Efficient Monte Carlo Device Simulation with Automatic Error Control

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***Abstract*—A single-particle approach to Monte Carlo device simulation is presented where the simulation is stopped when the error for the drain, substrate or gate current is below a predefined error bar. This is achieved by alternating an ensemble simulation in the contact elements, used for the injection of a carrier, with a single–particle simulation in the active device area, thus enabling stochastically independent current estimates. Together with efficient Monte Carlo techniques, leading to CPU times of typically one hour per bias point, this makes full-band Monte Carlo "affordable" for the simulation of submicron MOSFETs.

I. INTRODUCTION

Full–band Monte Carlo device simulation has been established as a powerful tool for the investigation of ballistic and hot–electron effects occurring in deep submicron MOSFETs [1], [2]. However, there are two drawbacks associated with this device simulation approach which have so far prevented its widespread use. One major concern was the computation time involved, but this problem has been greatly reduced by the frozen–field approach [3], a phase–space step–like propagation within the self–scattering scheme [4] and an efficient treatment of the state–after–scattering selection [5] as well as of impurity scattering [6]. The other obstacle is the statistical fluctuation of the current estimators, the (bias–dependent) error of which could not be determined without an a priori knowledge of the corresponding correlation times. So far, progress in this respect was only achieved for substrate current calculations [5], where a single–particle simulation is restricted to a window of the device, but this method may involve a more serious error by using beyond the frozen field also the drain current from the classical device simulation for the formulation of the boundary conditions on the window interface [3], [5]. It is therefore the aim of this paper to solve the error–control problem for drain, substrate and gate currents in submicron MOSFETs within the framework of the efficient full–band Monte Carlo algorithms mentioned above.

II. AUTOMATIC ERROR CONTROL METHOD

The central problem in achieving the above goal is the necessity to generate stochastically independent estimates of the currents, thus enabling the applicability of the textbook formula for the standard deviation, and at the same time to fulfil the ohmic boundary condition of the Boltzmann equation along all metallic contacts. The solution is based on a realization of the ohmic boundary condition within an ensemble Monte Carlo (MC) simulation [7], where an equilibrium MC simulation (i.e. with vanishing field) is performed in contact elements. When a particle in a contact element hits the border of the contact element, it is set back at the opposite side of the element with an unchanged momentum. If the border is adjacent to the semiconductor area of the MOSFET, a copy of this particle is injected. On the other hand, a particle from inside the device hitting the border to a contact element is taken out of the simulation.

Our new idea consists of the combination of an ensemble equilibrium simulation of equally weighted electrons in the contact elements, distributed according to the equilibrium density, and a single–particle approach (SPARTA) in the active

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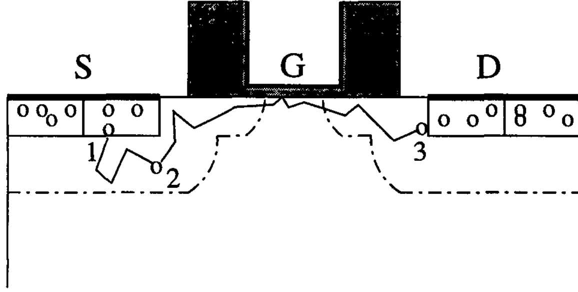

Fig. 1. Schematic structure of a MOSFET with 14 electrons in 4 contact elements. 1) During the ensemble simulation at thermal equilibrium in the 4 contact elements, one electron hits the border to the active region, and a single electron is injected. 2) While traversing the device, the electron suffers several scattering processes. 3) The single electron hits a contact element and is absorbed. A new ensemble simulation in the contact elements begins.

domain, where the single electron carries within the frozen–field approximation the integrated electron charge of the classical device simulation. This scheme is illustrated in Fig. 1. When an electron hits the border with the active domain during the ensemble simulation in the contact elements, it is injected at the corresponding position. In this way, the ohmic boundary condition is taken into account. The injected single electron is simulated until it hits the border of a contact element, where it is absorbed, and a new ensemble simulation in the contact elements begins. The statistics gathered along the electron trajectory by the just–before–scattering method [8] is, on the other hand, used for an estimate of the different currents, and the estimates for different electron trajectories are independent from each other due to the stochastic nature of the particle injection and absorption (Actually, for efficiency reasons, current computations are not performed for each single trajectory, but after 30000 trajectories).

