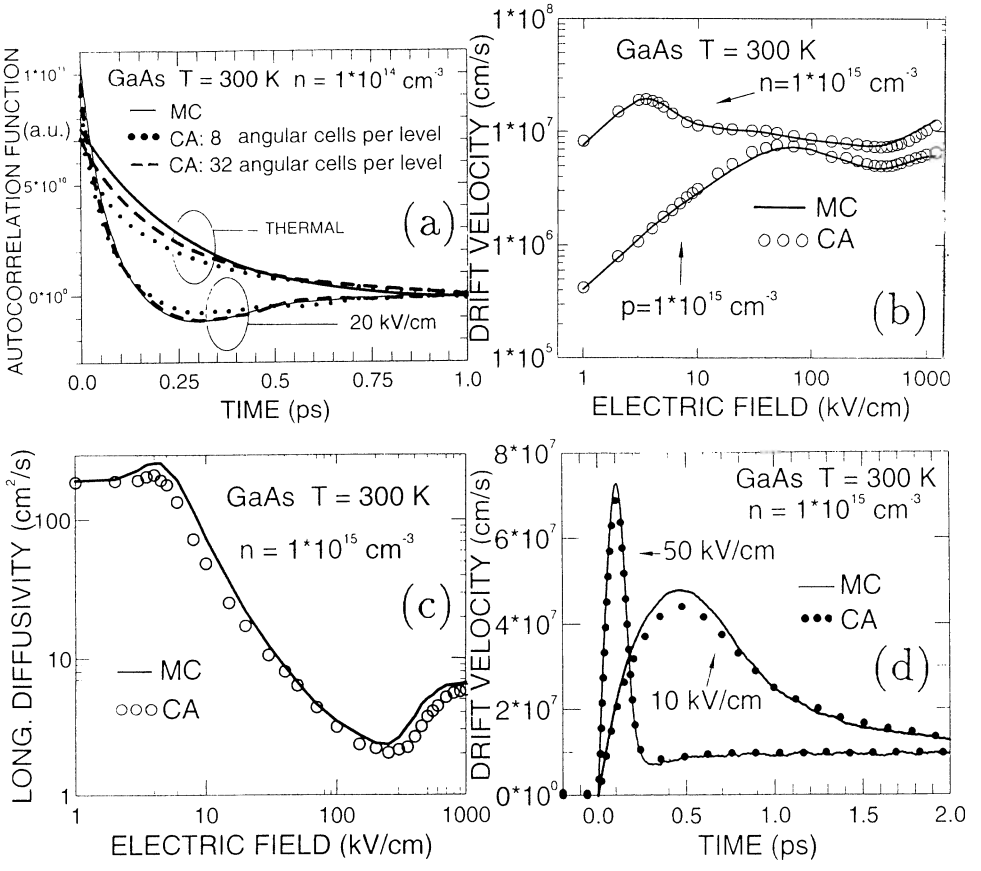

Figure 2: Comparison of stationary autocorrelation function (a), drift velocity (b), and longitudinal diffusivity (c), and of time-dependent velocity overshoot (d) calculated with the CA and the MC method

4. Conclusion

A new 3-dimensional Cellular Automaton method was presented. This method gives an accurate description of all relevant physical quantities and shows a factor of 10 - 40 higher computational speed compared to efficient standard Monte-Carlo codes. This makes the present method suitable to characterize the operation of mm-wave devices and to optimize their structure.

Acknowledgement

The author gratefully acknowledges the Deutsche Forschungsgemeinschaft for financial support.

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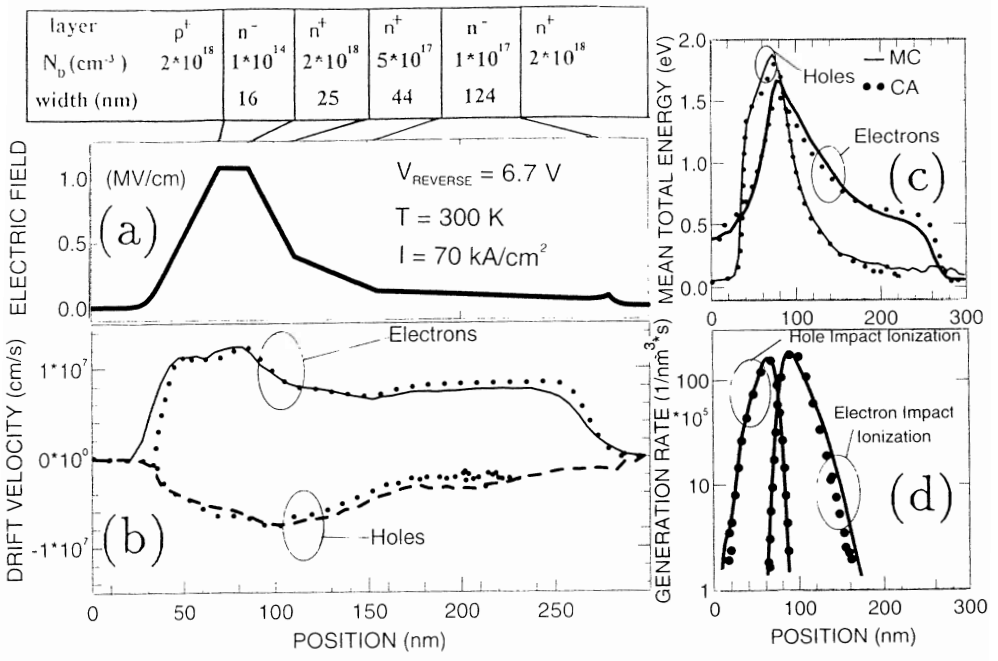

Fig.: 3 Comparison of the calculated distributions of electric field (a), drift velocity (b), mean energy (c), and impact ionization rate (d) for stationary operating conditions of the GaAs-IMPATT-diode