An efficient heat generation rate evaluation with electrothermal Monte Carlo simulations

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***Abstract*—In this paper we present an improved version of the Electrothermal Monte Carlo method. This modification has better approximation properties due to reduced statistical fluctuations. Simulation results in 2D structures are presented.**

I. Introduction

In sub-micron semiconductor devices the presence of very high and rapidly varying electric fields is the cause of non-equilibrium phenomena such as the production of hot electrons and the thermal heating of the crystal lattice. The external electric field transfers energy to the electrons and in turn to the crystal lattice through the scattering mechanisms. The self-heating can influence significantly the electrical performances since the dissipated electrical energy causes a temperature rise over an extended area of the device resulting in increased power dissipation. The transport of heat in semiconductors is due to the propagation of lattice vibrations (phonons), whereas the contribution given by the electrons (dominant in the case of metals) is estimated of the order 1 $\%$ even in the case of very large concentration [1].

In case of diffusive transport, where the device dimension L is much greater then the charge inelastic mean free path ($\simeq$ 10 nm in silicon at room temperature), the charge transport can be described by the drift-diffusion model [1] coupled to the heat diffusion equation

$$C_S \frac{\partial T_L}{\partial t} = \nabla_x \cdot (\kappa \nabla_x T_L(x)) + g(x,t) \qquad (1)$$

where the Fourier law has been assumed, T_L is the lattice temperature, C_S and κ are the heat capacity per unit volume and the thermal conductivity respectively, and $g(x,t)$ represents the heat-generation rate per unit volume. But for small devices, the drift-diffusion model is no more valid, and the charge transport must be modeled in a more accurate way. An important issue that arises from the coupling of any electronic transport algorithm to any thermal model is the significant difference in the characteristic time scales of electronic and thermal transport. The transfer of energy from the electrons to the silicon lattice occurs in a time scale of about 0.3 ps through interactions between electrons and phonons, while the transport of thermal energy by phonons has an effective relaxation time of $\simeq$ 80 ps, yielding a difference of two order of magnitude [2]. Consequently, the energy transfer from the electrons to phonons is assumed to occur instantaneously when compared to the heat transport scales, and the charge and heat transport can be decoupled. Under this ansatz, the charge transport can be described by Electrothermal Monte Carlo simulations [3]-[11] where a traditional electron MC solver is coupled to the heat diffusion equation (1). The coupling between this equation and the charge transport is guaranteed by means of the g term. One of the critical points is the determination of this heat-generation rate. In the context of traditional semiconductor device simulations, this term is typically computed starting from the dot product on the electric field and the current density [1], but numerical simulations show that this is not correct when the transport become ballistic [9]. In a Monte Carlo framework, the lattice heating rate can be calculated by accounting for the exchange of phonons between the electrons and the lattice. This net phonon emission method was applied for the first time in [12] without including heat diffusion effects. The purpose of the paper is to study this methodology and to present a modification which allows a reduction in the statistical fluctuations.

II. Electrothermal Monte Carlo

The main steps of this algorithm are the following:

1) Run the standard isothermal MC algorithm until the steady-state is reached [13], [14].

2) As the steady state is approached, various electronic parameters are sampled for typically 20 ps to generate the results from this iteration. In particular, the sum over all phonon emission minus phonon absorption events per unit time is **counted**, i.e.

$$g(x) = \left\langle H^C \right\rangle (x) = \frac{1}{N_{obs}} \sum_{j}^{N_{obs}} \left\{ \frac{n}{N_p \Delta t} \sum_i \hbar\omega_i \left[C_i^+ - C_i^- \right] \right\} \quad (2)$$

where N_{obs} is the total number of observation times, n and N_p are respectively the electron density and the particle number in the x-cell, Δt is the time interval in which the counting is made, $\hbar\omega_i$ is the energy of the exchanged phonon, and C_i^+, C_i^- are the numbers of the i-th phonon emitted and absorbed respectively. This quantity is used as an approximation to the rate of heat generation at position x.

3) The spatially varying lattice temperature distribution $T_L(x)$ is obtained by solving the steady-state heat diffusion equation (1).
4) In the next iteration the MC algorithm is rerun, where the scattering rates are updated according to the new lattice temperature distribution T_L, which is a function of the position.
5) This iterative procedure is performed until the terminal currents converge to the electrothermal steady-state values.

