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The MicroMOS 3D Monte Carlo Simulation Program – a Tool for Verifying the MINIMOS Mobility Models

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Abstract.

A molecular dynamics Monte Carlo simulation method was developed for examining the behaviour of submicron MOSFET devices. A brief description of the simulation principles and physical backgrounds is presented. Special attention was paid to use first physical principles. An important advantage of the method is that the Coulomb scattering are taken into account inherently. A MOS structure of 0.25 μm channel length and 0.25 μm channel width has been analyzed on an Alpha-chip DEC 7000 computer.

1. Introduction

MiCroMOS is a *three-dimensional Monte Carlo semiconductor device simulation program* developed primarily for studying the behaviour of sub-halfmicron Si MOSFET devices.[2]. The *molecular dynamics method* [1] seems to be the best suitable technique[3]. The program development is concentrated on applying *first physical principles* in the active device region, without any fitting factors. [4]

2. The device structure

In the channel region, and in limited parts of the source, drain and bulk all carriers are examined individually. Outside this region classical approximations are

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2 The following considerations have lead us to apply this concept:
- the classical *drift-diffusion method* or the *hydrodynamic method* - both based on some statistical considerations for the distribution functions - are no more valid, since in such a structure the number of carriers is only in the order of thousands.
- for the relatively small number of particles, *the momentum and space-trajectories of each individual carrier can be followed* within acceptable CPU time.

3 The more sophisticated Monte Carlo methods (using charge clouds, superparticles, etc.) offer far more effective numerical solution tools, whereas the physics of the simulated system is obscured.

4 At present, the following effects are neglected: generation - recombination, impact ionization surface quantization, magnetic field, presence of split-off holes.

applied[5]. The dimensions of the examined device can be seen on Fig. 1. In the nondepleted parts of the source, drain and bulk charge neutrality is forced by introducing the required number of carriers.

L	= 250 nm
D	= 300 nm
W	= 250 nm
D_S	= 120 nm
D_{ox}	= 4.5 nm
N_A	= 10^{23} m^{-3}
N_D	= 10^{24} m^{-3}
N_{ss}	= -10^{15} m^{-2}
Al gate	

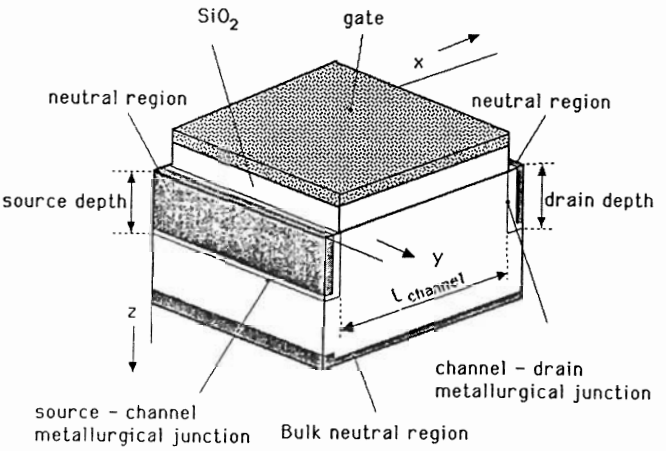

Fig. 1

3. Simulation principle[6]

The flow chart of the simulation can be seen on Fig. 2.

3.1 Potential calculation

A unique feature of the program, that the field and the potential distributions are not determined by solving the Poisson equation. Instead, the field and potential are separated into two parts, one originating from the *charges inside the active region* (and from the Si-SiO_2 interface charges) and calculated *analytically*, the other from the *charges outside the active region and external voltages* (representing the boundary conditions) and determined by solving the Laplace equation *numerically*. The potential distribution is given on Fig. 3.

3.2 The dispersion relation

For electrons, there are *six ellipsoid shaped constant energy surfaces*. For <100> oriented Si their principal axes lies on the positive or negative coordinate axes of the **k** - space and their centre is located at 0.85 $\mathbf{k}_{Max}$ [3]. The constant *effective mass concept* is used, and only diagonal elements of the effective mass tensor differ from zero. Different transversal and longitudinal effective masses are considered. The relationship between the k-vector, velocity and momentum for the i^{th} ellipsoid electrons is given by

$$\mathbf{p} = \mathbf{m}_i^{-1}\,\mathbf{v} = \hbar(\mathbf{k} - \mathbf{k}_{oi})$$

The effective masses of heavy and light holes correspond to two concentric constant energy spheres (ie. the warped shape of the valence band is approximated by spheres). Caused by the spherical symmetry, the diagonal elements are equal, ie. two scalar effective mass can be considered for the light and heavy holes.

