

# Comparison of Single-Particle Monte Carlo Simulation with Measured Output Characteristics of an 0.1 $\mu\text{m}$ n-MOSFET

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A comparison between non-selfconsistent single-particle Monte Carlo (MC) simulations and measurements of the output characteristics of an 0.1  $\mu\text{m}$  n-MOSFET is presented. First the bulk MC model, which features a new simplified treatment of inelastic acoustic intravalley scattering, is validated by comparison with experimental literature data for mobilities and velocities. The dopant distribution of the MOSFET is obtained from a 2D process simulation, which is calibrated with SIMS and electrical measurements and fine-tuned by a comparison of the measured transfer characteristics in the subthreshold regime with a coupled Schrödinger drift-diffusion (DD) simulation. Then the quantum effect is replaced by a shift of the work function and the DD, hydrodynamic (HD) and MC models are adjusted to reproduce the measured drain current in the linear regime. The results of the three models in the non-linear regime are compared without further adjustment to the measured output characteristics. While good agreement is found for the MC model, the on-current is significantly overestimated by the HD model and underestimated by the DD model.

**Keywords:** Monte Carlo simulation; Single-particle approach; Submicron n-MOSFET; Measurement of output characteristics; Full band; Phonon scattering

## INTRODUCTION

As metal-oxide semiconductor field-effect transistors (MOSFETs) are scaled into the sub 0.1  $\mu\text{m}$  regime, the question arises to what extent the saturation drain current increases and which simulation models are able to take the involved quasiballistic transport accurately into account [1]. The most elaborate method to address this issue is a self-consistent ensemble Monte Carlo simulation [2–6]. However, due to the problem of time stability [7], these approaches have been applied only to simplified device structures with uniform substrate doping [4–6], with maximum doping levels of  $3 \times 10^{19} \text{cm}^{-3}$  [3],  $8 \times 10^{19} \text{cm}^{-3}$  [4] and  $1 \times 10^{19} \text{cm}^{-3}$  [5] (Refs. [2,6] do not specify the maximum doping level), or with too thick oxides [2], and none of the aforementioned works contains comparisons with experimental data. In contrast, realistic 0.1  $\mu\text{m}$  MOSFETs involve non-uniform substrate doping and maximum doping levels above  $3 \times 10^{20} \text{cm}^{-3}$ . Apart

from the lack of experimental verification, there remains some uncertainty to what extent the results from those structures can be extrapolated for realistic devices and, in particular, how realistic devices can be simulated.

It is therefore the aim of this paper to investigate the issue of quasiballistic transport and saturation drain current for a real state-of-the-art MOSFET. In our approach we will use simpler transport models, which can be applied without problems to realistic devices, i.e. drift-diffusion (DD), hydrodynamic (HD) and single-particle Monte Carlo (MC) simulation where a frozen field from the DD simulation is used. The dopant distribution of the 0.1  $\mu\text{m}$  n-MOSFET is obtained from a calibrated 2D process simulation, which is fine-tuned such that the measured transfer characteristics in the subthreshold regime is accurately reproduced by a coupled Schrödinger DD simulation. After adjusting the transport models in the linear regime to the measured drain current, the non-linear regime of the output characteristics is simulated without

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further adjustment and compared to the measurements. In conjunction with the minimization of uncertainties of the doping profiles, this simulation methodology allows us to access the accuracy and the limits of the transport models in a realistic example.

The paper is organized as follows. In the second section, information about the models for band structure and scattering mechanisms is provided, with particular emphasis on the new approach to inelastic acoustic intravalley scattering. This Monte Carlo model is subsequently validated by comparing the simulation results for drift mobility and drift velocity with corresponding experimental data. The third section reports the new methodology for the fine calibration of the doping profile with the help of a coupled Schrödinger drift-diffusion simulation. In the fourth section, the simulation results of the transport models in the non-linear regime are compared to the measured output characteristics. The findings are summarized in the fifth section.

## MONTE CARLO MODEL

The band structure of the four conduction bands is computed by the non-local empirical pseudopotential method including spin-orbit interaction. The band energies are stored on an equidistant mesh in momentum space with a mesh spacing of  $1/96 \times 2\pi/a$  where  $a$  denotes the lattice constant of silicon.

