Simulation of Nanometer MOS-Devices with MINIMOS

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1 INTRODUCTION

In the last decade two dimensional device simulation based on the Drift-Diffusion (DD) model has been widely used and is still of remarkable importance for industrial purposes. When device size shrinks below one micron the electric field often becomes very high and undergoes rapid changes over a small distance. In this situation the DD model begins to fail, while the Monte-Carlo (MC) method being based on more accurate physical models is capable to describe the occuring effects. On the other hand for low field transport or in regions with retarding fields the DD model with adequate parameter models has proven to be sufficiently accurate. In terms of computational effort the solution of the DD model can be seen as very efficient compared to a MC simulation. For these reasons we have tried to find a coupling scheme for MC and DD model which is rigouros in a physical sense and cheap in terms of demands on computational resources.

2 THE PHYSICAL MODEL

If we assume the Boltzmann transport equation (BTE) to be valid, the full spectrum of carrier transport phenomena such as velocity overshoot and ballistic transport can also be extracted from its first momentum equation which can be expressed in following terms.

$$J_i = q\, n\, \mu \left(E_i + \frac{1}{n} \sum_{i=1}^{2} \frac{\partial n U_{ij}}{\partial x_j} \right), \qquad i = 1,2 \tag{1}$$

Mobility μ and thermal voltage U_{ij} $(U_{ij} = k_B T_{ij}/q)$ has to be treated as functionals of the local distribution function in k-space. For the notation of these functionals we use subsequently the average operator $< A >$ which has the meaning of $\int A(\mathbf{k}) f(\mathbf{k},\mathbf{x}) d^3\mathbf{k} / \int f(\mathbf{k},\mathbf{x}) d^3\mathbf{k}$. μ and U_{ij} can not longer be treated simply as parameters as usually done in the DD model, even when they are modeled space dependent, field dependent and the like.

The Monte Carlo method is well known to allow a direct solution of the BTE. By means of a MC facility we evaluate the space dependent parameters μ and U_{ij} and solve (1) with our device simulator MINIMOS [1]. This coupling method of MC and conventional simulation can be justified rigourosly from the BTE [2].

To find the correct form of mobility we start with the mechanism of momentum relaxation, which is described by the momentum loss integral $\int(\hbar\mathbf{k}-\hbar\mathbf{k}')S(\mathbf{k},\mathbf{k}')d^3\mathbf{k}'$. For our band structure model the vector valued integral is colinear with the momentum $\hbar\mathbf{k}$. The proportionality factor is the momentum scattering rate $\lambda_m(E)$ which differs due to the anisotropic nature of coulomb scattering slightly from the total scattering rate. Mobility is now the ratio of local velocity and local momentum loss.

$$\mu = q \frac{\| < \mathbf{v} > \|}{\| < \hbar\mathbf{k}\ \lambda_m(E) > \|} \tag{2}$$

It should be noted that the mobility does not rely on the relaxation time approximation.Therefore extension to general bands is straight forward, but in that case the scalar property of μ would not be valid anymore. The definition of the thermal voltage tensor results directly from the derivation of the momentum conservation equation from the BTE.

$$\left(U_T\right)_{ij} = \frac{1}{q} < \hbar k_i\ v_j > \tag{3}$$

Again should be noted that the definitions (2) and (3) do not contain the effective mass and are thus suited for general band structures. As reported in [3] the need for a more general temperature definition (the definition $< E >= \frac{3}{2}k_BT$ is restricted to parabolic bands) has also arised in the field of hydrodynamic modeling.

The physical model in the MC program is mainly that described in [4] and contains six anisotropic, nonparabolic valleys for the band structure, several phonon modes for inter- and intravalley scattering and the Brooks-Herring formulation for impurity scattering. We have no need to assume any velocity distribution at the boundary of the MC-window, since electrons are always injected in the source of a MOSFET, where they fully thermalize before entering the channel. In the region of interest, usually near drain, a sufficiently large number of particles is supplied by a particle split algorithm as proposed in [5], thus reducing the statistical uncertainty of the resulting profiles.

3 RESULTS

A n-channel MOSFET with $L_{gate} = 0.25\mu m$, $t_{ox} = 5nm$ was simulated with our combined technique. The device has a metallurgical channel length of $L_{eff} = 0.15\mu m$ and exhibits a threshold voltage $U_t = 0.2V$ at $U_{DS} = 2.5V$. The results depicted in Fig1. to 4. were obtained under a bias condition of $U_{GS} = U_{DS} = 2.5V$. Fig. 1. indicates the lateral temperature T_{xx} to have a maximum at the surface, while the maximum of T_{yy} is shifted away from surface. We suppose that degradation due to hot electron injection into the oxide is dominated by the distribution of T_{yy}. In our simulations the off-diagonal temperatures never exceeded 15% of the main-diagonal elements. Thus we estimate their contribution to the driving force of minor importance and assume diagonal form $T_{ij} = T_{ij}\delta_{ij}$.
Fig. 2. and Fig. 3. compares the lateral electric field and the driving force acting on the electrons. At the coordinate 0.3 μm lying already in the highly doped drain the lateral field has nearly vanished. But the driving force has still a value of about 35 kV/cm which is mostly contributed by the spatial gradient of carrier-energy and -concentration.

