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Single-Particle Approach to Self-Consistent Monte Carlo Device Simulation

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SUMMARY The validity and capability of an iterative coupling scheme between single-particle frozen-field Monte Carlo simulations and nonlinear Poisson solutions for achieving self-consistency is investigated. For this purpose, a realistic $0.1\,\mu$m lightly-doped-drain (LDD) n-MOSFET with a maximum doping level of about $2.5 \times 10^{20}\,\mathrm{cm}^{-3}$ is simulated. It is found that taking the drift-diffusion (DD) or the hydrodynamic (HD) model as initial simulation leads to the same Monte Carlo result for the drain current. This shows that different electron densities taken either from a DD or a HD simulation in the bulk region, which is never visited by Monte Carlo electrons, have a negligible influence on the solution of the Poisson equation. For the device investigated about ten iterations are necessary to reach the stationary state after which gathering of cumulative averages can begin. Together with the absence of stability problems at high doping levels this makes the self-consistent single-particle approach (SPARTA) a robust and efficient method for the simulation of nanoscale MOSFETs where quasi-ballistic transport is crucial for the on-current.

key words: *ballistic transport, Monte Carlo simulation, nanoscale MOSFETs, nonlinear Poisson equation, self-consistency*

1. Introduction

As scaling of silicon microelectronics has now reached the $0.1\,\mu$m regime, the on-current I_{on} is increasingly influenced by quasi-ballistic transport which is not accurately taken into account by classical device simulation based on the drift-diffusion or the hydrodynamic model [1], [2]. In contrast, this effect can be adequately investigated by self-consistent full-band Monte Carlo simulation [3], [4] and this approach has been often adopted in recent works for studying the performance of nanoscale MOSFETs [1], [5]–[9]. However, in these works the ensemble Monte Carlo technique was employed which requires very small time steps on a femtosecond scale in order to avoid stability problems [10]. This has limited the practical applicability to simplified device structures with a maximum doping level considerably or even far below $1 \times 10^{20}\,\mathrm{cm}^{-3}$. The stability problem does not exist in an alternative self-consistency scheme where Monte Carlo solutions of the Boltzmann equation are iteratively coupled with the nonlinear Poisson equation until convergence is achieved [11]. In the present work we adopt the latter approach by coupling single-particle frozen-field Monte Carlo simulations [12] with solutions of the nonlinear Poisson equation where the electron density in the low-density bulk regions, which are never visited by the single particles, is taken from the initial classical simulation. It is, on the one hand, the aim of this paper to assess the validity of this approach by investigating whether there is a sensitivity to the type of the initial classical simulation (DD or HD) or to the length of the time interval after which the Poisson equation is solved because these variations involve different bulk densities. On the other hand, the capability of this method for treating realistic devices is demonstrated and illustrated by the simulation of an $0.1\,\mu$m LDD n-MOSFET structure which is obtained from process simulation [13] according to a realistic process flow.

2. Monte Carlo Model and Device Structure

The full band structure is obtained from nonlocal empirical pseudopotential calculations including spin-orbit interaction and the energies of four conduction bands are stored on an equidistant mesh with a spacing of $1/96 \times 2\pi/a$ with a denoting the lattice constant. The scattering mechanisms include phonon scattering, impurity scattering, impact ionization and surface roughness scattering. The phonon system consists of three f-type and three g-type intervalley processes with the same values for the coupling constants as reported by Jacoboni and Reggiani [14] and acoustic intravalley scattering. Impurity scattering is taken into account via a calibrated Ridley model [12] where a doping-dependent prefactor of the rate is adjusted such that the measured doping dependence of the ohmic mobility [15] is reproduced. The present impact ionization scattering rate is taken from Ref. [16]. The semi-empirical surface roughness scattering model involves a combination of diffusive and specular scattering where the percentage of diffusive scattering is 15%. Details of the propagation algorithm are reported in Refs. [12], [17].