The scattering model includes phonon scattering and impurity scattering. Three f-type and three g-type intervalley phonons are considered using exactly the same values for the coupling constants as Jacoboni and Reggiani [8]. Concerning acoustic intravalley scattering, a new approach is used. It constitutes a compromise between a model, which considers explicitly the acoustic phonon dispersion thereby involving a wave-vector dependent scattering rate, and the elastic equipartition approximation where the scattering rate depends only on energy thereby facilitating the search of after-scattering states during full-band Monte Carlo simulation. The new idea is to replace both the phonon energy and the square of the wave vector in the scattering rate by constants that are determined by an adequate averaging procedure. As a consequence, the scattering rate depends only on energy, but involves at the same time energy dissipation as in the wave-vector dependent model. The starting point for the development of the new model is the expression for the scattering rate which can be written in the form

$$S(\mathbf{k}) = \sum_{\mathbf{k}'} \frac{\pi}{\rho\omega(q)} \Delta^2(q) \left( N_q + \frac{1}{2} \mp \frac{1}{2} \right) \times \frac{1}{V} \delta(\epsilon(\mathbf{k}') - \epsilon(\mathbf{k}) \mp \hbar\omega(q)) \quad (1)$$

where  $\rho$  denotes the mass density,  $V$  the volume of the crystal and  $N_q$  the Bose-Einstein distribution. Upper and

lower signs correspond to phonon absorption and emission, respectively, and the phonon wave-vector  $\mathbf{q} = \mathbf{k}' - \mathbf{k}$  results from wave vector conservation. In the isotropic approximation, the coupling constant for acoustic intravalley scattering is given by  $\Delta(q) = \mathcal{E}q$ . For the phonon dispersion we use the parametrization  $\hbar\omega(q) = \hbar(\nu_{SL}q - c_Lq^2)$  where  $\nu_{SL} = 9.0 \times 10^5$  and  $c_L = 2.0 \times 10^{-3} \text{ cm}^2/\text{s}$  [9]. For the averaging procedure, first the modulus of the phonon wave vector,  $q = \|\mathbf{k}' - \mathbf{k}\|$ , is averaged over a sphere in the spirit of an isotropic, parabolic band structure with the result  $q = (4/3)k$ . Then the phonon energy is averaged with a Maxwell-Boltzmann distribution according to

$$k_B \theta_{ac} \equiv \hbar\omega_{ac} = \frac{\int d\epsilon \hbar\omega(\frac{4}{3}k(\epsilon)) \mathcal{D}(\epsilon) e^{-\epsilon/(k_B T)}}{\int d\epsilon \mathcal{D}(\epsilon) e^{-\epsilon/(k_B T)}}. \quad (2)$$

Here,  $\mathcal{D}(\epsilon)$  denotes the density of states,  $k_B$  the Boltzmann constant and  $k(\epsilon) = \sqrt{2m(\epsilon)\epsilon}/\hbar$  with the effective mass  $m(\epsilon)$  taken to be the energy-dependent effective density-of-states mass. An analogous procedure is applied for the square of the phonon wave vector. Of course, this approximation becomes inaccurate at higher electric fields, but in this regime energy dissipation is dominated by intervalley processes. As a consequence, the phonon energy and the square of the phonon wave vector depend on the lattice temperature as is shown in Fig. 1. Finally, the acoustic coupling constant  $\mathcal{E}$  is adjusted to reproduce the experimental Ohmic drift mobility at room temperature. This yields a value of  $\mathcal{E} = 7.73 \text{ eV}$ .

For the electronic band structure with ellipsoidal equienergy surfaces in the low-energy region, another

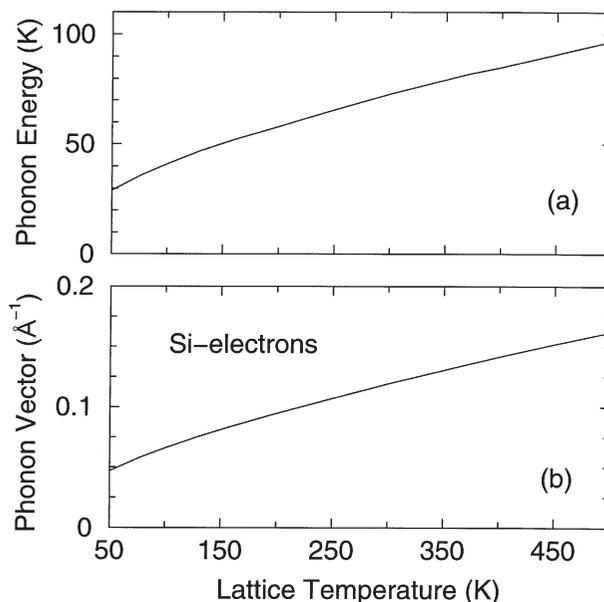


FIGURE 1 Phonon energy (a), expressed in terms of the equivalent phonon temperature  $\theta_{ac} = \langle \hbar\omega(q) \rangle / k_B$ , and mean modulus of the phonon wave vector (b), defined via  $\sqrt{\langle q^2 \rangle}$ , as a function of the lattice temperature.

