Microelectronic Engineering 15 (1991) 53–56
Elsevier

Monte-Carlo – Poisson Coupling Using Transport Coefficients

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Abstract
A coupling scheme between Poisson's equation and a combined Monte Carlo – Drift Diffusion transport model is presented. In an iterative procedure the mobility- and temperature profiles are updated. The method which exhibits a very good convergence rate is applied to study non-equilibrium transport in a one-dimensional semiconductor structure.

1 Introduction

For the simulation of submicron devices a hybrid approach to the modeling of carrier transport has several benefits [1][2]. The Drift Diffusion (DD) model provides an accurate description in the low field areas of a device. Since the Monte Carlo (MC) method is computationally expensive, it is desirable to restrict its application to areas were the DD-model becomes inaccurate, which is the case when the electric field is high an its spatial variation is large. One difficulty in this kind of regional MC analysis is the accurate handling of boundary conditions at the interface between the various regions. Furthermore in very small devices the hybrid transport model and the Poisson equation must be solved selfconsistently.

In the standard iteration technique the updated MC-carrier concentrations are substituted in the Poisson equation [3]. However stability problems can arise in areas with high carrier concentrations. In more recent work [4] the quasi fermi level has been proposed to be taken as MC-output and to serve as input for the Poisson equation. This algorithm solves the above mentioned stability problems and shows a better convergence rate [4]. In the following we describe a new selfconsistent iteration scheme which takes into account the hybrid nature of the transport model. During each MC-step the coefficients mobility and thermal voltage are updated. Their new values are then substituted in a set of equations consisting of Poisson-, the continuity equation and a generalized current relation. This procedure allows in low regions the required coefficients to be related analytically to the electric field. The current relation then simplifies to the DD-relation. Just in device regions far off equilibrium the coefficients have to be calculated by MC. The area in which MC-calculation is performed is larger then the area where the coefficients are recorded. This leads to an overlap of the MC-domain with the DD-areas, which makes the boundary condition problem less stringent.

2 Iteration Technique

The basis of our method is the following set of equations, which is assumed to be valid both near equilibrium and in the hot carrier regime. Neglecting pair generation and

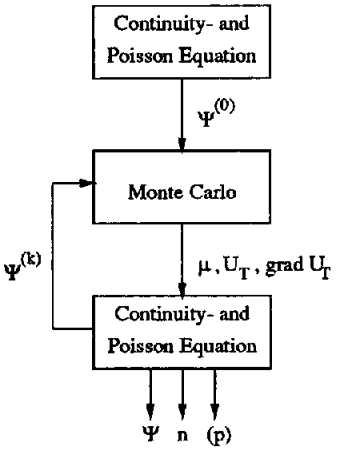

Figure 1: Flow chart of the main iteration loop.

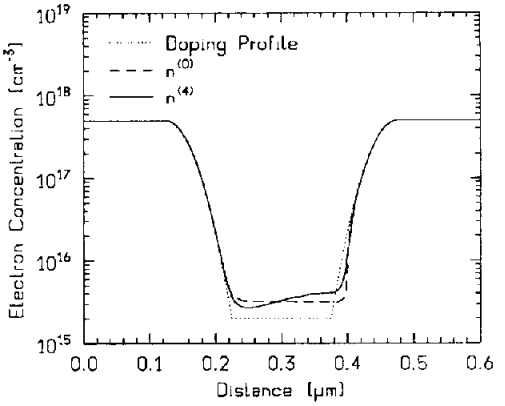

Figure 2: Doping profile and carrier concentrations in an n^+-n-n^+ structure.
$n^{(0)}\cdots$ initial solution (DD)
$n^{(4)}\cdots$ after four MC–Poisson iterations

recombination and impact ionization this set reads for electrons

$$\Delta\psi = \frac{q}{\epsilon}\cdot(n-C) \tag{1}$$

$$\nabla j_n = 0 \tag{2}$$

$$j_n = q\cdot n\cdot\mu\cdot(-\nabla\psi + \nabla U_T + \frac{U_T}{n}\cdot\nabla n)\,. \tag{3}$$

Poisson equation (1) and continuity equation (2) are valid in the whole device regardless to the energy distribution of the electrons. The equation for the first moment of the Boltzmann Transport equation can be cast in the form of the generalized current relation (3). It states momentum balance for electrons and includes nonlocal effects such as velocity overshoot and the occurrence of an energy gradient field ∇U_T.

In device areas where the electric field is low or the situation is homogeneous, the energy gradient field vanishes in (3) leading to the conventional DD-current relation. Furthermore the mobility μ and the electron thermal voltage U_T can be related analytically to local quantities such as doping concentration, electric field or the driving force.