III. Current Estimators

The drain current $I_{\rm D}$ is estimated by the test–function method of Yoder [9], [10], taking the densities and velocities entering the test–function optimization [10] from the drift–diffusion solution. The substrate and gate currents are computed via

$$I_{Subs} = e \int_{Device} d^2r \; n(\mathbf{r}) \; \langle S_{\rm II} \rangle (\mathbf{r}) \qquad (1)$$

and

$$I_{\rm G} = e \int_{Gate} dx \; n(\mathbf{r}) \; \frac{1}{2} \langle v_n T \rangle (\mathbf{r}), \qquad (2)$$

respectively, with $S_{\rm II}$ denoting the impact ionization scattering rate, n the electron density, v_n the velocity normal to the gate interface, and T the tunneling probability calculated with the WKB approximation. The two–dimensional integration in Eq. (1) is over the whole active device area and the one–dimensional integration in Eq. (2) is along the gate oxide. Since only one electron is simulated, phase–space elements are visited according to the distribution of real electrons. In deep–submicron MOSFETs under normal operation conditions, this is advantageous for the above current estimators, because the relevant regions (source–side of the channel for the gate current $I_{\rm G}$ in the dominant direct–tunneling regime [11], high–velocity region at the drain–side of the channel for the drain current $I_{\rm D}$, and the drain–side LDD region for the substrate current I_{Subs}) exhibit high electron densities and/or high electron temperatures. Hence, a large amount of statistics is gathered by the just–before–scattering technique in those phase–space elements, which determine the respective currents within the above estimators. Other details of the full–band Monte Carlo model are published elsewhere [12], [13].

IV. Simulation Results

The simulated n–MOSFET is displayed in Fig. 2, and the resulting current characteristics can be seen in Figs. 3 and 4, where the simulations were performed until the relative error had reached a predefined value. Fig. 5 shows for an example the evolution of the error as a function of the number of current computations. Finally, the number of current computations necessary for typical errors are reported in Fig. 6 for all three kinds of currents as a function of the applied voltage. It can be seen that

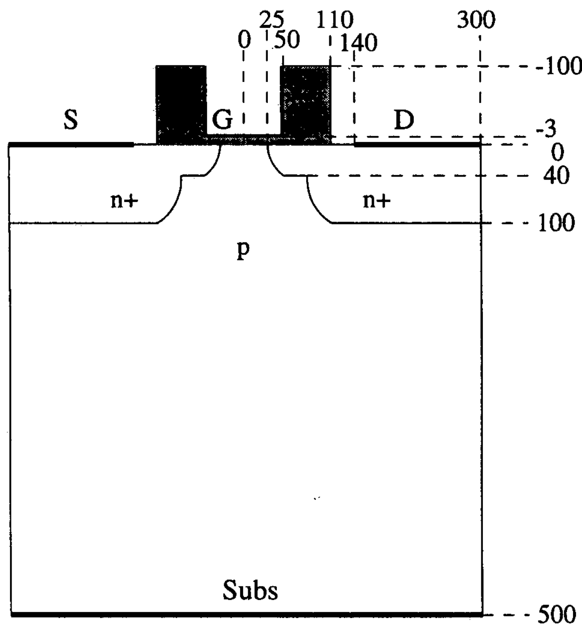

Fig. 2. Structure of the simulated n–MOSFET. The maximum n–type dopings are $N_D = 1.5 \times 10^{20}$ cm^{-3} and $N_D = 5 \times 10^{19}$ cm^{-3}, respectively, and the constant p–type doping is $N_A = 1 \times 10^{18}$ cm^{-3}. The measure in the figure is nm.

