

A Monte Carlo MOSFET simulator based on a new method for the Poisson-transport iteration

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Abstract

A two-dimensional, steady state Monte Carlo (MC) device simulator which is especially suited for the simulation of submicron MOSFETs is described. A unique Monte Carlo-Poisson coupling scheme has been adopted, which exhibits a significantly better convergence rate than conventional schemes. This technique is based on MC-Drift-Diffusion (DD) coupling, a method which proves to be correct within the Boltzmann formalism. In addition, MC-DD coupling allows to tackle equilibrium- and non-equilibrium transport, both of them occurring in different device regions, by one and the same transport equation, while using transport coefficients of different origin. An implementation in MINIMOS [3] has been performed and simulation results are shown.

1 Introduction

MC simulation of a submicron MOSFET employing the potential distribution obtained by a selfconsistent DD simulation leads to unrealistic results. Due to non-local transport effects, which are not included in the DD model but are properly treated by the MC method, a change in the distribution of mobile charge may occur, which in turn has strong impact on the electrostatic potential distribution in the device. Therefore a selfconsistent treatment of Boltzmann's transport equation (BTE), solved by the MC method, and Poisson's equation is mandatory for such small devices.

Previously published algorithms couple the BTE with either the linear [4] or the nonlinear [7] Poisson equation. In [6] we have presented a one-dimensional implementation of an algorithm, which adds to the BTE and the Poisson equation a redundant continuity equation. At first glance the solution of an additional unrequired equation may seem somewhat strange, however, this treatment is formally correct within the Boltzmann picture and, as a practical consequence, leads to a new algorithm requiring significantly less iterations than conventional techniques do. The reason why this method works is that the additional continuity equation together with a drift-diffusion-like current relation exactly reproduces the MC transport phenomena, provided that the mobility and the temperature voltage stem from a correct solution of the BTE.

In MINIMOS [3] a two-dimensional version of the new algorithm has been implemented. Simulation results for a quarter micron MOSFET performed with MINIMOS/MC are discussed in detail.

2 The MC–DD Coupling Scheme

The momentum balance equation which can be derived directly from the BTE can be written as

$$\vec{j}_n = q \cdot n \cdot \hat{\mu} \cdot \left(-\vec{\nabla}\psi + \frac{1}{n} \cdot \vec{\nabla}(n\hat{U}_T) \right). \quad (1)$$

Here $\hat{\mu}$ and \hat{U}_T denote the mobility tensor and the thermal voltage tensor, respectively. Both quantities depend on the distribution function, and are evaluated by means of the MC method according to their correct definitions

$$\left(\hat{U}_T \right)_{ij} = \frac{1}{q} \langle \hbar k_i \cdot v_j \rangle. \quad (2)$$

For the definition of the mobility two different expressions, which are formally equivalent, are possible. Neglecting the tensor property one gets

$$\mu(\vec{x}) = \frac{|\langle \vec{v} \rangle|}{|-\vec{\nabla}\psi + \frac{\hat{U}_T}{n} \vec{\nabla}n + \vec{\nabla}\hat{U}_T|} \quad (3)$$

$$\mu(\vec{x}) = q \cdot \frac{|\langle \vec{v} \rangle|}{|\langle \int (\hbar \vec{k} - \hbar \vec{k}') S(\vec{k}, \vec{k}') d^3 k' \rangle|} \quad (4)$$

The first expression (3) defines the mobility by using as the denominator the LHS of the momentum balance equation, which can be interpreted as the driving force acting on the electrons. A quite similar definition has been proposed in the original work of Bandyopadhyay [1]. However difficulties arise when this non-local mobility is evaluated by the MC-method. In particular the evaluation of both the diffusion term $\vec{\nabla}n$ and the energy gradient field $\vec{\nabla}\hat{U}_T$ requires differentiation of MC quantities, which leads to inaccurate results.