advantage of the energy-dependent scattering rate is that the Ohmic drift mobility can be calculated directly via [10]

$$\mu = \frac{e \int_0^\infty d\epsilon \tau(\epsilon) \mathcal{V}^{-2}(\epsilon) \mathcal{D}(\epsilon) e^{-\epsilon/(k_B T)}}{k_B T \int_0^\infty d\epsilon \mathcal{D}(\epsilon) e^{-\epsilon/(k_B T)}} \quad (3)$$

where non-degeneracy has been assumed,  $\mathcal{V}^{-2}(\epsilon)$  is (e.g. the  $x$ -component of) the square of the group velocity averaged over an equienergy surface and  $\tau(\epsilon)$  is the microscopic relaxation time. The lattice-temperature dependence of the Ohmic drift mobility computed according to Eq. (3) is shown in Fig. 2 in comparison with experimental data [11,12]. Note, however, that the fields applied in the time-of-flight experiments [11] were too large for the Ohmic regime at low lattice temperatures. This can be seen from the Monte Carlo simulations in Fig. 2, which were performed at the same field strengths as used in the experiments, and is in accordance with the results of Monte Carlo simulations considering the full acoustic phonon dispersion [9]. Hence, this constitutes an improvement of the new model over the elastic equipartition approximation where this feature was not captured [10]. Since the finite discretization tends to overestimate the mobility at low lattice temperature and low fields, good agreement between the results of the theoretical model and the experimental data can be concluded from Fig. 2. In Fig. 3, the velocity-field characteristics at different lattice temperatures are displayed. In view of the experimental uncertainties, there is also satisfactory agreement between the full-band Monte Carlo simulations and the time-of-flight measurements [13,14].

Further details about the single-particle approach (SPARTA) to Monte Carlo device simulation are reported elsewhere [15].

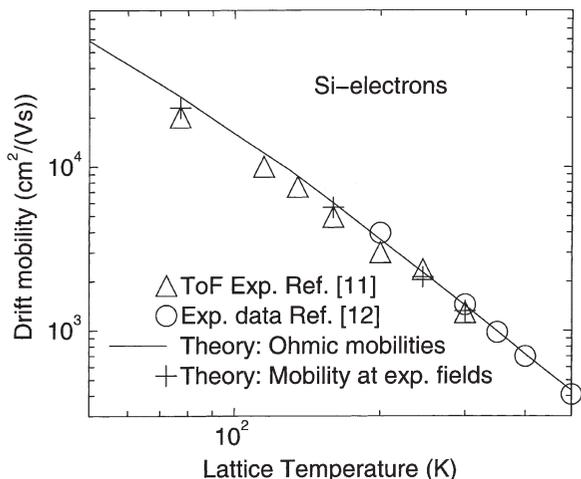


FIGURE 2 Theoretical results for the drift mobility as a function of the lattice temperature in comparison with experimental data.

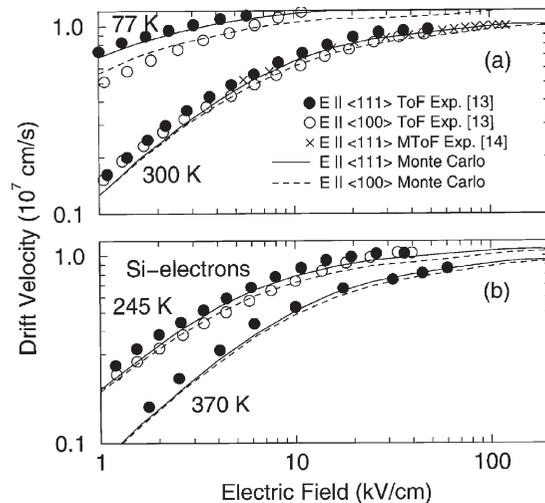


FIGURE 3 Full-band Monte Carlo results for the velocity-field characteristics at different lattice temperatures in comparison with corresponding time-of-flight (ToF) measurements and microwave time-of-flight (MToF) measurements.

## CALIBRATION METHODOLOGY IN THE LINEAR REGIME

The investigated device structure is a LDD (lightly-doped drain) n-MOSFET with a gate length of  $L_G = 0.12 \mu\text{m}$  and a metallurgical gate length of approximately  $L_{\text{eff}} = 0.085 \mu\text{m}$ . The non-uniform p-type channel doping is in the order of  $10^{18} \text{cm}^{-3}$  and the maximum doping in source and drain is about  $3 \times 10^{20} \text{cm}^{-3}$ . The oxide thickness is  $2.6 \text{nm}$ .

