Hot Carrier Study Including e-e Scattering Based on a Backward Monte Carlo Method

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***Abstract*—Degradation models for MOSFETs require accurate knowledge of the carrier distribution function, which is determined by the Boltzmann equation. It is well known that the high-energy-tail of the carrier distribution is affected by electron-electron (e-e) scattering. An e-e scattering model has been implemented in a full-band Monte Carlo device simulator. The high-energy-tail has been calculated using the Backward Monte Carlo method. Our results show an enhancement of the high-energy-tail due to e-e scattering, which, however, is not as pronounced as predicted by spherical-harmonics-based simulations.**

I. Introduction

The physically 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 was proposed in 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 has been proposed [3]. Since the backward transition rates now obey the principle of detailed balance, a runaway of the energy along a backward trajectory is avoided. In this way, the scattering rates of the FMC method can be used in BMC method as well [3]. The principle of the BMC method for the solution of a boundary value problem is to chose a set of rare states in phase space and trace trajectories from these states back in time until they reach a contact. The statistical weight of the backward trajectory and consequently its contribution to the estimator of interest is determined via the known distribution function (DF) at the contact.
The BMC method has been implemented in the full-band simulator VMC [4] [5].

II. Monte Carlo Method

The Boltzmann transport equation (BTE) classically describes the motion of gas molecules. It considers acceleration, diffusion, and scattering [6] [7]. In the semi-classical transport theory of semiconductors, the motion of the electron gas is also described by the BTE. The scattering rates are calculated using Fermi's Golden Rule [6] and the electron group velocity is obtained from the full-band structure of the semiconductor [8] [9].
The Monte Carlo (MC) method is a stochastic method for the solution of integrals and integral equations such as the BTE [6] [10]. Trajectories of carriers are simulated in $\vec{r}$- and $\vec{k}$-space under the influence of acceleration by the electric field and scattering mechanisms. The duration of free-flight, the selection of the scattering mechanism and the final state are calculated using random numbers. With a sufficiently large number of trajectories, the averages of observables can be calculated [7].

III. The Backward Monte Carlo Method

The DF in a given point ($\vec{k}_0$,$\vec{r}_0$) can be calculated by [3]:

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

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 $\sum_j \Delta E_j^{(i)}$ is the sum of all energy changes due to phonon emission and phonon absorption processes for the i-th trajectory.
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 $<A>=\int A(\vec{k}_0,\vec{r}_0)\,f(\vec{k}_0,\vec{r}_0)\,d^3k_0 d^3r_0$ can be derived from (1) straightforwardly.

To calculate the current through the channel of a MOSFET, we randomly generate the states $\vec{k}_0$ from a Boltzmann distribution at some arbitrary temperature and the positions $\vec{r}_0$ in the channel cross section where the energy barrier has its maximum. This arbitrary distribution will be referred to as $p_0(\vec{k}_0, y_0)$.
We start with the general definition of the current density,

$$\vec{J} = \frac{2\,q}{(2\pi)^3} \int\limits_{\mathrm{BZ}} \vec{v}(\vec{k})\, f(\vec{k},\vec{r})\, \mathrm{d}^3k, \tag{2}$$

where $f(\vec{k},\vec{r})$ is the unknown solution of the BTE. The current through the injection plane can be written as

$$I = \frac{q}{4\pi^3}\, W \int\limits_{y=0}^{y_{\max}} \int\limits_{\mathrm{BZ}} v_x(\vec{k}_0) f(\vec{k}_0,\vec{r}_0)\, \mathrm{d}^3k_0\, \mathrm{d}y_0\,. \tag{3}$$

Here, $f(\vec{k}_0,\vec{r}_0)$ is given by (1). With the artificial distribution function $p_0(\vec{k}_0, y_0)$ the integral can be estimated by MC integration

$$I = q\, W \int\limits_{y=0}^{y_{\max}} \int\limits_{\mathrm{BZ}} \nu(\vec{k}_0, y_0)\, p_0(\vec{k}_0, y_0)\, \mathrm{d}^3k_0\, \mathrm{d}y_0 \tag{4}$$

$$\approx q\, W\, \frac{1}{N} \sum_{i=1}^{N} \nu(\vec{k}_{0,i}, y_{0,i}), \tag{5}$$

where N is the number of sampling points $(\vec{k}_0, y_0)$. The estimator $\nu(\vec{k}_{0,i}, y_{0,i}) = \nu_i$ can be identified from (4). More details are presented in a forthcoming publication.