In the latter expression (4) the RHS of the momentum balance equation, namely the averaged momentum loss rate is used. Since this term can accurately be evaluated without any differentiation, this mobility definition is well suited for implementation. The denominator in (4) can be expressed by the energy dependent momentum relaxation time

$$\left(\frac{dp}{dt} \right)_c = \langle \hbar \vec{k} \cdot \tau_m^{-1}(E) \rangle \quad (5)$$

$$\tau_m(E)^{-1} = \int (1 - \cos \theta) S(\vec{k}, \vec{k}') d^3 k'. \quad (6)$$

The momentum relaxation time is the superposition of the individual scattering mechanisms.

$$\tau_m(E)^{-1} = \lambda_{ac}^{tot}(E) + \lambda_{opt}^{tot}(E) + \lambda_{surf}^{tot}(E) + \tau_{ion,m}^{-1}(E) \quad (7)$$

In the present model we have taken into account acoustic and optical phonons, surface roughness scattering and ionized impurity scattering.

In conclusion of this section we note that by knowledge of the correct distribution function insertion of the coefficients (2) and (4) exactly recovers the the non-local current density $\vec{j}_n = -qn \langle \vec{v} \rangle$. Especially in low field regions μ and U_T can be related analytically to the electric field and (1) simplifies to the conventional DD-relation.

3 The MC–DD–Poisson Coupling Scheme

In the semiclassical theory transport of charged carriers is determined by the following set of equations:

- Poisson’s equation
- BTE (MC)

This problem can be solved selfconsistently within real devices [2][4][7]. In the algorithm we propose, the continuity equation and the current relation (1) are added.

- Poisson’s equation
- continuity equation
- current relation
- BTE (MC)

The additional equations are the zeroth and first moment equations of the BTE and therefore neither any information is added nor any approximation is introduced. This extended set allows a new solution strategy to be applied.

At first an initial guess for the electrostatic potential is calculated by a conventional DD-simulator. In the second step the resulting potential serves as input for the BTE, which is solved by the MC method. Mobility and thermal voltage profiles are recorded in the critical device regions according to (4) and (2), respectively. These profiles are then extended over the remaining regions, which are near equilibrium.

In the third step the DD-simulator solves the Poisson equation and the continuity equation together with the extended current relation (1) in the entire device. During this step the profiles (μ, U_T) remain unchanged. The algorithm continues with the solution of the BTE until the change of the potential is sufficiently small. A flow chart of this algorithm is shown in Fig.1.

4 Results

The MC-code is based on the physical model of silicon as it is described in [5]. The algorithm has been implemented in the two-dimensional device simulator MINIMOS [3], which both serves as front end and controls the simulation. As an example, an n-MOSFET at room temperature with a gate mask length of $L = 0.25\mu m$ has been simulated at $U_G = U_D = 2.5V$. Fig. 2 (a) shows the relative updates of carrier concentration and electrostatic potential as a function of the number of iterations. The norms first decrease rapidly but then are limited by the statistical noise inherent in the MC-method. The drastically increased drain current (Fig. 2 (b)) occurring after the first iteration can be attributed to velocity overshoot. However in the subsequent iterations the Poisson coupling reduces the impact of velocity overshoot on the drain current. The final drain current is obtained after just five iterations. Compared to the data reported in [7] that means a reduction of the costly MC-iterations by a factor of two.

Fig.3 (a)–(d) compares DD (dashed lines) and MC (solid lines) results. The DD result served as initial solution, and the MC results have been taken after five MC-DD-Poisson

iterations. The lateral effective velocity shown in Fig. 3 (a) is defined as the average $v_{x,\text{eff}} = \int v_x(y) \cdot n(y) \cdot dy / \int n(y) \cdot dy$. The initial DD-solution for the velocity is clearly bounded by the bulk saturation velocity ($1 \cdot 10^7 \text{ cm/s}$). In the pinch-off area MC leads to velocity overshoot, and one should keep in mind that this velocity profile was reproduced by the DD-like current relation (1) by including the MC-generated coefficients (2) and (4). In Fig.3 (b) the corresponding electron concentrations at the Si-SiO₂ interface are shown. The impact of velocity overshoot on the drain current is compensated by a reduced carrier concentration. This difference in MC- and DD-carrier concentration has significant influence on the potential within the device (Fig.3 (c)). In the MC case the potential profile in the high field region becomes smoother, because the lower carrier concentration results in a lower space charge in that area. As a consequence MC predicts a lower lateral electric field (Fig.3 (d)) than DD.

