P:21 Investigation of hot-carrier effects using a backward Monte Carlo method and full bands

M Kampl and H Kosina

TU Wien, Austria

Degradation models for MOSFETs require accurate knowledge of the carrier distribution function which is determined by the Boltzmann equation. This equation can be solved by the Monte Carlo method. However, calculation of the high-energy-tail of the carrier distribution which requires the simulation of statistically rare events often poses a problem on the standard Monte Carlo methods. Using a backward Monte Carlo algorithm it is possible to selectively simulate the rare events of interest and to avoid simulation of the uninteresting common events. A stable backward Monte Carlo algorithm has been implemented in a full-band Monte Carlo code and its properties have been analyzed. High-energy tails of the distribution function and I/V curves in the sub-threshold regime can be easily calculated with this new method.

The pysically transparent and commonly used forward Monte Carlo (FMC) method produces a large statistical error when used for the simulation of statistically rare events. In the field of semi- classical transport, the backward Mont Carlo (BMC) method has been proposed at the end of the 1980's [1] [2]. These early algorithms turned out to be numerically instable as the transition rates did not satisfy the principle of detailed balance. In 2003 a numerically stable algorithm was proposed [3]. Because now the backward transition rates obey the principle of detailed balance, a runaway of the energy along a backward trajectory is avoided. The BMC method uses the scattering rates of the FMC method [3] and can thus be easily implemented in an already existing Monte Carlo simulator, Vienna Monte Carlo (VMC).

The principle of the BMC method is to create a set of rare events in phase space, and to trace the trajectories back in time until they reach a contact. From the known distribution function (DF) at the contact the statistical weight of the backward trajectory, consequently its contribution to the estimator of interest, is determined.

THE BACKWARD MONTE CARLO METHOD

A stable estimator for the DF in a given point $(\vec{k}_0,\vec{r}_0)$ is given by [3]:

$$f(\vec{k}_0,\vec{r}_0) = \frac{1}{M}\sum_{i=1}^{M} f_b(\vec{k}_{b,i},\vec{r}_{b,i})\,\mathrm{e}^{\sum_j \Delta E_j/k_B T}\,, \qquad (1)$$

where f_b represents the boundary distribution at the contact, M is the number of backward trajectories injected at the point $(\vec{k}_0,\vec{r}_0)$ and $\Sigma_j \Delta E_j$ is the sum of all energy changes due to phonon emission and phonon absorption processes.

This approach allows one to calculate the DF in only one point of the device, neglecting all other trajectories which do not pass through that point. Monte Carlo estimators for statistical averages of the form $< A >= \int A(\vec{k}_0,\vec{r}_0) f(\vec{k}_0,\vec{r}_0) d^3k d^3r$ can be derived from (1) straightforwardly.

We investigated a 65 nm MOSFET presented in [5].

To calculate the current, we generate the states $\vec{k}_0$, from a Maxwellian distribution at different temperatures and the positions $\vec{r}_0$ in the channel cross section where the energy barrier has its maximum. The BMC method allows to compute the whole I/V curve, including the sub-threshold region as shown in Figure 1. The statistical error of the current as a function of the injection temper- ature is plotted in Figure 2. While the estimated current is independent of this temperature, the statistical error shows a clear minimum where the injection distribution most closely resembles the real distribution. The energy distribution is calculated pointwise in energy at some fixed locations at the interface, see Figure 3.

Additionally, a combined backward-forward MC (BFMC) method has been developed. After having calculated a backward trajectory from the starting point $\vec{k}_0, \vec{r}_0$, a weighted forward trajectory is started from that point as well, see Figure 4. The combined backward-forward technique has been used to calculate the acceleration-integral employed for hot-carrier degradation modeling, see Figure 5.

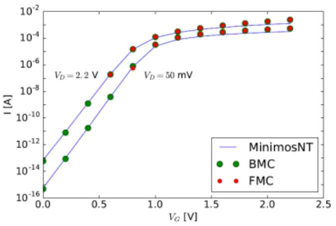

Fig. 1. Transfer characteristics of an nMOS device, simulated with MinimosNT [4] (drift-diffusion), the FMC and BMC methods. Drain voltage is varied between 2.2 V and 50 mV. Each point of the Monte Carlo methods is calculated with 10^6 trajectories.

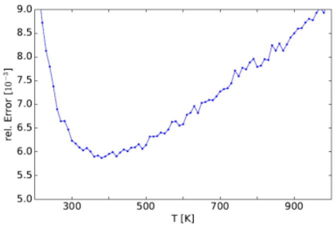

Fig. 2. Relative error of the BMC estimator on a 65 nm nMOS channel at $V_{GS} = 0.6$ V and $V_{DS} = 2.2$ V with different injection temperatures.

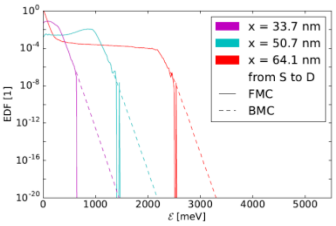

Fig. 3. Energy distribution at some cuts through a 65 nm nMOS channel at $V_{GS} = 2.2$ V and $V_{DS} = 2.2$ V. Solid lines show FMC at with 10^{10} scattering events. Dashed lines show BMC with 10^4 trajectories per energy point.

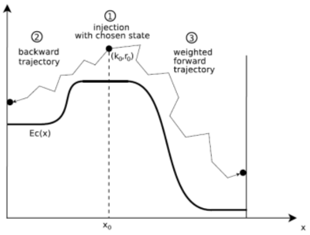

Fig. 4. Principle of the BFMC method for a MOSFET. The injected particle has a chosen state in r- and k-space. It is traced back in time to its origin to calculate the weight (probability) of itself. The observables are calculated from the weighted forward trajectory

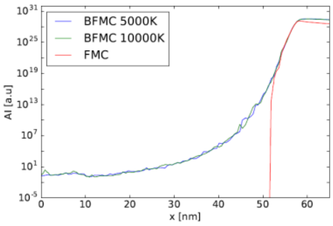

Fig. 5. The results of the acceleration integral [5] from two BFMC simulations, at different injection temperatures, and one FMC simulation with 10^{10} scattering events were compared with each other. Furthermore the graph shows that the backwards estimator is independent of the injection temperature.

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