In regions far off equilibrium the set of parameters $(\mu(x), U_T(x))$ depend on the local distribution function. Extracting these parameters from the equation for the first moment in its rigorous form they would have tensor property. However to deal with scalar quantities we adopt the following definitions [5].

$$\mu = \frac{q\ v_d}{(dp/dt)_c} \tag{4}$$

$$U_T = q^{-1}\cdot\frac{1}{3}\cdot Tr <\hbar k_i\ v_j> \tag{5}$$

Here v_d and $(dp/dt)_c$ denotes the magnitude of drift velocity and momentum loss rate, respectively. With the energy dependent momentum relaxation time $\tau_m(E)$ the average

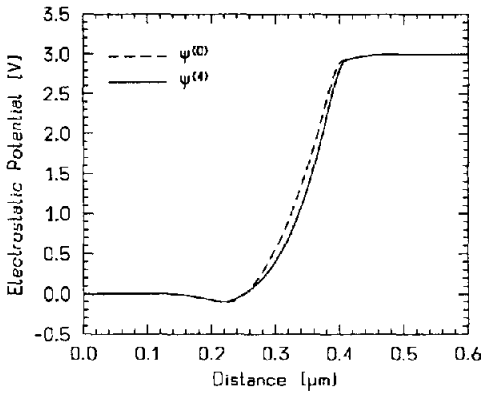

Figure 3: Initial solution ($\Psi^{(0)}$) of the electrostatic potential and its profile after four iterations ($\Psi^{(4)}$).

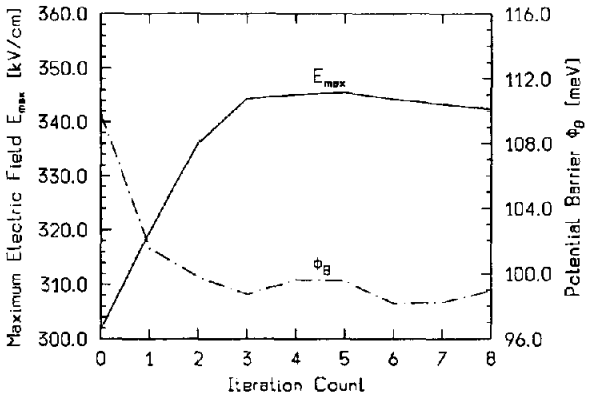

Figure 4: Evolution of the maximum of the electric field and the retarding potential barrier with the number of iterations.

momentum loss rate is defined as: $(dp/dt)_c = <\hbar k \cdot \tau_m^{-1}(E)>$. In (5) we use the trace of the energy tensor to get the scalar approximation U_T. Provided that the same potential distribution is used in both the current relation (3) and in the MC-procedure, this current relation employing the parameters (4) and (5) recovers exactly the MC-results $n(x)$ and $v_d(x)$. Therefore nonlocal transport effects such as velocity overshoot and ballistic transport are included in this drift-diffusion like current relation.

In the first step of our algorithm an initial guess for the electrostatic potential is calculated by a conventional DD-simulator (Fig. 1).

In step two the updated potential serves as input for the MC-procedure. Mobility and thermal voltage profiles are calculated in the critical device regions according to (4) and (5). These profiles are then extended over the remaining regions, which are near equilibrium.

In step three the set of equations (1),(2) and (3) is solved in the entire device by means of a conventional continuity–Poisson solver. During this step the coefficients (μ, U_T) are kept constant. The algorithm continues with step two until the change of the potential is sufficiently small.

3 Results

As an example we have simulated is an n^+–n–n^+ structure, where the n-region has a length of $0.15\mu m$. Bias voltage has been $3V$. To tackle the Poisson- and continuity equation we have used PROMIS, a general solver for partial differential equations of second order [6]. The MC-simulator is based on the physical model of Si mainly as it is described in [7].

Since the simulation domain is very small ($0.6\mu m$) we performed the MC-simulation from contact to contact. The decision where to use the MC-calculated parameters and where the analytical near-equilibrium values has be made by the carrier temperature profile. In the region, where the thermal voltage U_T exceeds 5% of the equilibrium value the MC-parameters have been used.

To characterize the potential distribution the maximum electric field in the device and the potential barrier at the $n^+ - n$ junction have been observed. This barrier is of some importance for the MC-method, because a particle split algorithm is required to achieve

significant injection into the n-region. Fig. 2 compares the initial carrier concentration obtained by the DD-simulator and the selfconsistent concentration after four MC-Poisson iterations. Fig. 3 shows the change of the potential due to the redistribution of the mobile charge. Fig. (4) shows the convergence rate of the two observed quantities. After three MC-Poisson iterations the maximum field evolved from $320kV/cm$ to $345kV/cm$. The values of the following iterations spreads within $\pm 0.45\%$. The potential barrier decreases from $110meV$ to $99meV$ within a range of $\pm 0.9\%$.

To get reliable results in the present one-dimensional example only three of the time consuming MC-Poisson iterations are actually required. Thus the proposed MC-Poisson coupling scheme proves very efficient.

4 Conclusion

A new coupling scheme between Poisson equation and MC-transport has been proposed. The algorithm which allows combined Monte Carlo – Drift Diffusion analysis is efficient for two reasons: Firstly, few MC-Poisson iterations are required due to the very high convergence rate. Secondly, if significant portions of the device allow accurate modeling by the DD-model, MC-calculation can be restricted to the critical device regions.

Acknowledgements

This work is supported by: AUSTRIAN INDUSTRIES – AMS International Unterpremstätten, Austria; DIGITAL EQUIPMENT Corporation Hudson, USA; SIEMENS Corporation Munich, FRG; and SONY Corporation Atsugi, Japan.

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