5 Conclusion

A MC-Poisson coupling method, which is based on MC-DD coupling, has been implemented in a two-dimensional device simulator for the first time. The expectation of a high convergence rate has been confirmed. Application to a quarter micron MOSFET has demonstrated the applicability of the new algorithm as well as the necessity of selfconsistent simulation for such small devices.

Acknowledgements

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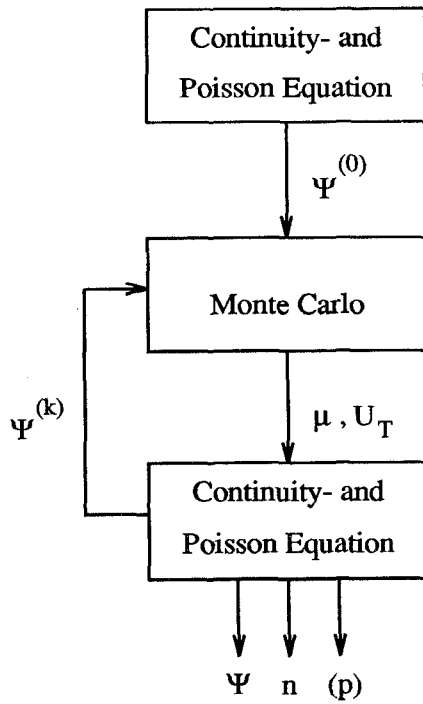


Figure 1: Flow chart of the selfconsistent MC-Poisson algorithm.

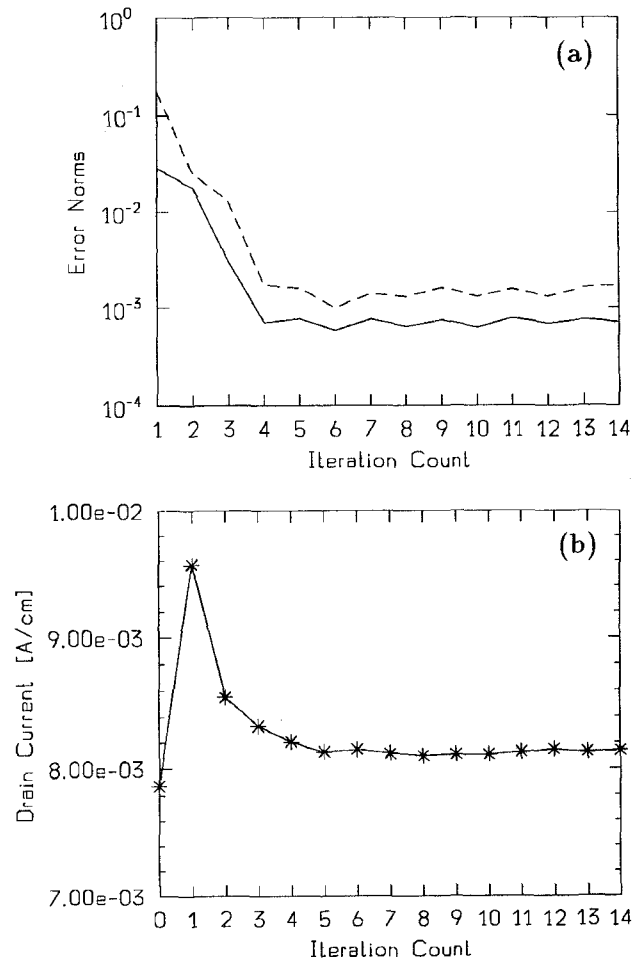


Figure 2: (a) relative norm of carrier concentration updates $\|\Delta n_k\|/\|n_k\|$ (dashed line) and potential updates $\|\Delta \psi_k\|/\|\psi_k\|$ (solid line) versus the number of iterations. (b) evolution of the drain current with the iteration number.

