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

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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 bandstructure and scattering mechanisms, such as electron-phonon scattering, impact ionization and other carrier-carrier scattering [1]. However, the practical usefulness of Monte Carlo device simulation has not entirely lived up to its promise, as evidenced by the observed propensity to simulated simplified or imaginary device structures.

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  $D_{IOS-ISE}$  [2] to begin with a process simulation. Drift-diffusion or hydrodynamic simulations can be performed with the mixed-mode multi-dimensional device simulator  $D_{ESSIS_{-ISE}}$  [3, 4] as a preprocessing step. The full-band Monte Carlo simulator VEGAS\_ISE [1] was imbedded into DESSIS\_ISE by a window technique. The domain of the Monte Carlo simulation may be chosen either as the entire device, or as a simply connected subregion. 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 [5, 6]. In this paper initial and boundary conditions are extracted from a hydrodynamic solution calculated by DESSIS-ISE. Carrier densities, velocities and temperatures are passed to the Monte Carlo part. The Monte Carlo simulations can be performed self-consistently or using a frozen field from DESSIS\_ISE, either in one or two dimensions.



Figure 1:  $0.5\mu$ m nMOSFET with arbitrarily shaped Si-SiO<sub>2</sub> interface from process simulation.

We present three examples: a  $0.5\mu$ m MOS-FET, a 40nm MOSFET and a  $0.5\mu$ m nin structure.

The  $0.5\mu$ m nMOSFET was fabricated and measured by Fujitsu. The process was simulated with DIOS<sub>-ISE</sub> leading to a nonflat Si-SiO<sub>2</sub> interface (Figure 1). Figure 2 shows that the drift-diffusion Ansatz completely fails in this example.



Figure 2: Drain current at  $V_{subs}=0V$  and  $V_{gate}=2V$ .

The hydrodynamic simulation leads to good agreement with the measurements until about 4V drain voltage. Only the Monte Carlo method predicted accurately the avalanche breakdown. The terminal currents are evaluated by a powerful domain integration technique. The convergence of the terminal current as a function of simulation time is shown in Figure 3. After about one picosecond convergence is obtained also for the substrate current.



Figure 3: Convergence of terminal current during the Monte Carlo simulation

The second example is a 40nm LDD-MOSFET. In Figure 4 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 4: Comparison of electron temperatures computed by the hydrodynamic and the Monte Carlo method. ( $V_{gate}=2V, V_{drain}=4V, V_{sub}=0V$ )

The third example is a nin structure with doping concentrations of  $5 \times 10^{17}$  and  $2 \times 10^{15}$ , where the intrinsic region has a length of 0.5  $\mu$ m. In Figure 5 the need for Monte Carlo sim-

ulations 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 mirror the nonlocality needed for this example.



Figure 5: Avalanche generation and electric field at 10V applied bias

The presented coupling of the hydrodynamic Ansatz with the Monte Carlo method in 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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