III. VARIANCE-REDUCED

Let us introduce the transition scattering rate $S(k,k')$, which represents the probability that, in the unit time, an electron with wave-vector k passes into a new state k'. In silicon, the main scattering mechanisms, at room temperature, are due to scattering with acoustic and optical phonons, where

$$S_{ac}(k,k') = K_0 \delta \left[\varepsilon(k) - \varepsilon(k') \right]$$

$$S_{op}(k,k') = \sum_{i=1}^{6} \left\{ S_i^+(k,k') + S_i^-(k,k') \right\} \quad (3)$$

$$S_i^+ = K_i \delta \left[\varepsilon(k') - \varepsilon(k) + \hbar\omega_i \right] (g_i + 1) \quad (4)$$

$$S_i^- = K_i \delta \left[\varepsilon(k') - \varepsilon(k) - \hbar\omega_i \right] g_i \quad (5)$$

where $\varepsilon(k)$ is the electron kinetic energy, $g_i(T_L)$ is the thermal equilibrium number of optical phonons

$$g_i(T_L) = \frac{1}{\exp\left(\frac{\hbar\omega_i}{k_B T_L}\right) - 1} \quad (6)$$

and the coupling constants are given in [16]. From the previous equations one can evaluate the **integrated scattering probability** per unit time, where the signs + and - indicate emission and absorption of the i-th phonon, i.e.

$$\lambda_i^{\pm}(\varepsilon) = \int S_i^{\pm}(k,k') dk' \quad . \quad (7)$$

Now we can modify Step 2 of the algorithm described in previous section. The heat generation rate is approximated as

$$g(x) = \langle H \rangle (x) \quad (8)$$

where

$$\langle H \rangle (x) = \frac{1}{N_{obs}} \sum_{j}^{N_{obs}} \left\{ \frac{n}{N_p} \sum_{ip=1}^{N_p} G\left[\varepsilon(k_{ip}(t_j)) \right] \right\} \quad (9)$$

N_{obs} is the total number of observation times t_j, and

$$G(\varepsilon) = \sum_i \hbar\omega_i \left[\lambda_i^+(\varepsilon) - \lambda_i^-(\varepsilon) \right]. \quad (10)$$

In [15] we have proved why this algorithm reduces the variance.

IV. NUMERICAL EXPERIMENTS

As first benchmark we have simulated a Silicon MESFET doped to 3 $\times 10^{17}$ cm^{-3} in the n+ zone and 10^{17} cm^{-3} in the n zone, with Vsource = 0 V, Vgate = -0.8 V and Vdrain = 1 V [17]. In the figure 1 we have plotted the heat generation rate obtained with the counting formula (2), and in the figure 2 that evaluated with the integrated probability formula (9), using the same particle number and simulation time. From these figures it is evident that the integrated probability estimator shows significantly lower fluctuations compared to the counting estimator.
Then, we have simulated an ultra-scale MOSFET, formed by a p-type silicon substrate and n-type source and drain region [18]. The source/drain regions have a uniform n-type doping of 10^{20} cm^{-3}, and the substrate has an uniform p-type doping of 10^{16} cm^{-3}, while the channel region has a uniform p-type doping of 10^{18} cm^{-3}. The gate and source/drain voltages are set to be 1 V each. The results are shown in the figures (3), (4) confirming again the goodness of the integrated probability estimator.

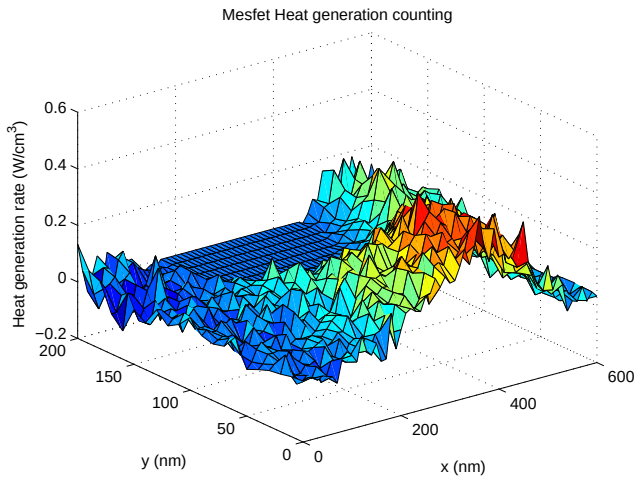

Fig. 1. The heat generation rate versus the position in the MESFET [17], evaluated by means of the counting estimator (2).

