Boundary Condition Models for Terminal Current Fluctuations

M. Nedjalkov, T. Grasser, H. Kosina, and S. Selberherr
Institute for Microelectronics, TU Vienna, Gusshausstrasse 27–29, A-1040 Vienna, Austria
Phone: +43-1-58801/36014, Fax: +43-1-58801/36099, Email: Nedjalkov@iue.tuwien.ac.at

Abstract

A stochastic approach to a recently proposed model of terminal current fluctuations is presented. Two kinds of boundary conditions suitable for noise simulations in semiconductor devices are proposed. The properties and the domain of application of the two models are investigated and the conclusions are drawn from numerical experiments.

1 Introduction

The importance of current fluctuations in semiconductor devices and the physical and numerical complexity of their characterization stimulated a mutual development of the basic models and appearance of novel models for the current noise. Fundamental is the Ensemble Monte Carlo (EMC) method which provides both a model and numerical approach to the phenomena. The method is based on the notion that a direct emulation of the stochastic processes underlying the transport phenomena provides along with the physical mean values also their fluctuations. If the transport process is emulated and the current $i(t)$ is recorded in the time interval $(0, T)$ [1], the autocovariance function which characterizes the fluctuations is retrieved from its basic definition:

$$C_i(t,\tau) = \langle i(t)i(t+\tau)\rangle - \langle i\rangle(t)\langle i\rangle(t+\tau) \Rightarrow C_i(\tau) = \frac{1}{T}\int_0^T i(t)i(t+\tau)dt - \langle i\rangle^2 \quad (1)$$

where the brackets denote ensemble averages. A stationary process is considered ($\langle i\rangle$ = const) so that C_i becomes independent on the reference time t and the ensemble average is replaced by the time average in (1). The advantages and the drawbacks of this stationary EMC model are well known. The latter are particularly due to the fact that boundary conditions (BC) determine the device behavior. The EMC which is appropriate for evolution problems requires an initial transient period until the ensemble becomes stationary inside the device. The leaving particles must be re-injected to maintain the stationary process. Different models for re-injection from the boundaries are studied [2], [3] and it is shown that they affect the fluctuation characteristics.

Recently an alternative model for the current noise has been proposed [4], [5]. The autocovariance function has been obtained as a statistical average:

$$C_i(\tau) = \langle i\rangle \int d\mathbf{k} \int_L dx\; i(\mathbf{k},x)g(\mathbf{k},x,\tau) - \langle i\rangle^2; \quad \langle i\rangle = \int d\mathbf{k}\int_L dx\; i(\mathbf{k},x)f_s(\mathbf{k},x) \quad (2)$$

The space coordinate x is for a one-dimensional device with a length L and $\mathbf{k}$ denotes the wave vector. Here $i(\mathbf{k}, x)$ is the current contribution from a particle in the particular phase space point according to the Ramo-Shockley theorem and g is an effective distribution function. The latter is the solution of the time dependent Boltzmann equation for an initial condition (IC) $g_0(\mathbf{k}, x) = i(\mathbf{k}, x)f_s(\mathbf{k}, x)/\langle i\rangle$, f_s being the stationary solution in the device. In [3] the model has been applied to a bulk semiconductor using a deterministic method.

2 Boundary conditions

As applied to devices, the model requires proper BC. They are formulated in the framework of the stochastic method developed for evaluation of (2). A Monte Carlo approach to the latter simulates an evolution of the effective distribution function in contrast to the direct emulation of the current fluctuations.

The first BC model can be deduced from the limit $C_i \to 0$ when $\tau \to \infty$. The effective distribution g must evolve from g_0 to f_s in this limit. Practically C_i becomes zero after some time t_c typical for the concrete device. The stationary distribution f_s is ensured by the physical BC and it is thus concluded that they are the proper BC for (2). The particles that leave the device are re-injected according the BC in the way also used by the stationary EMC. The following effect can be encountered in this picture: particles exiting the device contribute to C_i after being reinjected with the BC, commonly taken to be the equilibrium distribution. If the exiting particles are not thermalized in the contact, the sudden cooling by the BC affects the autocovariance function. This problem is typical also for the stationary EMC which relies on the re-injection to maintain the steady state current. Special algorithms have been developed to avoid this effect [3].