Geometry and doping profiles for the device simulation have been calculated with a 2D process simulation using DIOS [16], which has been calibrated in two steps. The first step was based on secondary ion mass spectroscopy (SIMS) and transmission electron microscopy (TEM) measurements as well as electrical data for 50 process variants, which covered experimental splits for various implantation and annealing parameters. It led to a good agreement between SIMS profiles and 1D process simulation results as well as between measured threshold voltage roll-off curves and device simulation results obtained with the DD model and a Van Dort quantum correction. In the second step, this calibrated process simulation was fine-tuned for the  $0.1 \mu\text{m}$  n-MOSFET with the help of a coupled Schrödinger DD simulation. In contrast to other quantum mechanical methods such as the Van Dort model or the quantum drift-diffusion approach, the coupled Schrödinger DD simulation [17,18] has the advantage that it does not involve any adjustable parameters. As a consequence, all uncertainty in the subthreshold regime can be attributed to process simulation. For the fine-tuning, a small variation of the diffusivity of negatively charged arsenic vacancy pairs was used to adjust the lateral diffusion into the channel and to obtain an excellent agreement between measured

and simulated transfer characteristics in the subthreshold regime at a drain voltage of 50 mV. Subsequently, the quantum effect is taken into account via a shift of the work function of 70 mV for the simulations with the DD, HD and MC model. The results of this procedure are compared in the upper part of Fig. 4 to the measured transfer characteristics.

Finally, the channel mobility reduction had to be adjusted above the threshold in order to reproduce the measured drain current at a gate voltage of 1.5 V. For the DD and HD simulation, the mobility model of Darwish *et al.* [19] has been adopted and the parameters B and C had to be divided by a factor of 2 for the Schrödinger-DD simulation and by a factor of 2.2 for the classical DD and HD simulations, respectively, whereas for the MC simulation the diffusive part of surface roughness scattering had to be set to 80%. This mobility adjustment, the results of which are displayed in the lower part of Fig. 4, is certainly also influenced by effects such as some distortions of internal variables due to non-selfconsistency in the MC case. However, the strong adjustments needed in all models suggest that the structure was probably affected by some other effects not taken into account in the process and/or device simulation.

## SIMULATION RESULTS IN THE NON-LINEAR REGIME

In the previous section, the reproduction of the measured MOSFET characteristics in the linear regime by different transport models was achieved by a comprehensive

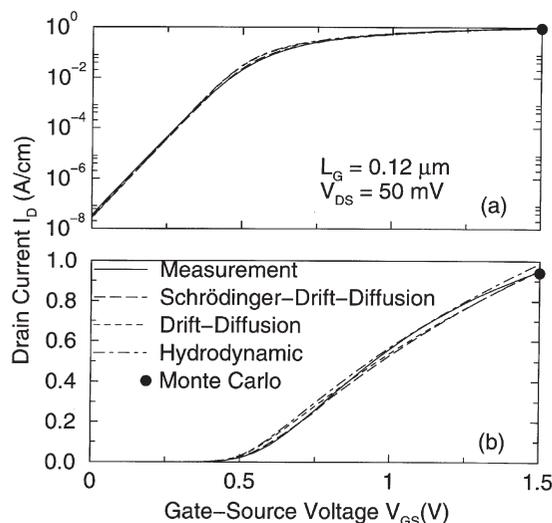


FIGURE 4 Logarithmic (a) and linear (b) plot of the transfer characteristic: Results of the adjusted models in comparison with the measurement (The quantum effect is considered via a shift of the work function in the case of the drift-diffusion, hydrodynamic and Monte Carlo model).

calibration methodology. In contrast, the aim of this section and the central goal of this paper is to compare the results of the transport models without further adjustment in the non-linear regime to the measured output characteristics.

There are at least two requirements to be met for a meaningful comparison. Firstly, the transport models have to agree at bulk level, i.e. especially the field-dependence of the drift velocity and the doping-dependence of the low-field mobility have to be the same. The former criterion is fulfilled via the Caughey-Thomas parameterization of the velocity-field characteristics in the DD and HD models, while the latter is ensured by a doping-dependent adjustment of the MC impurity scattering rate [15] to the measured mobility data [20] that are used in the classical device simulation [21]. Secondly, the transport models have to agree in the linear operation regime of the MOSFET which was achieved by the calibration procedure described in the previous section. Nevertheless, the models are not entirely consistent. For example, the carrier-concentration-dependence of the mobility due to screening is different between DD/HD and MC. Also, the channel mobility degradation is modeled in different ways, i.e. either through the Darwish-model [19] or through surface roughness scattering. Therefore, a useful comparison has to focus on integrated quantities such as the drain current relative to the corresponding measurements rather than on details of the simulations.