The bulk mobility model of the initial classical device simulations corresponds to the bulk Monte Carlo

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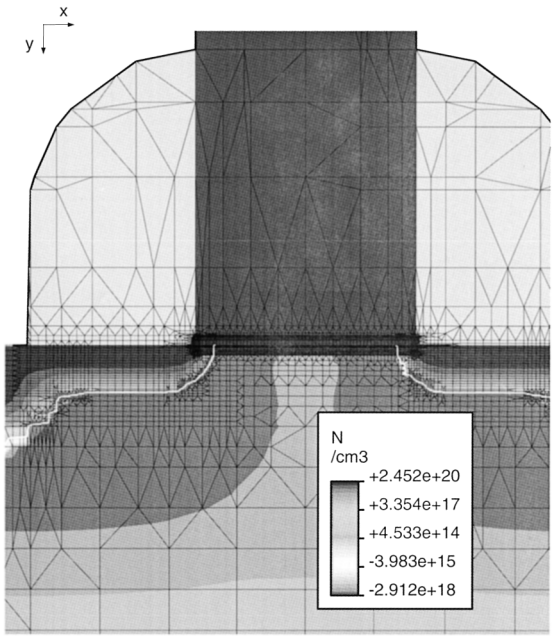

Fig. 1 Simulated n-MOSFET with $L_{\rm ch} = 90\,{\rm nm}$, $L_{\rm eff} = 75\,{\rm nm}$ and $t_{\rm ox} = 2.2\,{\rm nm}$. The white lines indicate the *pn* junctions.

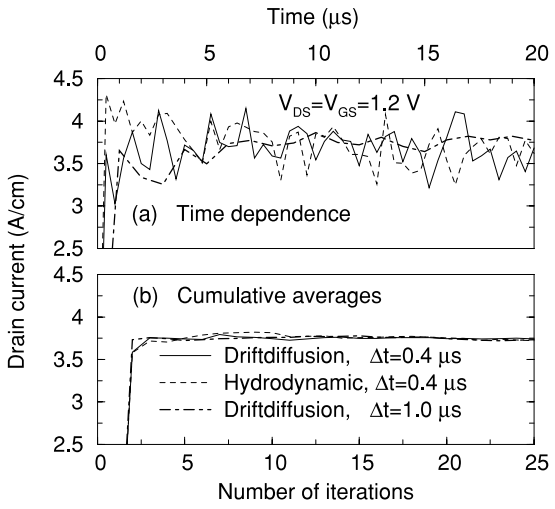

Fig. 2 (a) Drain current as a function of the time, during which single particles are simulated, and (b) cumulative averages as a function of the number of iterations taken over the values of (a) after ten iterations (i.e. after $4\,\mu{\rm s}$ for $\Delta t = 0.4\,\mu{\rm s}$ and $10\,\mu{\rm s}$ for $\Delta t = 1.0\,\mu{\rm s}$, respectively). The different curves correspond to Monte Carlo simulations based either on an initial drift-diffusion or a hydrodynamic simulation and involve different lengths Δt of the time intervals after which the nonlinear Poisson equation is solved.

result which entails in particular an energy relaxation time of $\tau_w = 0.3\,{\rm ps}$ for the hydrodynamic model. The model of Darwish [18] for surface mobility reduction is adopted and bandgap narrowing, equally attributed to the valence and the conduction band edge, is modeled according to Slotboom [19]. Boltzmann statistics is used as in the Monte Carlo simulation. Finally, the above surface mobility model is adjusted in order to reproduce the Monte Carlo result for the drain current in the linear regime for the simulated $0.1\,\mu{\rm m}$ LDD n-MOSFET shown in Fig. 1. The device structure in Fig. 1 is obtained from process simulation [13] and features a channel length of $L_{\rm ch} = 90\,{\rm nm}$, an effective gate length of $L_{\rm eff} = 75\,{\rm nm}$, an oxide thickness of $t_{\rm ox} = 2.2\,{\rm nm}$ and a maximum doping level of about $2.5 \times 10^{20}\,{\rm cm}^{-3}$. The channel direction, i.e. the x axis in Fig. 1, corresponds to the crystallographic $\langle 110 \rangle$ direction as is usual in standard complementary metal-oxide-semiconductor (CMOS) technology.