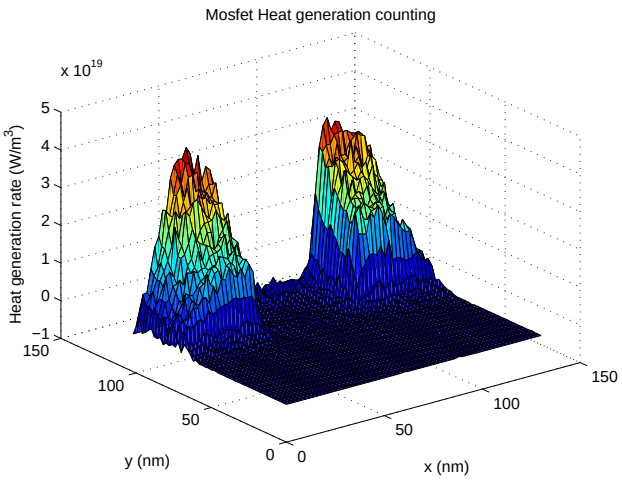

Fig. 3. The heat generation rate versus the position in the MOSFET [18], evaluated by means of the counting estimator (2).

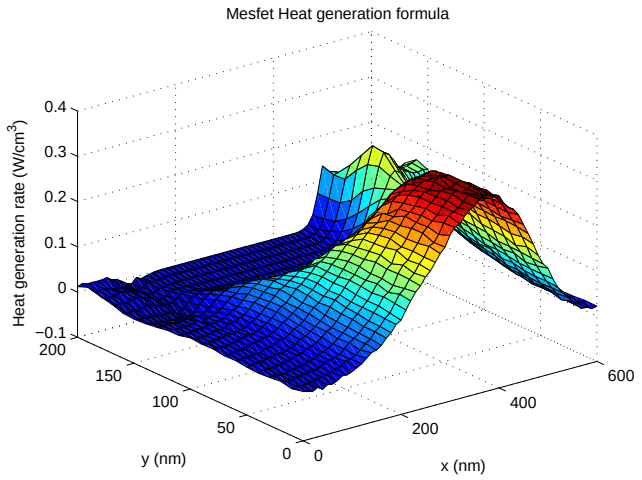

Fig. 2. The heat generation rate versus the position in the MESFET [17], evaluated by means of the integrated probability estimator (9).

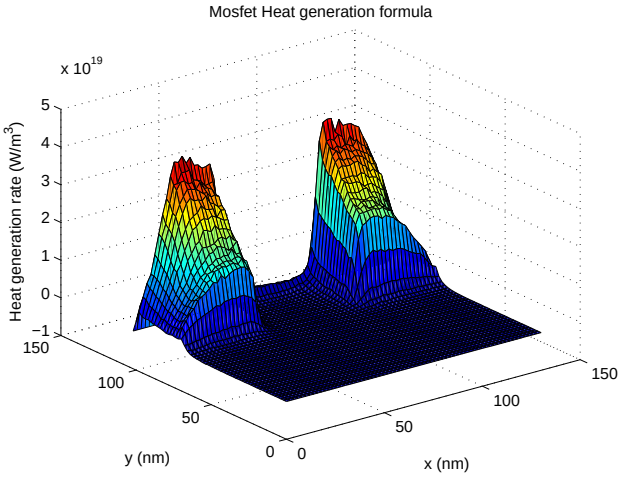

Fig. 4. The heat generation rate versus the position in the MOSFET [18], evaluated by means of the integrated probability estimator (9).

V. Conclusion

The electrothermal Monte Carlo algorithm provides a rather efficient tool for studying heat generation and transport in small semiconductor devices, at expense of huge computational effort. The coupling between the MC charge transport and the heat diffusion equation is given by a term called heat generation rate. Usually this term is determined by counting, during the steady-state, the number of phonons emitted/absorbed. In this paper we have presented a new estimator of the heat generation rate, based on the integrated scattering probability function (7). In such a way, it reduces to the usual calculation of functionals such as the mean velocity or mean energy.

We have shown that, by running 2D simulations, the new estimator reduces the variance. Moreover, it indicates that the electrothermal Monte Carlo algorithm solves the steady state Boltzmann transport equation coupled with a steady state heat diffusion equation. Efficient ETMC simulations can be also a useful benchmark for testing hydrodynamic models based on the Boltzmann equation [19]-[26].

VI. Acknowledgment

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