Another advantage of the BMC method is, that the statistical error of an estimator can be easily calculated from the sample variance s^2 [11]

$$s^2 = \frac{1}{N-1} \sum_{i=1}^{N} (q\, W\, \nu_i - I)^2 \tag{6}$$

$$\sigma_I^2 = \frac{s^2}{N}, \qquad \sigma_{\mathrm{rel}} = \frac{\sigma_I}{I} \tag{7}$$

where σ_I^2 is the variance and σ_{rel} is the relative standard deviation of the current estimator. This equation is applicable because all trajectories of a BMC simulation are statistically independent, and so are the random variables ν_i.

IV. Backward-Forward Monte Carlo Method

The BMC method works well if energies above the top of the energy barrier are considered. For energies below the top of the barrier (drain region) BMC suffers from increasing variance. To treat this region properly, a combined forward/backward method has been developed.

Subsequent to the backward trajectory, from the starting point ($\vec{k}_0$,$\vec{r}_0$) a weighted forward trajectory is computed. The probability of the backward trajectory gives the statistical weight of the forward trajectory. The combined backward-forward technique can be used to calculate the mean values of interest from the weighted forward trajectories. The combined Backward-Forward Monte Carlo (BFMC) method was introduced in [4] and is schematically described in Figure 1.

V. The Electron-Electron-Scattering model

A physically relevant effect that affects the distribution of hot carriers is e-e scattering. Starting with a two-body screened Coulomb interaction potential

$$V(\vec{r}_1 - \vec{r}_2) = \frac{e^2}{4\pi\epsilon_s} \frac{\mathrm{e}^{-\beta_s|\vec{r}_1-\vec{r}_2|}}{|\vec{r}_1-\vec{r}_2|} \tag{8}$$

the matrix element can be written as

$$\langle \vec{k}_1', \vec{k}_2' |\, V\, | \vec{k}_1, \vec{k}_2 \rangle = \left(\frac{e^2}{\epsilon_s \Omega}\right) \frac{\delta_{\vec{k}_1+\vec{k}_2, \vec{k}_1'+\vec{k}_2'}}{\left|\vec{k}_1 - \vec{k}_1'\right|^2 + \beta_s^2}. \tag{9}$$

Using Fermi's Golden Rule the total scattering rate between two electrons in the states $\vec{k}_1, \vec{k}_2$ is given by the following expression:

$$\lambda_{\mathrm{ee}}(\vec{k}_1, \vec{k}_2) = \frac{n}{2} \frac{e^4}{(2\pi)^2 \hbar \epsilon_s^2} \int \frac{\delta\left[\epsilon(\vec{k}_1+\vec{q}) + \epsilon(\vec{k}_2-\vec{q}) - \epsilon(\vec{k}_1) - \epsilon(\vec{k}_2)\right]}{\left(q^2+\beta_s^2\right)^2}\, d^3q \tag{10}$$

Here, β_s is the inverse screening length and $\vec{q}$ the momentum transfer. The total scattering rate for a one-particle simulation is obtained by summing over all possible states of the partner electron. Since we are interested in the effects of mixing the channel hot electrons with the cold electrons in the drain, we assume the partner electrons to obey the equilibrium distribution of the drain. Out

of the two summations over initial and final states of the partner electrons, one summation has to be carried out numerically taking into account the numerical band structure. This leads to a scattering rate $\Gamma_{ee}(p, \eta)$, depending only on the scaled group velocity p and the Fermi-Level η, see Figure 2.

VI. Results and Discussion

We investigated a $65\,\mathrm{nm}$ MOSFET described in [12]. The BMC method allows us to calculate the whole I/V curve, including the sub-threshold region as shown in Figure 3. While the estimated current is independent of the injection distribution, the statistical error shows a clear minimum where the injection distribution most closely resembles the real distribution, shown in Figure 4.

The EDF presented in [12] were computed by the spherical-harmonics-expansion simulator ViennaSHE [13] and are used as a reference for the present work. In order to calculate the hot-carrier related values we used the BFMC method, schematically described in Figure 1. To resolve the high-energy tail more accurately we included e-e scattering.

The combined backward-forward technique has been used to calculate the EDF at different positions along the channel, see Figure 5. We observed an additional heating at high energies, where the slope of the EDF clearly deviates from the Maxwellian tail. However, this additional heating is less pronounced than predicted by ViennaSHE, see Figure 6. Consequently, the acceleration-integral employed for hot-carrier degradation modeling, which depends sensitively on the high energy tail, is also altered due to e-e scattering as shown in Figure 7.