3. Self-Consistency Scheme

When the first single-particle frozen-field Monte Carlo simulation based on the electrostatic potential ψ resulting from the initial classical simulation is completed, an estimate for the electron density $n_{\rm MC}$ has been obtained. It enters the Poisson equation

$$-\nabla \cdot (\varepsilon \nabla \psi) = -e\left(n_{\rm MC} - p + N_{\rm A}^- - N_{\rm D}^+\right) \qquad (1)$$

which gives the new electric field to be used in the next Monte Carlo simulation. Here, ε is the dielectric constant, $e > 0$ the elementary charge, p the hole density, $N_{\rm A}^-$ the acceptor concentration and $N_{\rm D}^+$ the donor concentration. However, Eq. (1) which is linear in ψ gives rise to stability problems at high doping concentrations necessitating very small time steps on a femtosecond scale during ensemble Monte Carlo simulations [10], [11]. Therefore we adopt the alternative stable self-consistency scheme proposed by Venturi et al. [11]. In this scheme an electron quasi-fermi level is defined via

$$\phi_n \equiv \psi - \frac{k_B T_L}{e} \ln\left(\frac{n_{\rm MC}}{n_{\rm i,eff}}\right) \qquad (2)$$

and likewise for holes with k_B denoting the Boltzmann constant, T_L the lattice temperature and $n_{\rm i,eff}$ the effective intrinsic carrier concentration. Keeping the quasi-fermi level fixed and resolving Eq. (2) for $n_{\rm MC}$ leads to an expression for the density which depends on the potential, i.e. $n_{\rm MC}(\psi)$. Inserting this expression into Eq. (1) makes the Poisson equation nonlinear in ψ. Then, solutions of the nonlinear Poisson equation have to be iterated with Monte Carlo solutions of the Boltzmann transport equation until convergence versus the steady-state is achieved after which gathering of cumulative averages can begin to reduce the Monte Carlo noise for the final result.

Figure 2(a) shows the evolution of the drain current as a function of the time, during which single particles are simulated, and Fig. 2(b) shows the corresponding cumulative average as a function of the number of iterations after the steady-state has been reached. In the framework of the single-particle approach without statistical enhancement, the bulk region is hardly ever visited by Monte Carlo electrons due to the small elec-

tron density in the bulk. Therefore the electron density in this region is taken from the initial classical simulation as is the hole density in the whole device. However, the electron bulk densities are significantly different between DD and HD. Also the extension of the inversion channel into the bulk, which is visited by Monte Carlo electrons, varies depending on the length Δt of the time interval after which the nonlinear Poisson equation is solved, because during a longer time interval also regions with a lower density and hence a lower probability of being visited are sampled. This raises the question how those density differences affect the solution of the Poisson equation and the resulting drain current. Therefore three different simulations are displayed in Fig. 2 based either on an initial HD or DD simulation or on different time interval lengths ($\Delta t = 0.4\,\mu$s or $\Delta t = 1.0\,\mu$s) of a single frozen-field Monte Carlo simulation. It can be seen in Fig. 2(a) that the drain current begins in all three cases to fluctuate around the steady-state after rougly ten iterations, i.e. after $4\,\mu$s for $\Delta t = 0.4\,\mu$s and after $10\,\mu$s for $\Delta t = 1.0\,\mu$s. Despite different shapes in the initial phase (e.g. the simulation based on an initial HD simulation features a kind of overshoot) the currents tend afterwards to fluctuate around the same value. This becomes obvious in Fig. 2(b) where the cumulative averages after ten iterations over the values in Fig. 2(a) are shown. Hence, the same results for the drain current in Fig. 2(b) suggest that the differences between the three kinds of simulation for the electron density in the bulk, where the density level is small compared to the source/drain regions and the inversion channel, are negligible for the solution of the Poisson equation. While the number of iterations necessary for reaching the steady-state seems to be the same for DD and HD, it is also clear that a time interval as small as possible is to be preferred because it reduces the simulation time for reaching the stationary state. Of course, in any case sufficient statistics for the electron density in the inversion channel must be gathered so that Δt must not be too small. In this respect, the value of $\Delta t = 0.4\,\mu$s is close to the minimum which can be safely used in the present example.

Finally, the statistical nature of the Monte Carlo simulations is illustrated in Fig. 3. There the cumulative average, i.e. the mean value

$$\bar{I} \equiv \frac{1}{n}\sum_{i=1}^{n} I_i \tag{3}$$

of the current values I_i with n denoting the number of iterations, can be seen for (a) the drain current and (b) the substrate current where all three simulations are based on the same initial simulation (DD) and the same time interval length ($\Delta t = 0.4\,\mu$s). In Fig. 4, the corresponding relative errors