The second BC model is obtained from (2) by noting that C_i contains as an integrand the difference $\phi(\mathbf{k}, x, \tau) = g(\mathbf{k}, x, \tau) - f_s(\mathbf{k}, x)$. Both, g and f_s satisfy the Boltzmann equation which has the following integral form:

$$\begin{aligned} f(\mathbf{k}, x, \tau) \;&=\; \int_0^\tau dt' \int d\mathbf{k}' f(\mathbf{k}', x(t'), t') S(\mathbf{k}', \mathbf{k}(t')) e^{-\int_{t'}^\tau dy \lambda(\mathbf{k}(y))} \\ &+\; f_0(\mathbf{k}(0), x(0)) e^{-\int_0^\tau dy \lambda(\mathbf{k}(y))} + f_b(\mathbf{k}(t_b), x(t_b)) e^{-\int_{t_b}^\tau dy \lambda(\mathbf{k}(y))} \end{aligned} \quad (3)$$

with a trajectory determined by the electric force F and velocity $\mathbf{v}$:

$$\mathbf{k}(t') = \mathbf{k} - \int_{t'}^\tau F(x(y)) dy \qquad x(t') = x - \int_{t'}^\tau v_x(\mathbf{k}(y)) dy \quad (4)$$

The initial condition f_0 and the boundary conditions f_b participate explicitly in the integral form (4). f_b is zero inside the device and is specified only on the boundaries, while f_0 is zero if $x(0)$ is placed outside the device. The time t_b is determined from the position where the Newton trajectory (4) crosses the device boundary $x(t_b) = x_b$. f_s is a solution of (4) for IC given by $f_0 = f_s$, while for the function g the IC are given by $f_0 = g_0$. Both, f_s and g utilize the same BC given by the term f_b. It follows that the equation for ϕ does not contain f_b:

$$\begin{aligned} \phi(\mathbf{k}, x, \tau) \;&=\; \int_0^\tau dt' \int d\mathbf{k}' \phi(\mathbf{k}', x(t'), t') S(\mathbf{k}', \mathbf{k}(t')) e^{-\int_{t'}^\tau dy \lambda(\mathbf{k}(y))} \\ &+\; g_0(\mathbf{k}(0), x(0)) e^{-\int_0^\tau dy \lambda(\mathbf{k}(y))} - f_s(\mathbf{k}(0), x(0)) e^{-\int_0^\tau dy \lambda(\mathbf{k}(y))} \end{aligned}$$

This equation describes a purely transient problem, where two ensembles with initial conditions g_0 and f_s evolve in time as $\phi_0(\mathbf{k}, x, \tau)$ and $\phi_s(\mathbf{k}, x, \tau)$ and give the solution as the difference $\phi = \phi_0 - \phi_s$. The boundaries absorb all particles that leave the device without re-injection.

The autocovariance (2) becomes:

$$\begin{aligned} C_i(\tau) &= \langle i \rangle \int d\mathbf{k} \int\limits_L dx\, i(\mathbf{k},x)\,(\phi_0(\mathbf{k},x,\tau) - \phi_s(\mathbf{k},x,\tau)) \\ &= \langle i \rangle \int d\mathbf{k} \int\limits_L dx\, i(\mathbf{k},x)\phi_0(\mathbf{k},x,\tau) - \langle i \rangle(\tau)\langle i \rangle(0) \end{aligned} \quad (5)$$

where

$$\langle i \rangle(\tau) = \int d\mathbf{k} \int\limits_L dx\, i(\mathbf{k},x)\phi_s(\mathbf{k},x,\tau); \qquad \langle i \rangle(0) = \langle i \rangle$$

By using the definition of g_0 it is seen that (5) is the autocovariance function of the process of evolution of an ensemble of particles initially distributed according the stationary distribution f_s in the device. With the absorbing BC the particles leak trough the device boundaries which corresponds to a transient process. (5) resembles the basic definition of the autocovariance function given by the first equation in (1).

