An efficient lattice heating evaluation with electrothermal Monte Carlo device simulations

O. Muscato, W. Wagner* and V. Di Stefano
Dipartimento di Matematica e Informatica
Universita' di Catania, Viale A. Doria 6, 95125 Catania, Italy
e-mail: muscato@dmi.unict.it
*Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstrasse 39 - 10117 Berlin, Germany
e-mail: wagner@wias-berlin.de

INTRODUCTION

The Monte Carlo (MC) method is one of the common techniques for modelling electron transport in semiconductors [1]. It is based on Boltzmann transport equations, which describe the time evolution of the distribution of electrons with respect to position and wave-vector. One of the main advantages of the Monte Carlo method is its ability to include a large range of physical effects. The continued miniaturization of semiconductor devices has resulted in new challenges related to the modelling of heat generation. Recently an electrothermal Monte Carlo method has been developed [2], [3],[4]. The method couples a stochastic algorithm for the Boltzmann transport equation with a steady-state solution of the heat diffusion equation. 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 [5] without including heat diffusion effects. The purpose of the paper is to study the electrothermal Monte Carlo method and to present a modification with reduced statistical fluctuations.

ELECTROTHERMAL MONTE CARLO

The main steps of the algorithm are the following:

1) Run the standard isothermal MC algorithm until the steady-state is reached.
2) Various electronic parameters are sampled to generate the results from this iteration. In particular, the sum over all phonon emission minus phonon absorption events per unit time is calculated, i.e. [4]

$$\left\langle H^C \right\rangle (x) = \frac{n}{N_p \Delta t} \sum_j \hbar\omega_j \left[C_j^+ - C_j^- \right] \tag{1}$$

where n is the electron density, N_p is the particle number in the x-cell, Δt is time interval in which the counting is made, $\hbar\omega_j$ the energy of the exchaged phonon, and C_j^+, C_j^- are the numbers of the j-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

$$\nabla_x \cdot (\kappa \nabla_x T_L(x)) + g(x) = 0 \tag{2}$$

where κ is the thermal conductivity and $g(x)$ is the rate of heat generation, given by eq.(1).
4) In the next iteration the MC algorithm is rerun, where the scattering rates are updated acoording 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.

VARIANCE-REDUCED

We modify Step 2 of the algorithm described in previous Section. The heat generation rate is approximated as

$$g(x) = \langle H \rangle (x) \tag{3}$$

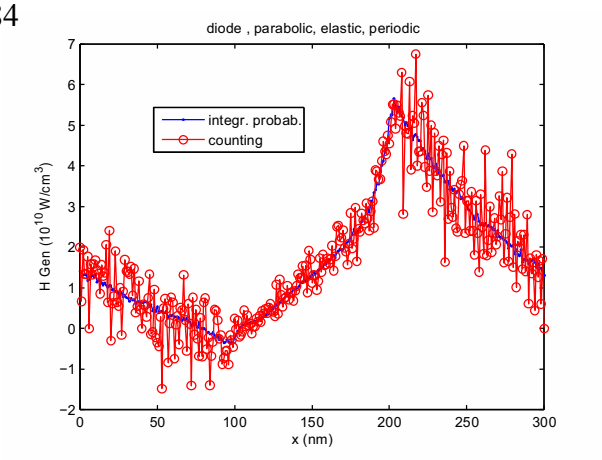

Fig. 1. The heat generation rate versus the position in the diode, evaluated by means of the counting estimator (1) and the integrated probability estimator (4).

where

$$\langle H \rangle (x) = \frac{1}{N_{obs}} \sum_{j}^{N_{obs}} \left[\frac{n}{N_p} \sum_{i=1}^{N_p} G(\varepsilon(k_i(t_j))) \right] \quad (4)$$

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

$$G(\varepsilon) = \sum_j \hbar\omega_j \left[\lambda_j^+(\varepsilon) - \lambda_j^-(\varepsilon) \right] \quad (5)$$

where

$$\lambda_j^+(\varepsilon) = \int S_j(k,k')dk' \quad (6)$$

is the integrated probability for the j-th scattering mechanism.

Numerical experiment

As first benchmark, we have considered silicon in the parabolic band approximation, and scattering mechanisms with optical and acoustic phonons. We have simulated a $n^+ - n - n^+$ diode, which consists of two highly doped regions n^+ (called cathode and anode) connected by a less doped region n (called channel). In our simulations, the n^+ regions are 100 nm-long doped to a density $N_D = 10^{19}\text{cm}^{-3}$, while the channel is 100 nm-long doped to a density $N_D = 10^{16}\text{cm}^{-3}$. The applied bias is Vb = 1.2 V, the total particle number is 201000, with a total simulation time of 20 ps. The result is shown in Figure 1, where the integrated probability estimator (4) shows significantly lower fluctuations compared to the counting estimator (1).

Acknowledgment

This work has been supported by Università degli Studi di Catania, by MIUR PRIN 2009 "Problemi Matematici delle Teorie Cinetiche e Applicazioni", and the CINECA Award N. HP10C3U0CA 2011 for the availability of high performance computing resources and support.

References

[1] C. Jacoboni and L. Reggiani, *The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent materials* , Rev. Mod. Phys., **55**, 645–705, (1983)

[2] T. Sadi, R. Kelsall, and N. Pilgrim, *Simulation of electron transport in InGaAs/AlGaAs HEMTs using an electrothermal Monte Carlo Method*, IEEE Trans. Elec. Dev., **53**(8), 1768–1774, (2006)

[3] K. Raleva, D. Vasileska, S.M. Goodnick, and M. Nedjalkov, *Modeling thermal effects in nano-devices*, IEEE Trans. Elec. Dev., 56(6), 1306–1316, (2008)

[4] E. Pop, S. Sinha and K. Goodson, *Heat generation and transport in namometer scale transistors*, Proc. IEEE,**94**(8), 1587-1601, (2006)

[5] C. Moglestue, F. A. Buot and W. T. Anderson, *Ensemble Monte Carlo particle investigation of hot electron induced source-drain burnout characteristics of GaAs field-effect transistors*, J. Appl. Phys., **78**(4), 2343–2348, (1995)