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Invited

Monte Carlo Simulation of Small Silicon Field-Effect Transistors

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The Monte Carlo method is able to model successfully some very small electronic devices. Yet, difficulties remain in order to simulate correctly electronic transport in small field-effect transistors, even when semi-classical transport is considered. We review in this paper some of those successes, such as the correct modeling of the transconductance of sub-0.1μm nMOSFETs, and the density dependence of the channel mobility when quantization in the inversion layer is accounted for. On the other side, the simulation of electron transport at high energies and in low-dimensionality situations presents significant problems. We discuss briefly these problems.

1. INTRODUCTION

The Monte Carlo method[1,2] has enjoyed some remarkable degree of success in the simulation of short-channel Si metal-oxide-semiconductor field-effect transistors (MOSFETs): 1. the transconductance of n-channel devices with 'effective' channel lengths down to 0.07μm has been predicted quite accurately[3] , both at 300 K and 77 K as shown in Fig. 1, the major uncertainty in the comparison with the experimental data being gated by the accuracy of the determination of the channel length and by the correction for parasitic effects to the 'as measured' (or 'extrinsic') characteristics in order to extract 'intrinsic' behavior[4]. 2. The behavior of hot carriers under extreme scaling[5], showing that it is not so much the strength of the field itself but, rather, the total voltage applied at the contact which begins to matter, as we approach 'quasi-ballistic' transport. 3. Recently, sophisticated self-consistent solutions of the Boltzmann transport equation (via the Monte Carlo method), of the Poisson equation, and of the one-dimensional Kohn-Luttinger equation have provided great insight on the behavior of quantized carriers in Si inversion layers in the ohmic and high-field regimes[6,7].

Yet, there are a few problems. The merits of Monte Carlo simulations are definitely their easy and intuitive implementation, and the large freedom from mathematical difficulties, such as discretization and convergence issues, which let us push physical models, rather than mathematical techniques, to their limits. However, our knowledge of the physics is obviously limited, and even Monte Carlo techniques cannot teach us what we do not know. Three examples of problems we may encounter in simulating small devices are discussed below: 1. the hot-carrier problem, dealing with high-energy processes, such as gate-injection, 2. the knowledge of the electron-phonon interaction in inversion layers, and 3. the problem of studying transport in narrow double-gated structures, which must deal with transport of carriers having large kinetic energy, yet confined in narrow regions.

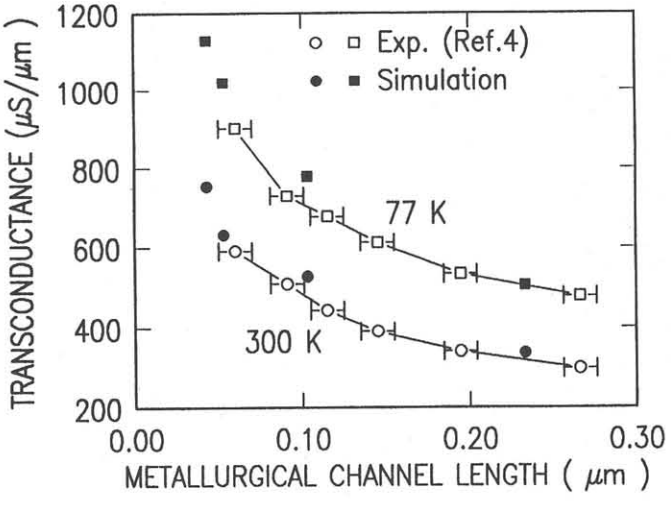

Figure 1. Simulated and measured transconductance as a function of channel length in n-channel Si MOSFETs.