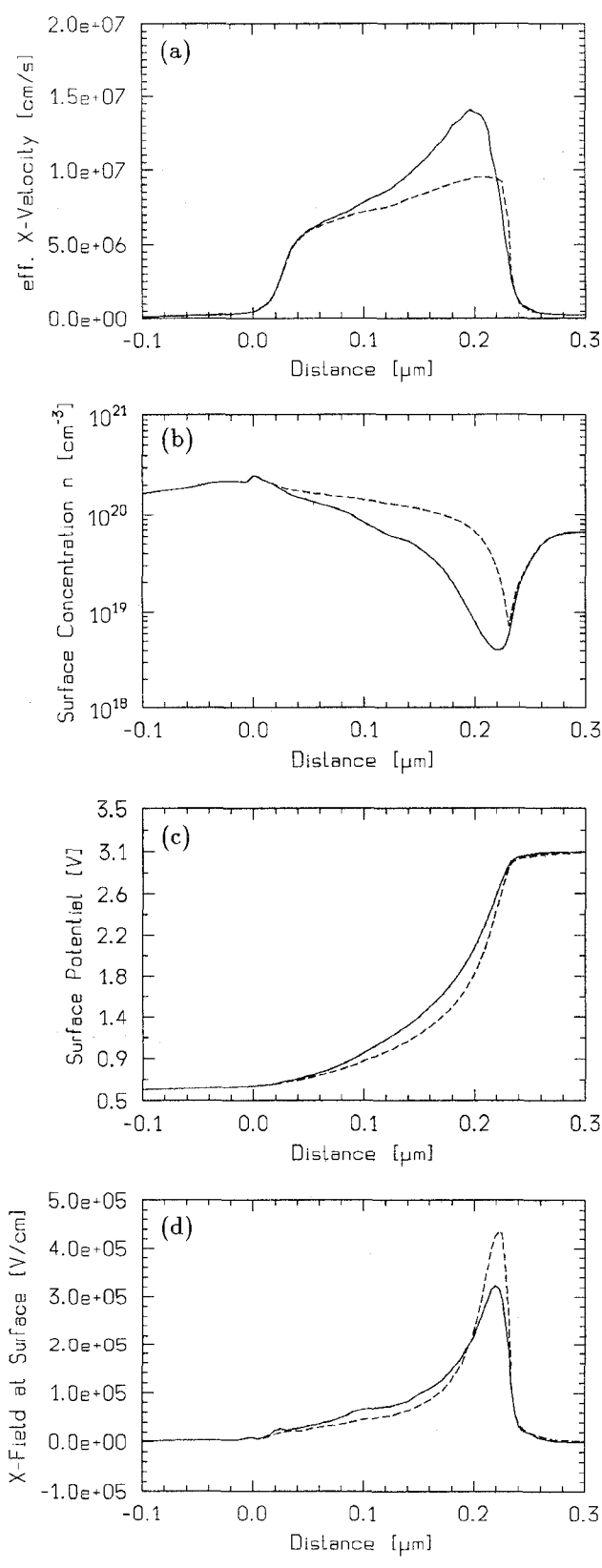


Figure 3:
 Comparison of different quantities in a $0.25\mu m$ MOSFET at $U_G = U_D = 2.5V$ obtained by selfconsistent DD- (dashed line) and selfconsistent MC- (solid line) simulation.
 (a) effective velocity in lateral direction
 (b) surface electron concentration
 (c) surface potential
 (d) lateral surface field.