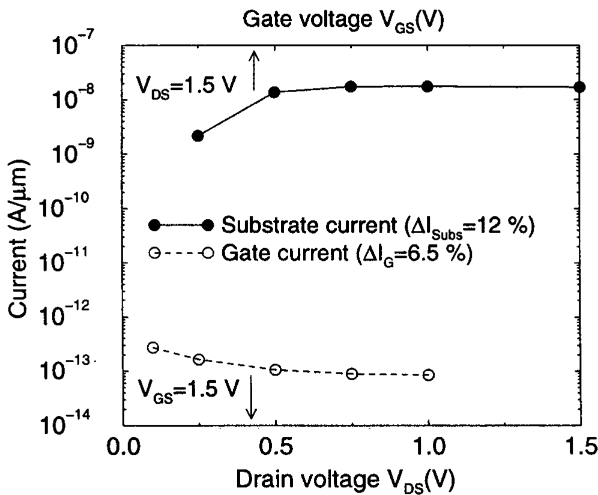

Fig. 3. Substrate current (at a drain voltage of V_{DS} = 1.5 V) as a function of the gate voltage, $I_{Subs}(V_{GS})$, and gate current (at a gate voltage of V_{GS} = 1.5 V) as a function of the drain voltage, $I_G(V_{DS})$, respectively.

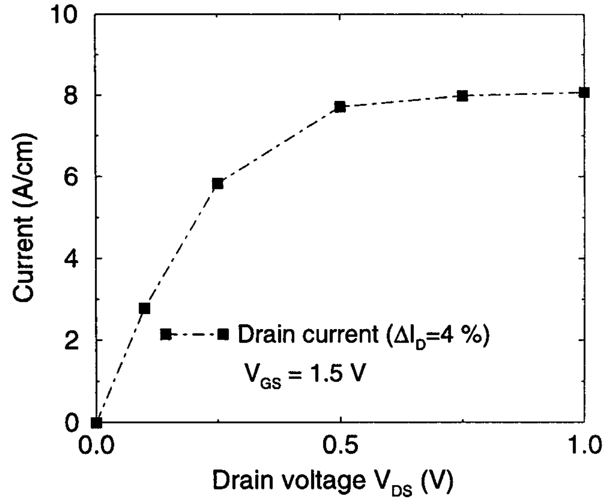

Fig. 4. Drain current (at a gate voltage of V_{GS} = 1.5 V) as a function of the drain voltage, $I_D(V_{DS})$.

these numbers are in the same order for all voltages except the smallest ones, so that with a single run also useful results for the two other currents will be obtained. The computational effort is in the order of one hour CPU time per bias point on a 500 MHz AlphaServer 21264 except for the lowest voltages.

V. Summary

In conclusion, a new single–particle approach (SPARTA) to Monte Carlo device simulation has been developed. It allows using predefined error bars for drain, substrate or gate currents, and typically requires one hour CPU time per bias point, thereby making the full–band Monte Carlo method viable for the simulation of MOSFETs in the deep submicron regime.

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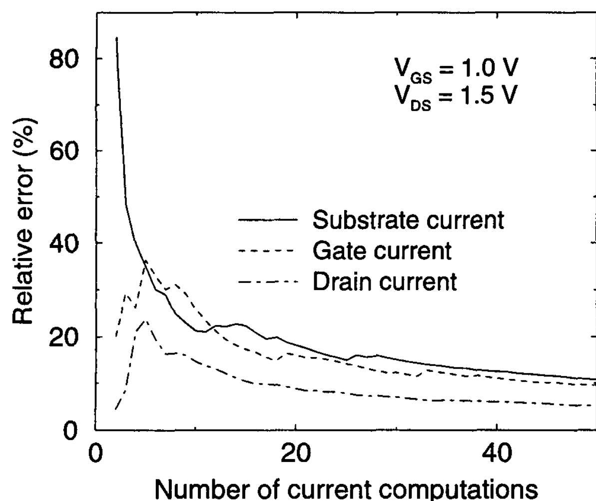

Fig. 5. Relative errors of substrate, gate and drain current as a function of the number of current computations. Each current computation refers to 30000 electrons, which have consecutively traversed the device.

