Full-Band Monte Carlo Transport Calculation in an Integrated Simulation Platform

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Abstract

We present a hierarchical CAD environment for realistic silicon device simulation, combining the utility of process, drift-diffusion/hydrodynamic, and Monte Carlo simulation in a unified platform. Monte Carlo simulation results are presented for the cases of an NIN diode and a 40nm LDD-MOSFET, using information given by a hydrodynamic pre-processing step. In addition we compare drift-diffusion, hydrodynamic and Monte Carlo results for an 0.5μm MOSFET whose geometry and doping profiles were generated by a 2-dimensional process simulation.

1. Introduction

The Monte Carlo method of charge transport simulation offers the possibility to extract information about all quantities derivable from the semiclassical distribution function, whose accuracy is limited explicitly by statistical convergence and implicitly by the quality of the physical models. To date, much effort has been devoted to improving models for band structure and scattering mechanisms, such as electron-phonon scattering [1, 2, 3, 4], impact ionization [5, 6, 7] and other carrier-carrier scattering [8, 9]. However, the practical usefulness of Monte Carlo device simulation has not entirely lived up to its promise, as evidenced by the observed propensity to simulate simplified device structures.

2. Degas – A Combined Hydrodynamic and Monte Carlo Simulator

A unique device simulation environment has been developed which unites the capabilities of process, drift-diffusion/hydro, and Monte Carlo simulation into a single platform. One may use DIOS_ISE [10] to begin with a process simulation. Drift-diffusion or hydrodynamic simulations can be performed with the mixed-mode multi-dimensional device simulator DESSIS_ISE [11, 12] as a preprocessing step. The full-band Monte Carlo simulator VEGAS was embedded into DESSIS_ISE by a window technique, which is called DEGAS_ISE [13]. The domain of the Monte Carlo simulation may be chosen either as the entire device, or as a rectangular sub-domain. When the Monte Carlo

simulation is invoked, it uses the precise device structure which has been generated by the process simulation. Former implementations of the window technique used the *drift-diffusion* information as initial and boundary conditions [14, 15]. In this work, carrier densities, velocities and temperatures are extracted from *hydrodynamic* simulation as calculated by DESSIS_ISE, and passed to VEGAS for use as initial and boundary conditions. Monte Carlo simulation may be performed self-consistently or using a frozen field provided by DESSIS_ISE, either in one or two dimensions.

3. Examples

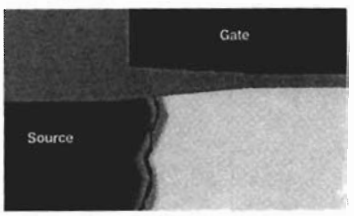

Figure 1: 0.5μm nMOSFET with arbitrarily shaped Si-SiO_2 interface from process simulation.

We present three examples: a 0.5μm MOSFET, a 40nm MOSFET and a 0.5μm NIN structure.

The 0.5μm nMOSFET was fabricated and measured by Fujitsu. The process was simulated with DIOS_ISE, and resulted in a non-planar Si-SiO_2 interface (Figure 1). Figure 2 shows that the drift-diffusion ansatz completely fails in this example.

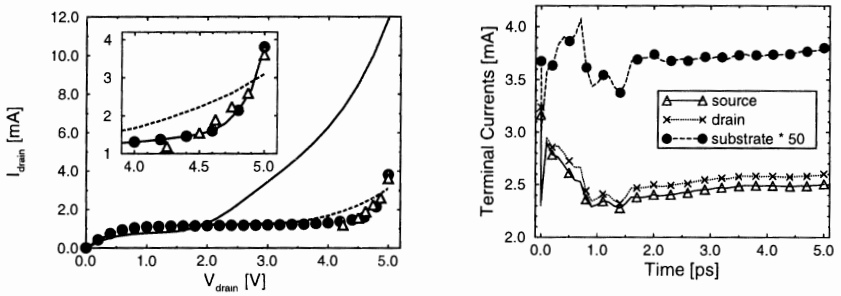

Figure 2: a) Drain current at V_{subs}=0V and V_{gate}=2V. (circles: experiment, solid line: drift-diffusion, dashed line: hydrodynamic, triangles: Monte Carlo) b) Convergence of terminal current during the Monte Carlo simulation at V_{drain}=4.875V.