4 DISCUSSION

The method to evaluate mobility- and temperature profiles with MC and than to solve the DD-like equation(1) with a conventional simulator has several benefits. Firstly, this method is capable to perform regional MC analysis. Only in the high field region of a device μ and U_{ij} have to be calculated with MC. In the low and moderate field regions traditional models assuming dependency on local quantities will suffice thus saving computer time. At the boundary of the MC window the smoothness constraints for the very sensitive quantities like carrier conentration and current density, are fullfilled automatically, since eq.(1) is solved globally in the whole device. Secondly, the selfconsistent solution of transport- and Poisson equation can be achieved with only few iterations between the conventional simulator and the MC routine. This is due to the fact that the definitions (2) and (3) do not explicitely contain any carrier concetration. Therefore our parameters are by for not so strongly coupled with the potential as the carrier concentrations are. Thirdly, we have the full capability of a MC simulator in conjunction with the advantages of a conventional simulator, which are, e.g., input specifications, coupling facilities to process simulators and links to graphic post processors, which have been developed to a considerable degree of sophistication in MINIMOS.

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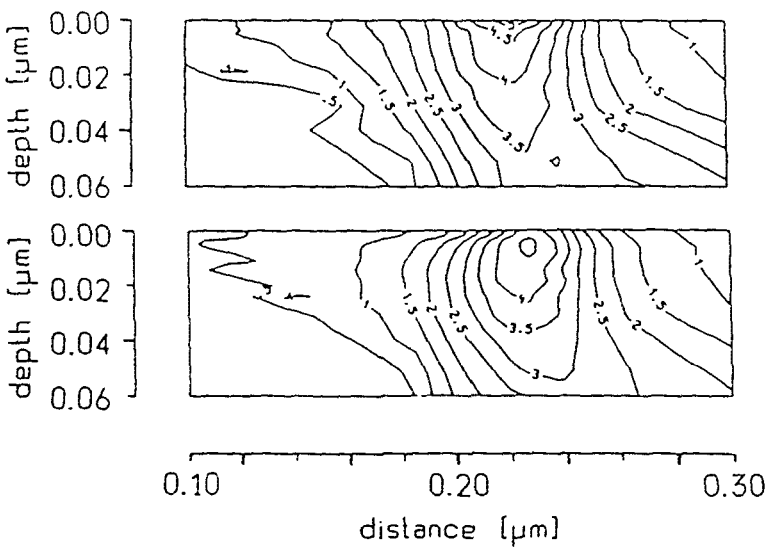

Fig. 1. Lateral (T_{xx}) and transversal (T_{yy}) electron temperatures in a quarter micron MOSFET (units [1000 K]).
$T_{ii} = \frac{1}{k_B} < p_i\ v_i >, \quad i = x, y$

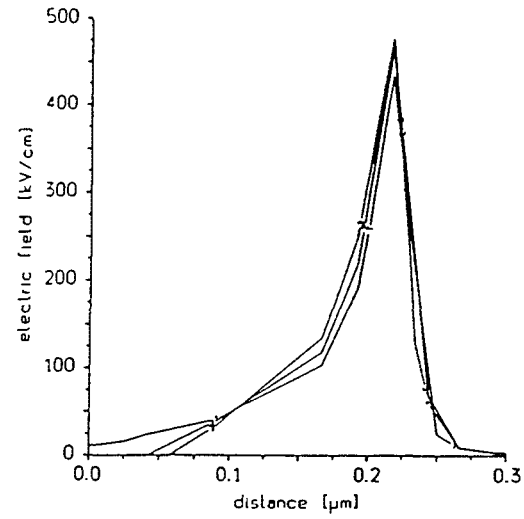

Fig. 2. Lateral electric field along the channel at 0, 50, 100 nm below the interface ($F_{max} = 490kV/cm$) . Results from MINIMOS with conventional DD model.

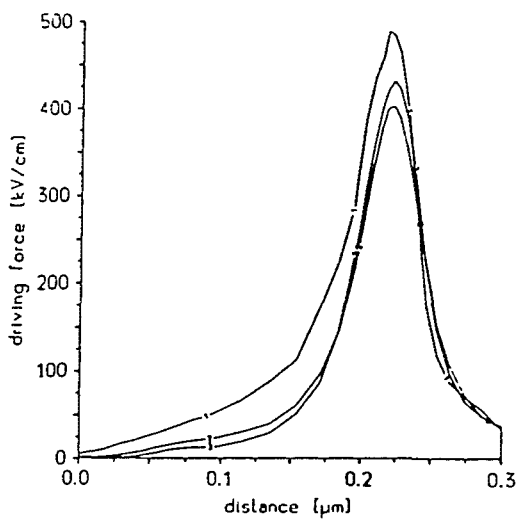

Fig. 3. Driving force along the channel (electric field plus diffusion term). This quantity equals to the momentum loss due to momentum balance. $\mathbf{DF} = \frac{1}{q} < \mathrm{p}\ \lambda_m >$

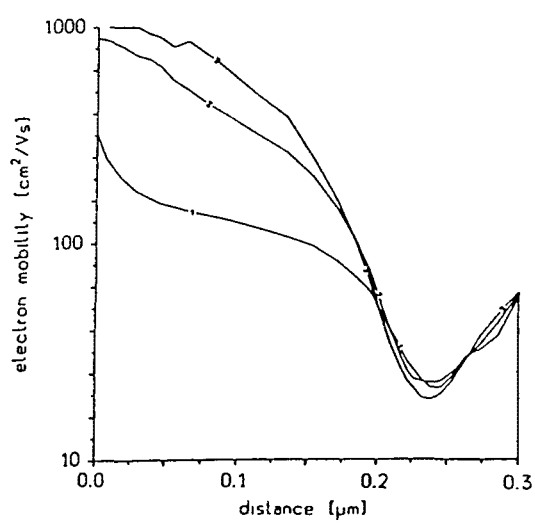

Fig. 4. Mobility according to eq (2). Curves 1,2,3 correspond to 0,50,100 nm below surface.