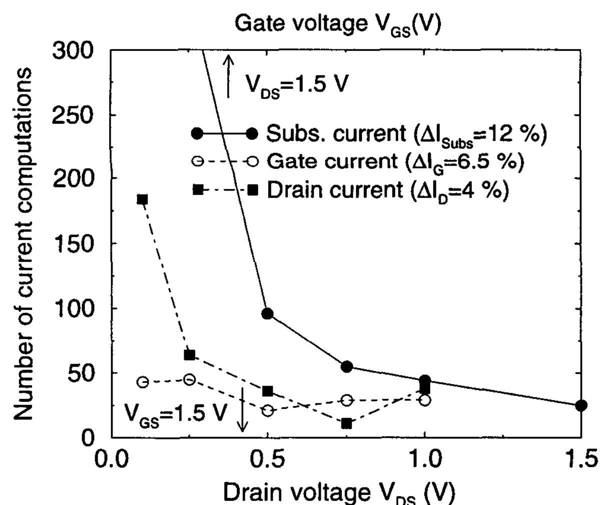

Fig. 6. Number of computations necessary for the error falling below the error bar. The bias point I_D=8 A/cm at V_{DS}=1.0 V requires e.g. 1 hour CPU time on a 500 MHz Compaq Alphaserver.

REFERENCES

[1] M. V. Fischetti and S. E. Laux, "Monte Carlo analysis of electron transport in small semiconductor devices including band–structure and space–charge effects," *Phys. Rev. B*, vol. 38, pp. 9721–9745, 1988.

[2] K. Hess, Ed., *Monte Carlo Device Simulation: Full Band and Beyond.* Boston: Kluwer, 1991.

[3] J. M. Higman, K. Hess, C. G. Hwang, and R. W. Dutton, "Coupled Monte Carlo–drift diffusion analysis of hot-electron effects in MOSFET's," *IEEE Trans. Electron Devices*, vol. 36, pp. 930–937, 1989.

[4] J. Bude and R. K. Smith, "Phase-space simplex Monte Carlo for semiconductor transport," *Semicond. Sci. Technol.*, vol. 9, pp. 840–843, 1994.

[5] C. Jungemann, S. Yamaguchi, and H. Goto, "Efficient full band Monte Carlo hot carrier simulation for silicon devices," in *Proc. ESSDERC*, G. Baccarani and M. Rudan, Eds., Bologna, 1996, vol. 26, pp. 821–824, Editions Frontières.

[6] H. Kosina, "A method to reduce small-angle scattering in Monte Carlo device analysis," *IEEE Trans. Electron Devices*, vol. 46, pp. 1196–1200, 1999.

[7] H.-J. Peifer, *Monte-Carlo-Simulation des Hochenergietransportes von Elektronen in submikron MOS–Strukturen.* Aachen: Augustinus–Buchhandlung, 1992.

[8] P. J. Price, *Semiconductors and Semimetals*, p. 249. New York: Academic, 1979.

[9] P. D. Yoder, K. Gärtner, and W. Fichtner, "A generalized Ramo–Shockley theorem for classical to quantum transport at arbitrary frequencies," *J. Appl. Phys.*, vol. 79, pp. 1951–1954, 1996.

[10] P. D. Yoder, K. Gärtner, U. Krumbein, and W. Fichtner, "Optimized terminal current calculation for Monte Carlo device simulation," *IEEE Trans. Computer–Aided Des.*, vol. 16, pp. 1082–1087, 1997.

[11] E. Cassan, S. Galdin, P. Dollfus, and P. Hesto, "Study of direct tunneling through ultrathin gate oxide of field effect transistors using Monte Carlo simulation," *J. Appl. Phys.*, vol. 86, pp. 3804–3811, 1999.

[12] F. M. Bufler, P. D. Yoder, and W. Fichtner, "Simple phase–space trajectory calculation for Monte Carlo device simulation including screened impurity scattering," in *Proc. SISPAD*, Kyoto (Japan), Sept. 1999, pp. 31–34.

[13] F. M. Bufler, A. Schenk, and W. Fichtner, "Efficient Monte Carlo device modeling." *IEEE Trans. Electron Devices*, in press.