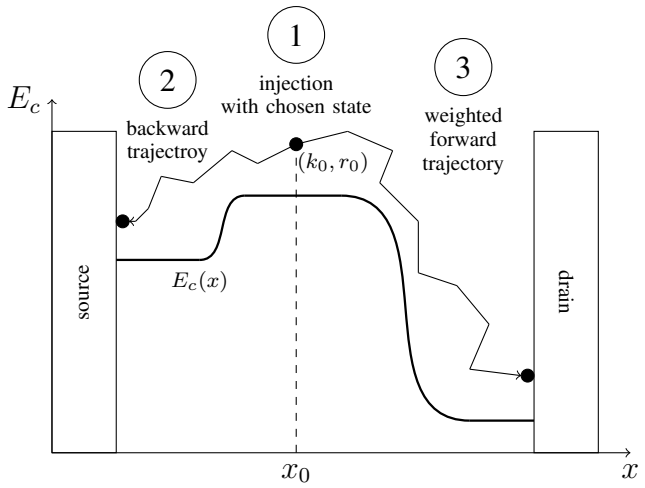

Fig. 1. Principle of the BFMC method for a MOSFET. The injected particle has a chosen state in r- and k-space. It is traced back in time to its origin to calculate the weight (probability) of itself. The observables are calculated from the weighted forward trajectory.

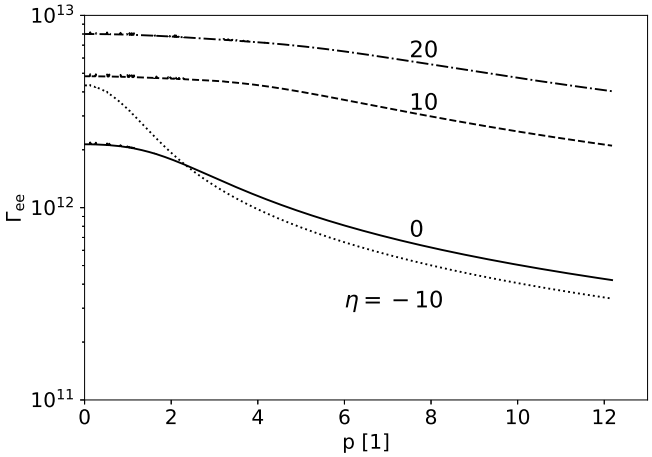

Fig. 2. The e-e scattering rate $\Gamma_{ee}(p, \eta)$ depends on the scaled group velocity $p = \frac{m v_g(\vec{k}_1)}{\hbar\sqrt{2} k_T}$ and the electron concentration via the Fermi-Level η. The parameter $\eta = \frac{E_F - E_C}{k_B T}$ takes the values $-10, 0, 10, 20$.

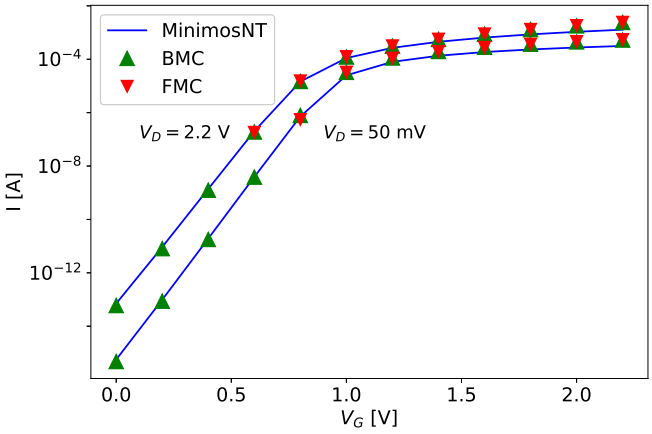

Fig. 3. Transfer characteristics of an nMOS device, simulated with MinimosNT [14] (drift-diffusion), the FMC and the BMC methods. Each point of the Monte Carlo methods is calculated with 10^6 trajectories.