$$\Delta I \equiv 2\bar{\sigma}/\bar{I} \tag{4}$$

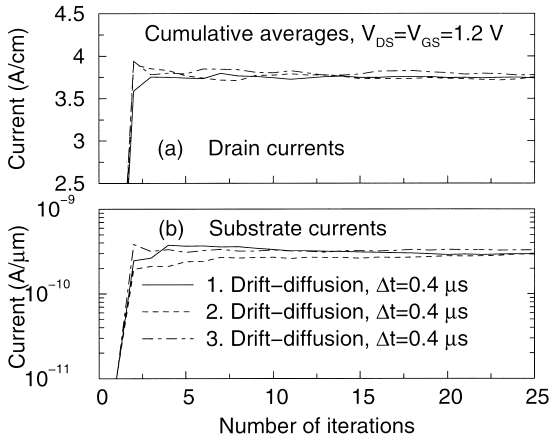

Fig. 3 Cumulative averages for (a) the drain current and (b) the substrate current as a function of the number of iterations for three simulations all based on the same initial classical device simulation and the same time interval length Δt.

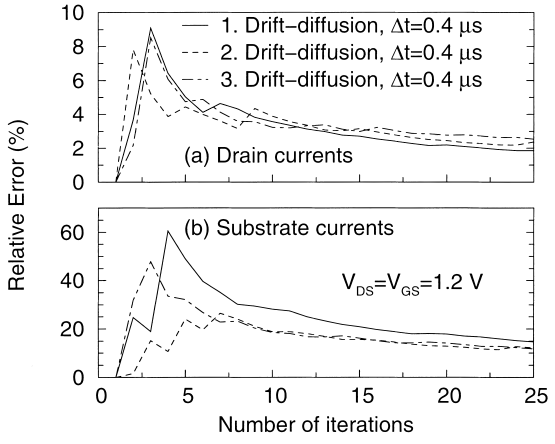

Fig. 4 Relative error corresponding to the averages in Fig. 3 for (a) the drain current and (b) the substrate current as a function of the number of iterations for three simulations all based on the same initial classical device simulation and the same time interval length Δt.

$$\bar{\sigma}^2 \equiv \frac{1}{n}\,\frac{1}{n-1}\sum_{i=1}^{n}(I_i - \bar{I})^2 \tag{5}$$

are shown with $\bar{\sigma}^2$ being the variance of the mean value. As discussed before, gathering of cumulative averages begins only after the stationary state has been reached. However, the current estimations of the subsequent iterations are not exactly stochastically independent, as it is the case for non-selfconsistent simulations [20], because two successive iterations are still coupled via the Poisson equation. As a consequence, the usual interpretation of the relative error for the confidence interval of the expectation value does not hold exactly. Nevertheless, from a practical point of view, the 'relative errors' in Fig. 4 still show the usual $1/\sqrt{n}$ behavior and can therefore be used as stopping criteria to discriminate between the different simulation times necessary at different bias points for a similar level of accuracy. The

results of one simulation after 25 iterations following steady-state as shown in Figs. 3 and 4 correspond to a CPU time of 14 h on one 667 MHz alpha processor. Note, however, that the simulation time for one bias point strongly depends on geometry and doping profiles of the device under consideration.

4. Device Simulation Results

In this section, the simulation results of the drift-diffusion model, the hydrodynamic model and the Monte Carlo model are compared. Figure 5 shows the output characteristics corresponding to the three transport models. Note that apart from the modification of the DD/HD surface mobility in order to reproduce the MC drain current at $V_{DS} = 50\,\mathrm{mV}$ no further adjustment was performed. The agreement with the Monte Carlo results continues for the hydrodynamic simulation to higher drain voltages than for the drift-diffusion simulation, but the overestimation of the on-current is considerably stronger by HD than the underestimation by DD.

The differences of the on-current are related to the distribution of internal variables which are displayed in Figs. 6 and 7. The figures show the profiles of the internal variables along the channel, i.e. along the x axis in Fig. 1. They are computed by averaging the quantity perpendicular to the Si/SiO_2 interface with the relative electron density according to

$$v_x(x) \equiv \frac{\int v_x(x,y)\; n(x,y)\, dy}{\int n(x,y)\, dy} \tag{6}$$

as for the x-component of the drift velocity in Fig. 7(a) and likewise for the electron density $n(x)$ in Fig. 6(b) and the longitudinal electric field $E_x(x)$ in Fig. 7(b) or by integration of the quantity over y according to

$$n_{\mathrm{inv}}(x) \equiv \int n(x,y)\, dy \tag{7}$$

as for the inversion layer density n_{inv} in Fig. 6(a), respectively. The figures show that the different on-currents are associated with a different drift velocity in the source-side of the channel which mainly determines I_{on}. The behavior in the drain-side of the channel is then determined by the continuity equation for the charge density. This requires e.g. the compensation of the low DD drift velocity, which cannot be higher than the saturation velocity, by a higher electron concentration so that the current remains constant in the channel.

