# Comparison of Monte Carlo Transport Models for Nanometer-Size MOSFETs

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#### Abstract

This paper presents the results of a comparison among five Monte Carlo device simulators for nano-scale MOSFETs. These models are applied to the simulation of the I-V characteristics of a 25 nm gate-length MOSFET representative of the high-performance transistor of the 65 nm technology node. Appreciable differences between the simulators are obtained in terms of simulated  $I_{ON}$ . These differences are mainly related to different treatments of the ionized impurity scattering (IIS) and pinpoint a limitation of the available models for screening effects at very large carrier concentrations.

### 1 Introduction

Monte Carlo transport models [1, 2] are often taken as a reference for lower-order but more efficient simulation approaches. A general consensus on the validity and accuracy of these models is therefore of great importance. In [2] several Monte Carlo simulators were compared by analyzing electron transport in bulk silicon. This activity proved very valuable as it led to building up a general consensus on the selection of key ingredients such as band structure and scattering models. This paper aims at a substantial step forward with respect to [2] by comparing simulations of on advanced n-type nanoMOS-FET obtained with five well assessed MC simulators [3, 4, 5, 6, 7]. Our results put in evidence a non-satisfactory status of the modeling of IIS at large doping concentrations and for far-from-equilibrium conditions.

#### 2 Transport Models

Most of these transport models [3, 5, 6, 7] (hereafter referenced as A, C, D and E, respectively) adopt a full-band description of the energy-wavevector dispersion relationship with usual  $0^{th}$  order phonon description and parameter values suggested in [1], with the exception of acoustic phonons in model A. Model B [4] assumes a non-parabolic ellipsoidal analytical model for the conduction band;  $0^{th}$  order phonon model

is assumed for  $f_2$ ,  $f_3$ ,  $g_3$  intervalley transitions, while a 1<sup>st</sup> order model is assumed for the  $f_1$ ,  $g_1$ ,  $g_2$  phonons.

Concerning IIS, different approaches are adopted by the different groups: A adopts the Brooks Herring model with a screening length evaluated assuming equilibrium Fermi-Dirac electron energy distribution, with temperature coincident with lattice temperature  $(T=T_L)$ ; groups B and D implement a model similar to the one of A, with screening calculated assuming non-degenerate conditions (Maxwell-Boltzmann distribution); groups C and E use the Ridley model with a screening length computed according to a Maxwell-Boltzmann distribution with temperature self-consistently related to the carrier mean energy  $(T=T_e=2 < E > /(3K_B)$ , rescaled, so that  $T_e=300$  K is recovered at equilibrium). Finally, while A computes the exact k-dependent scattering rate, B, C, D and E adopt a more efficient scheme in which the scattering rate is calculated according to an energy-dependent inverse microscopic relaxation time and the final state is randomly selected. All the adopted models present limitations:

- A, B, D assume equilibrium distributions;
- C and E assume a simple heated-maxwellian approximation for the non-equilibrium distribution;
- B, C, D and E do not account for degeneracy effects.

As it is well known IIS models fail to properly model mobility in the high-doping concentration limit ([6] and references therein); all the groups tried to compensate this effect by adopting a doping concentration dependent pre-factor for the IIS-rate, whose value is tuned to obtain agreement with experimental mobility data for majority carriers at large doping densities.

Surface roughness (SR) is treated by the reflective-diffusive model in [4, 5, 6, 7], while [3] adopts an effective-field dependent scattering rate. In all cases, SR parameters are tuned in order to fit the universal mobility curve for n-MOSFETs.

While A, B, D and E adopt an ensemble time-dependent Monte Carlo algorithm with self-consistency achieved through the frequent solution of the linear Poisson equation, C achieves self-consistency by iterating single-particle Monte Carlo transport simulations with solutions of the non-linear Poisson equation until convergence is reached. In order to focus on the comparison of semiclassical transport models, quantum corrections that mimic the effects of carrier confinement are not included in the simulation.