2. THE HOT-CARRIER PROBLEM

Substrate currents and gate currents in MOSFETs are more-or-less direct measures of the 'reliability' of small devices driven at very large fields. Yet, despite the wealth of publications dealing with subject, some key issues of the physics of hot-carrier transport remain almost completely unknown: We can only give an incomplete list of these genuine physics-problems: 1. Tunneling across the insulator: we still use empirical matching conditions at the Si-SiO_2 interface, we still ignore the (complex) dispersion in the gap of SiO_2, we still ignore how to handle conservation of crystal momentum in the context of the amorphous SiO_2 layer. 2. Band-to-band impact ionization is obviously very important in shaping the high-energy end of the electron distribution function, thus in gating all hot-electron related effects. Yet, we are still struggling trying to evaluate either theoretically[8,9,10] or empirically[11].

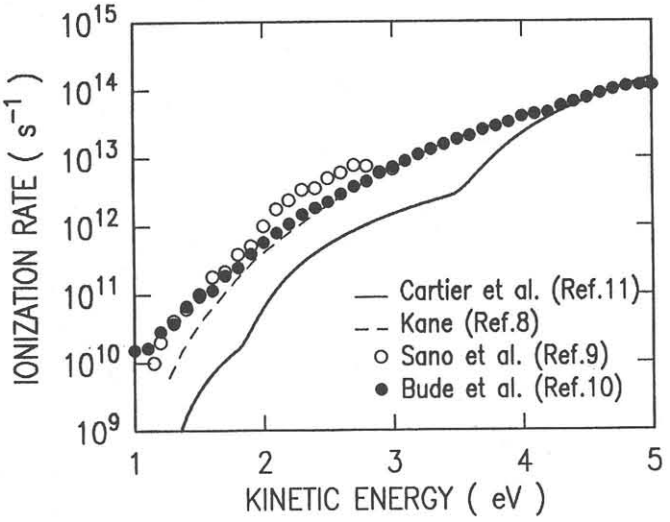

Figure 2. Electron band-to-band impact ionization scattering rate determined from Monte Carlo simulations of XSP, ionization-coefficient, and quantum-yield data. The results of calculations performed using empirical pseudopotential Bloch states and band-structures are also shown.

By using recent data obtained using x-ray photoemission spectroscopy, added to known data on ionization coefficient and probability, we have employed Monte Carlo simulations to determine the strength of the ionization rate relative to the electron-phonon scattering rate. The results show that, while at high energies ($\gtrsim$ 3 eV), calculations based on pseudopotentials[8,9,10] explain the data, at lower energies the ionization threshold is much softer that expected. Figure 2 shows the empirically determined rate, compared to theoretical calculations. 3. High-energy transport effects: the nature of the band-structure at high energies ($\sim$ 1eV-3eV) is till modeled, at best, with empirical pseudopotentials[12,13]. More often, oversimplified parabolic (or first-order $\mathbf{k}\cdot\mathbf{p}$ nonparabolic) bands are assumed. Similarly, the electron-phonon coupling constants are extrapolated from their know values near the band edges to the entire Brillouin Zone. 5. What is worse, even unexpected physical ingredients seem to matter at high energies: A striking example is given by our past work: we have shown[14] how 'a priori' small effects, such as Coulomb interactions, both long-range and short-range, can perturb the high-energy tail of the electron energy distribution to a very large extent. Figure 3 shows the result of a simulation performed on a 0.25μm-channel n-MOSFET device driven at a source-to-drain bias of 4 V. It can be seen that depending on whether the Coulomb interactions are included or not, the 'gate-current' (as measured by the relative fractions of carriers above an arbitrary threshold of 3 eV) could change by more than one order of magnitude.

This short discussion must necessarily end with a pessimistic note: despite claims made quite often, we still lack most of the knowledge about basic transport-physics to make any quantitative conclusion about hot-carrier effects in small MOSFETs. Common sense and good engineering practices have better chance of success than theoretical simulations, when dealing with reliability problems triggered by hot carriers.

3. ELECTRONS IN INVERSION LAYERS

Studies of the electron transport Si inversion layers have uncovered serious problems with our understanding. Three examples may suffice to make the point:

The role of surface modes, as analyzed in great depth by Ezawa[15] in the past, constituted a monumental problem. But their results have been disappointing: surface/interface modes, despite their complexity, do not change the electron-phonon coupling that much. Old theoretical estimates about the electron mobility in inversion layers were in striking disagreement with experimental data.