Acknowledgment

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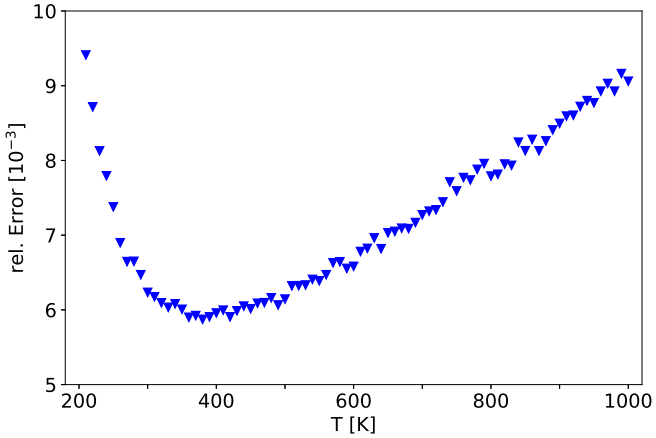

Fig. 4. Relative error of the BMC current estimator for a 65 nm nMOS device at $V_{GS} = 0.6\,\mathrm{V}$ and $V_{DS} = 2.2\,\mathrm{V}$ as a function of the injection temperature.

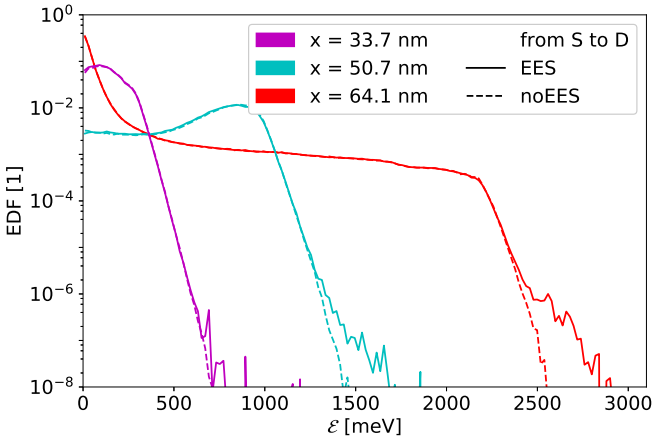

Fig. 5. Energy distribution at different points along a 65 nm nMOS channel at $V_{GS} = 2.2\,\mathrm{V}$ and $V_{DS} = 2.2\,\mathrm{V}$. Solid lines show BFMC with e-e scattering and 10^{10} scattering events. Dashed lines show BFMC without e-e scattering and 10^{10} scattering events. An injection temperature of 500K was assumed.

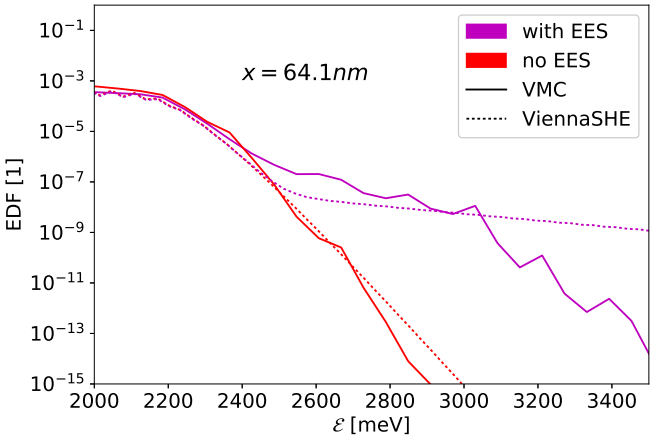

Fig. 6. Comparison of the high-energy-tail for the 65 nm nMOS device at $V_{GS} = 2.2\,\mathrm{V}$ and $V_{DS} = 2.2\,\mathrm{V}$ calculated by VMC using BFMC at an injection temperature of 1000K, and ViennaSHE. Results with and without e-e scattering are compared.

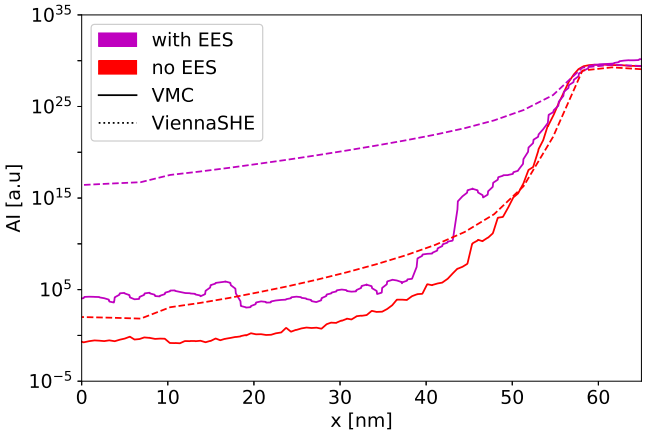

Fig. 7. Influence of e-e Scattering on the acceleration integral [12]. Results from BFMC simulation with 10^{10} scattering events and ViennaSHE are compared.

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