The stochastic method consists of alternative MC algorithms which obtain the IC, simulate the evolution process, and obey the BC. The main feature is that a One Particle MC (OPMC) simulation is used to obtain the stationary distribution f_s inside the device. The latter gives rise to initial points of an ensemble of particles, whose evolution provides the current autocovariance function. In this way the initial transient simulation required by the stationary EMC can be saved since OPMC is much more efficient in obtaining f_s. Indeed, while the EMC method collects the information at the end of each trajectory, the OPMC collects the information from each trajectory segment. In the present formulation of the task the ensemble is followed until the time t_c which is commonly few orders less than the averaging time T of the stationary EMC. The evolution process imposed by the first kind of BC resembles the physical transport in the device and thus can be simulated self-consistently by a coupling with the Poisson equation. Here we compare the two kinds of BC using non-selfconsistent simulations. In this case the electric field is stationary, so that the ensemble trajectories can be mapped onto the OPMC trajectory similar to the way discussed in [6].

The numerical experiments for the two BC models are summarized in Fig. 1 and Fig. 2 respectively. A silicon n^+nn^+ structure with a length of each segment of 0.2μm and doping concentration $10^{17} : 10^{16}$ cm^{-3} is considered at different applied voltages. The autocovariance functions are normalized as $C_i(\tau)/C_i(0)$. The curves for the absorbing and the injecting BC overlap each-other and relax to zero as expected. However this is not true for a resistor with the same total length $0.6\mu m$, considered on the right of Fig. 1. At equilibrium the results of the two models coincide. At $0.25V$ there is already a difference in the corresponding curves which increases with the increase of the applied voltage. At $1V$ the autocovariance for the absorbing BC relaxes to zero, while for the injecting BC remains well above zero as seen on the left picture of Fig. 2. We assign this to the influence of the ohmic contact on the autocorrelation during the process of re-injection: the carriers are hot when leaving the device and are injected back thermalized. This conclusion is supported by additional experiments showing a decrease of the effect when the length of the structure increases under a constant electric field inside. In this case the portion of the leaving carriers decreases with respect to the total number of particles in the resistor. Another experiment is shown on the right of Fig. 2. The simualted structure is formed by two tiny highly doped $0.05\mu m$

regions attached on both sides of the resistor which cool the exiting carries. The two autocorelation functions coincide again.

We conclude that the injecting BC can be applied if the contact regions thermalize the carriers before they leave the device. The absorbing BC model is universal and physically more transparent since it refers to the dwelling time of the particles in the device.

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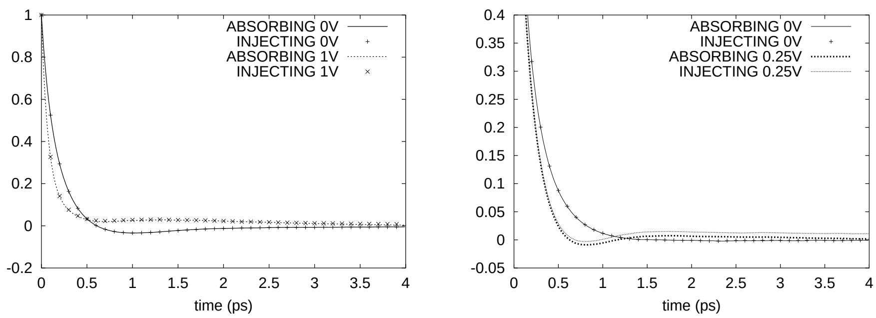

Fig. 1: Current Autocovariance for the n^+nn^+ diode (left) and the resistor (right)

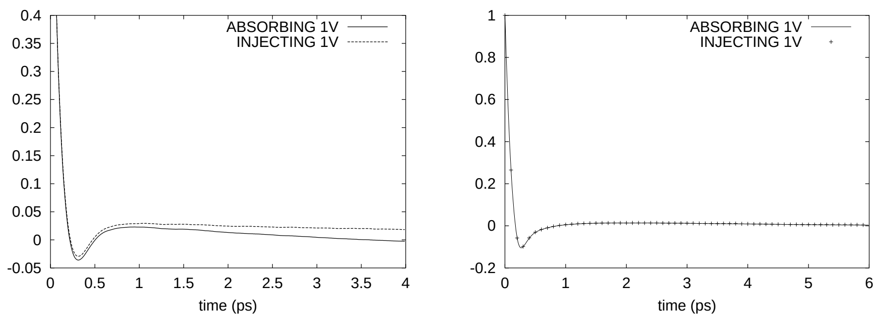

Fig. 2: Current Autocovariance at 1 Volt for the resistor (left) and the n^+nn^+ structure (right)

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