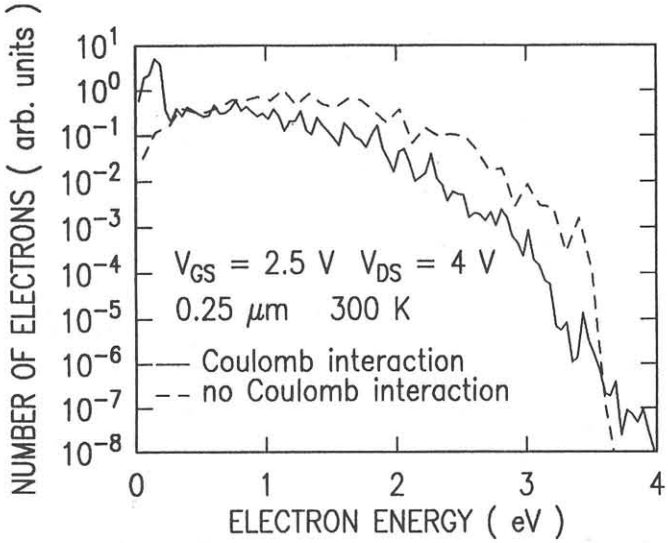

Figure 3. Simulated energy distributions for electrons in the channel of a Si MOSFET. The distributions are taken roughly 3.5 V 'downstream' along the channel. The simulation done excluding Coulomb interactions shows a cut-off at the expected energy of 3.5 eV, while single-particle excitations are responsible for an enhanced tail at high energy when Coulomb interactions are included. Note the signiture of the drain-plasmons, which shift the distribution by about $\hbar\omega_{Plasma} \simeq$ 250 meV towards lower energies, and the low-energy particles excited in the drain by single-particle collisions with the hot carriers.

Obviously, many effects not included in those early studies - such as inter-subband and inter-valley transitions - were believed to be important. At first, their incorporation into sophisticated Monte Carlo simulations seemed to yield good results using bulk modes and refined models for Coulomb and surface-roughness scattering.[6] But a deeper look we took at the some of these issues - nonparabolic corrections, the anisotropy and the dynamic screening of the deformation potential matrix element, the multisubband screening of the Coulomb interaction - has shown that there is still something missing, as also suggested by very early experimental data[16]: when phonons dominate the picture, the calculated mobility is still some 20% larger than observed. Additional scattering (interface strain?) or some missing piece in the puzzle of the electron-phonon interaction may be responsible for the disagreement. While this disagreement is hardly major from a theoretical viewpoint (not many parameter-free theory do much better than 20%!), a 20% error in the mobility is certainly not welcome by device designers. Figure 4 shows a comparison of experimental data and simulations for $<100>$ Si at 300K.

Finally, if we leave the ohmic regime and study the high-field behavior ($\gtrsim 10^4$ V/cm) of quantized carriers, we find difficulties in dealing with it. Necessarily, we must couple a 2-dimensional transport model to a bulk model at some critical 'threshold' energy, as pointed out already by Hayafuji and Imanaga[19]: we cannot (and perhaps we shouldn't) simulate

transport when too many subbands exhibit very narrow spacing. But, as we move to this 'hybrid' model, the velocity-field characteristics merge into the bulk behavior. Many reliable experimental data[22,23] show that this is not the case, saturated velocities ranging in the range of 6×10^6 to 8×10^6 cm/s.. Again, we are missing something. In this instance, the artificial algorithm chosen to match subbands to the bulk band-structure may be the source of our problems.