5. Conclusions

The validity of the single-particle approach for self-consistent full-band Monte Carlo device simulation has been investigated. In this approach, single-particle

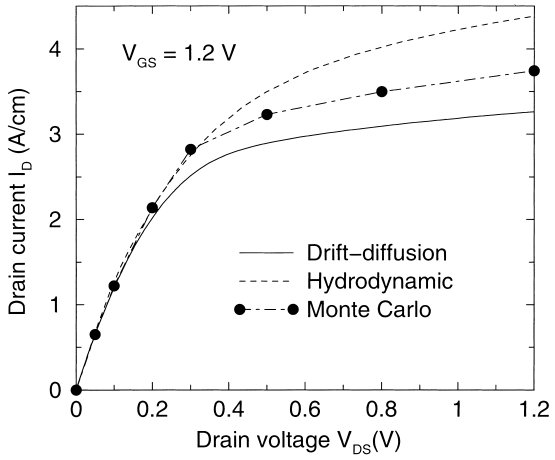

Fig. 5 Output characteristics of the 0.1 μm LDD n-MOSFET in Fig. 1 according to a drift-diffusion, a hydrodynamic and a self-consistent full-band Monte Carlo simulation.

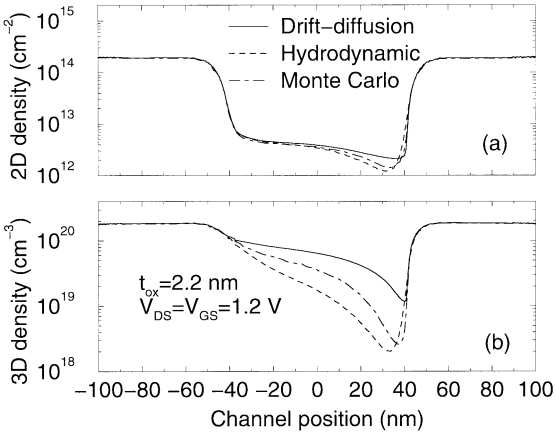

Fig. 6 Profiles along the channel of (a) the 2D inversion layer density obtained by integration of the density perpendicular to the Si/SiO_2 interface (i.e. in y-direction in Fig. 1) and (b) the mean 3D density resulting from averaging perpendicularly to the interface with the relative density.

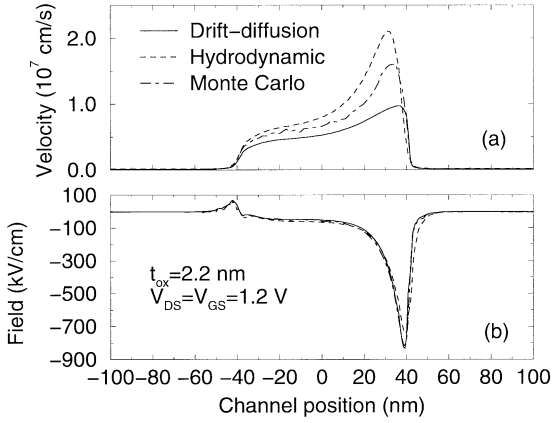

Fig. 7 Profiles along the channel of (a) the averaged electron velocity and (b) the averaged longitudinal electric field. Averaging is performed perpendicular to the Si/SiO_2 interface with the relative electron density.

frozen-field simulations are iterated with solutions of the nonlinear Poisson equation until convergence is achieved. It was found that different densities imposed for the bulk region, which is never visisted by Monte Carlo electrons, have a negligible influence on the final Monte Carlo result for the drain current and can be taken e.g. either from an initial drift-diffusion or a hydrodynamic simulation. The feasibility and importance of this Monte Carlo approach was demonstrated by the simulation of a realistic 0.1 μm n-MOSFET where the on-currents of the drift-diffusion and the hydrodynamic model strongly deviate from the Monte Carlo result. In conjunction with the stability of the nonlinear Poisson equation in high-doping regions this approach presents a viable and important tool for the consideration of quasi-ballistic transport in the sub 0.1 μm regime.

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