#### **3** Results and Discussion

The simulated device is a bulk n-MOSFET with 25 nm gate length and main characteristics defined in agreement with the specifications of the ITRS roadmap for the highperformance logic transistors of the 65 nm technology node. The distance between the source/drain contact and the gate edges is 50 nm, including a 23 nm long highly doped ( $N_D \approx 2 \times 10^{20} \text{ cm}^{-3}$ ) region and a 27 nm extension region with  $N_D \approx 10^{20} \text{ cm}^{-3}$ . Notice that these doping levels are larger than usually assumed in Monte Carlo device simulation. At large current levels a significant longitudinal electric field is present in the shallow moderately-doped extension regions, leading to appreciable carrier heating even at the source end of the channel. These latter characteristics make this simulation



**Figure 1:** Simulated I-V transfer characteristics for the 25 nm MOSFET without ionizedimpurity scattering;  $V_{DS}$ =0.1 V (left) and  $V_{DS}$ =1.1 V (right). Main device parameters are:  $L_G$ =25nm EOT=0.9 nm,  $N_{SUB}$ =3·10<sup>18</sup> cm<sup>-3</sup> (plus halo implant).



**Figure 2:** Longitudinal field (left) and average velocity (right) along the channel for the 25 nm MOSFET biased at  $V_{GS}=V_{DS}=1.0$  V. Ionized-impurity scattering not included in the simulation. Averages in the vertical direction have been performed according to the electron concentration.

particularly challenging, as the IIS models are developed for quasi-equilibrium conditions and tend to fail at very large doping densities.

Figure 1 reports the transfer characteristics in the linear and saturation regimes, calculated without including the effect of IIS. A good agreement is found in saturation, while model A predicts much lower current in the linear region. This is mainly due to the different deformation potential for the acoustic-phonons ( $D_{AC}$ ) compared to the other partners (14.6 eV vs. 9 eV), since the model used for SR requires, in order to fit the universal mobility curve, an increment of phonon scattering compared to the case of bulk silicon, as is required when computing mobility for a 2-D electron gas [8]. Furthermore, model A has been calibrated to work with quantum corrections, turned-off in this comparison. When model A is modified to become consistent with model D, i.e.  $D_{AC}$ =9 eV and specular/diffusive surface scattering (*A alt.* in Fig. 1 left), a much better agreement is found. Mutual agreement between models is confirmed also in terms of internal quantities (Fig. 2).

When IIS is included (Fig. 3), a significant disagreement between the models is found



**Figure 3:** Simulated I-V transfer characteristics for the 25 nm MOSFET with ionized-impurity scattering;  $V_{DS}$ =0.1 V (left),  $V_{DS}$ =1.1 V (right); open circle: model A using  $T_e$  in the evaluation of the screening length for ionized-impurity scattering.

at large  $V_{DS}$ , pinpointing the existence of subtle issues related to the treatment of this scattering mechanism. In particular, the analysis reveals the role played by the different treatment of screening effects. In an attempt to understand whether the discrepancies mainly involve electron transport in the channel or in the S/D regions, the MOSFET has been simulated with model A under  $I_{ON}$  bias condition, switching off the IIS inside the transistor's channel below the gate electrode. The calculated current was increased by a mere 3% with respect to the standard simulation, showing that the IIS inside the channel does not significantly affect the current and giving indirect indication of the fact that most of the ISS-related discrepancies involve the transport in the source and drain regions. The impact of different treatments of the screening effect has been addressed by changing model A in order to account for  $T_e$  instead of  $T_L$  as in models C and E. This led to a slight reduction of the ON-current (open circles in Fig. 3), still insufficient to eliminate the difference with respect to models C and E.

Based on our results and on the existence of limitations affecting the IIS models, we conclude that more work is needed in order to provide an improved description of this relevant scattering mechanism.

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