The hydrodynamic simulation leads to good agreement with the measurements until about 4V drain voltage. Only the Monte Carlo method predicted the breakdown. The terminal currents are evaluated by a powerful domain integration technique. The terminal current convergence as a function of simulation time is shown in Figure 2.b. After less than two picoseconds convergence is obtained also for the substrate current.

The second example is a 40nm LDD-MOSFET. In Figure 3 the hydrodynamic electron temperature and the Monte Carlo electron average energy are compared. The

rectangle denotes the boundary of the Monte Carlo simulation domain. While the hydrodynamic solution shows the highest temperatures at the highly doped drain edge, the largest Monte Carlo energies are at the bottom of the LDD implant and the region of hot carriers is much more extended into the drain.

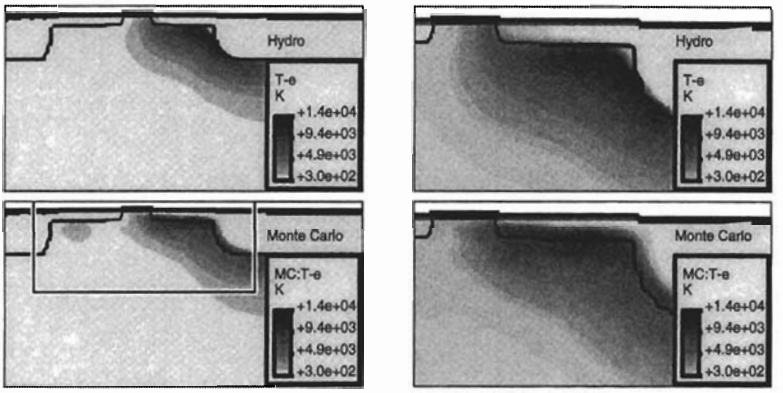

Figure 3: Comparison of electron temperatures computed by the hydrodynamic and the Monte Carlo method. (V_{gate}=2V, V_{drain}=4V, V_{sub}=0V) The plots on the right are zooms into the drain region.

The third example consists of an NIN structure with doping concentrations of $5x10^{17}$ and $2x10^{15}cm^{-3}$, where the intrinsic region has a length of 0.5 μm. In Figure 4 the need for Monte Carlo simulations is demonstrated by the impact ionization rate of the hydrodynamic in comparison with the Monte Carlo result. The hydrodynamic rate, a function of the carrier temperatures, cannot satisfactorily account for the non-locality needed in this example. Even when hydrodynamic temperatures and the average energies from Monte Carlo agree quite well, more detailed information about the non-local hot electron distribution is needed than the hydrodynamic formulation can model.

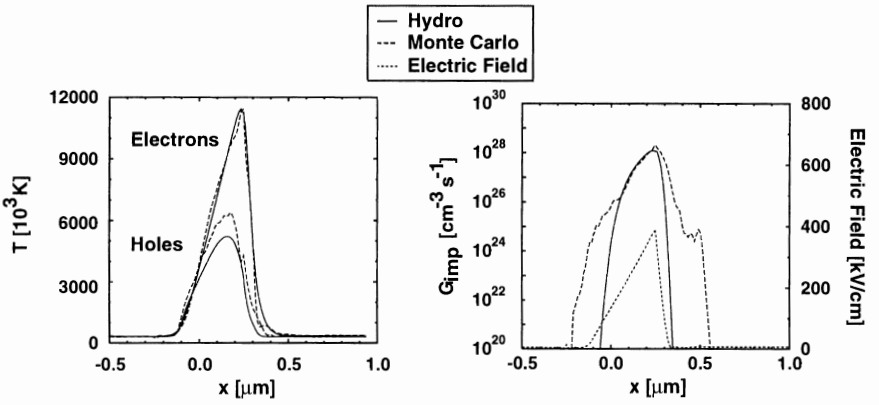

Figure 4: Carrier temperatures/average energies, avalanche generation, and electric field at 10V applied bias in the NIN example.

The coupling which has been presented between the hydrodynamic ansatz and the Monte Carlo method within the same software environment enables the user not

only to simulate deep submicron devices very accurately, but even to verify and adjust parameters of the hydrodynamic model. The mixed-mode and multi-device capabilities of DESSIS_ISE are not limited.

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