In Fig. 5, the measured output characteristics at a gate voltage of 1.5 V are compared with the simulation results of the drift-diffusion model, the hydrodynamic model where an energy relaxation time of  $\tau_w = 0.3$  ps is employed, and the single-particle Monte Carlo model which is based on the frozen field taken from the DD simulation. All data refer to a temperature of 300 K. It can be seen that there is a good agreement in the case of the MC model, whereas the HD model significantly overestimates and the DD model underestimates the saturation current. Of course, this does not imply that classical device simulation is not able to reproduce the output characteristics in the 0.1  $\mu\text{m}$  regime. For a given transistor structure, better agreement can e.g. be achieved by modifying the saturation drift velocity. However, such a procedure violates the first consistency requirement since in the limiting bulk case the experimentally established velocity-field characteristics is no longer recovered. In addition, the adjustment has to be repeated for different channel lengths.

Figure 6 reports the output characteristics at different gate voltages as obtained by measurement and Monte Carlo simulation. It should again be noted that a sensible comparison in the non-linear regime necessitates exact agreement in the linear regime requiring a gate-voltage dependent surface roughness scattering model. However, this dependence is relatively weak in Fig. 6 so that a satisfactory agreement is achieved without further adjustment.

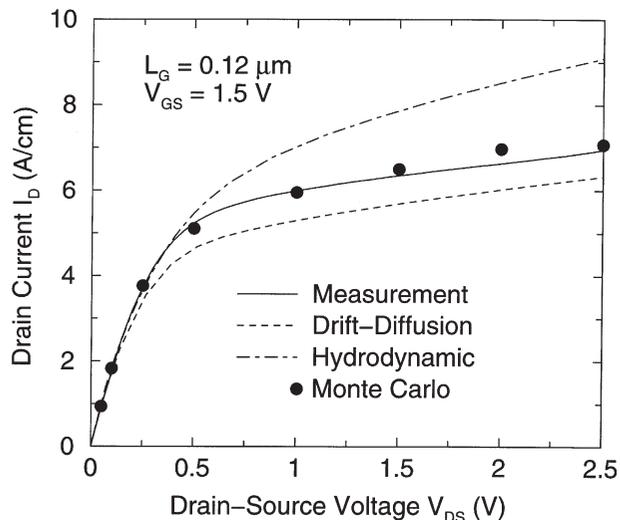


FIGURE 5 DC output characteristic of the n-MOSFET: Results of the different transport models without adjustment in the non-linear regime in comparison with the measurement.

## CONCLUSIONS

Non-selfconsistent single-particle Monte Carlo simulations of output characteristics have been performed and compared to corresponding measurements in an  $0.1 \mu\text{m}$  n-MOSFET. After an accurate calibration of the doping profile with the help of a coupled Schrödinger drift-diffusion simulation and a mobility adjustment in the linear regime, good agreement in the non-linear regime is found for the Monte Carlo model, while drift-diffusion and hydrodynamic simulations significantly deviate from the measured saturation current. The results obtained suggest that non-selfconsistent Monte Carlo simulation is—after adjustment of surface roughness scattering in the

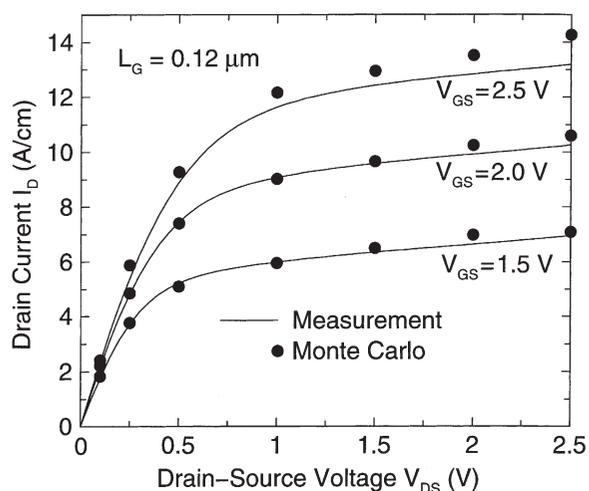


FIGURE 6 DC output characteristics of the n-MOSFET: Results of the Monte Carlo model without adjustment in the non-linear regime in comparison with the measurement for different gate voltages.

linear regime—able to reproduce with sufficient accuracy the non-linear part of the output characteristics.

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