4. DOUBLE-GATE DEVICES

At a recent conference, we reported a study a a small Si double-gate device, consisting of a Si channel sanwiched between two oxide gate-insulators[20]. The channel, about 30 nm long and 5 nm wide, was simulated in order to see how aggressively one can scale conventional field-effect devices, by minimizing short-channel effects, thanks to the double-gated structure. We shall not discuss here issues related to the particular choice of device. Rather, we'd like to stress our inability to simulate 'quantitatively' this device. The problem stems from the very narrow 'channel' with high potential barriers at both sides. This channel behaves as a quantum well. But now, subbands extend to very high energies. At these high energies, approximations usually employed to solve the problem fail dramatically. Let's recall the basic equation we must solve, the 'Schrödinger-like' equation

$$[\varepsilon(-i\nabla) + V(z)]\,\phi(\mathbf{r}, z) = E\,\phi(\mathbf{r}, z)\,, \qquad (1)$$

where z is the coordinate along the quantization direction (that is, normal to the $Si\text{-}SiO_2$ interface in our case), $\mathbf{r}$ is the spatial coordinate in the plane of the interface, $\varepsilon(\mathbf{K})$ is the energy dispersion, and $V(z)$ is the external confining potential. The unknown ϕ is the 'envelope' wave function, *i.e.*, a modulation of the periodic Bloch factor of the full wavefunction. Now, in principle, if we do not allow for the penetration of the wavefunction into the barrier (a satisfactory approximation), any band-structure model may be used in Eq. (1), including the empirical pseudopotential model we employ in bulk silicon[13,21], but computational stumbling blocks appear which prevent us from using such a complicated model in a transport situation. Therefore, we must fall back to a solution of based on a cruder the dispersion $\varepsilon(\mathbf{K})$, such as the usual first-order nonparabolic approximation. Nonparabolic correction can be handled with first-order perturbation theory. But its validity cannot extend to very high energies. In particular, nonparabolic corrections may yield non-monotonic kinetic energies at high subbands: clearly higher-order $\mathbf{k} \cdot \mathbf{p}$ terms are required. In such a case, we must fall back to a purely parabolic model and content ourselves with a comparison of the full-band-structure bulk model to the parabolic 2-dimensional model. Unfortunately, the difference we obtain in raw characteristics (transconductance, bare I-V characteristics) exceed 20% in some cases.

Finally, what these tiny devices teach us is that *fluctuations* become a major problem: Thickness fluctuations of the 'well' results in threshold fluctuations. They also cause extra scattering, similar to roughness scattering. The same effect is caused by the fluctuations of the number of dopants in the channel or also used a modulation-dopant, if so chosen. Again, this will affect channel mobility, threshold voltage, and subthreshold behavior. The much more studied conductance fluctuations may become the least of our worries, compared to more pressing and less understood effect of process fluctuations on the transport properties of tiny devices.

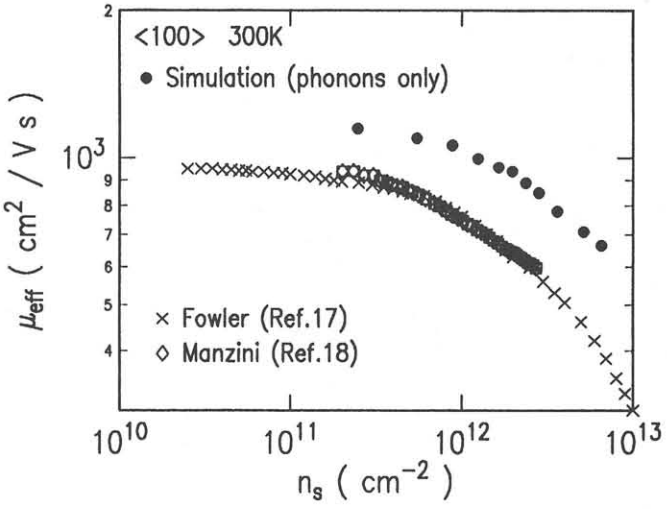

Figure 4. Simulated effective mobility of electrons in Si inversion layers as a function of sheet-charge-density including only scattering with phonons. Experimental data taken in samples with very low channel doping are shown for comparison. Note that at large densities ($\gtrsim 3 \times 10^{12}$ cm^{-2}) scattering with interface roughness dominates and the comparison becomes meaningless. Fowler's data are Hall mobilities.

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