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5 In this sense, the program is a hybrid Monte Carlo method

6 For a detailed discussion see Ref. [2]

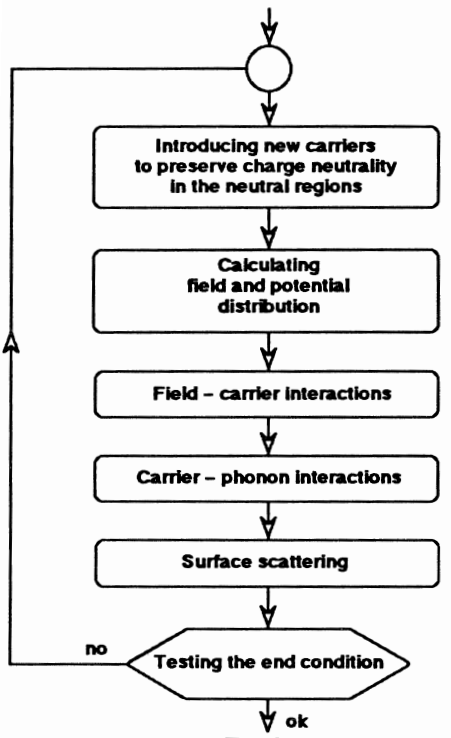

Fig. 2

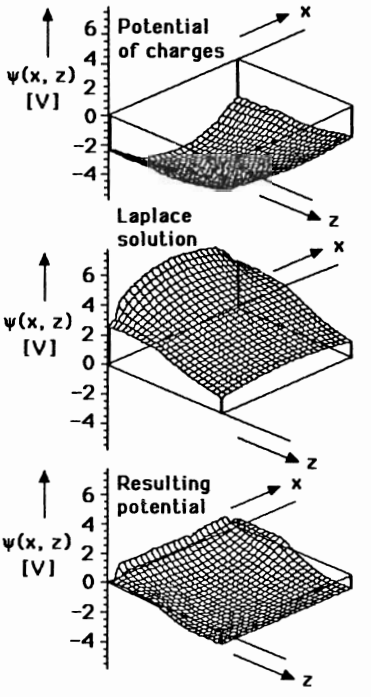

Fig. 3

3.3 Carrier Dynamics

The carrier motion is described by the classical *Newtonian law of motion,* using the reciprocal effective mass tensor. The force acting to carriers is proportional to the electric field, which consists of two parts. One of them can be analytically calculated from the positions of point charges, and the second one is derived from the potential distribution calculated by the Laplace solver. The first integral the of motion equation yields the *velocity,* and the second one the *position vector* of carrier[7]. This method enables exact simulation of carrier trajectories and thus the exact evaluation of all Coulomb scattering processes.

3.4 Scattering processes

Our approach for the field and potential calculation results in the exact simulation of all *Coulomb scattering* (ionized impurity scattering, scattering on charged interface states and carrier-carrier scattering)[8]. For the *intervalley scattering* of the electrons a *thermodynamic approach* is applied: an electron corresponds to that ellipsoid, where it has minimal energy. For *surface scattering* the *Coulomb*

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7 Applying a time increment Δt small enough to assume a constant force during this time, the integrations can be carried out by first order numerical quadrature formulae. Since the field is a strongly varying function of the position, using low order formula with small time step Δt yields better accuracy, than a higher order one with a larger time step.

8 An *empirical factor* (the only one in the program) must be used in the postprocessing phase to make a decision that the change of the direction of the particle movement is large enough to consider this as a Coulomb scattering or not.

scattering on charged interface states, further the *elastic* and *specular surface scattering*[9] are taken into consideration.

4. Results

In each time instant the circumstances in the structure (see Fig. 1) seem to be chaotic, there-fore *time averaging* is needed to get the stationary values of the currents, current densities, concentrations, etc. Fig. 4 shows (a) the current distribution along the x-axis vs. time, (b) the time average vs. x, and (c) the current distribution function. Special *postprocessor programs* must be used to evaluate results (to transform the results into the terms of classical semiconductor physics)[10] [5]. Table 1. compares the MicroMOS and MINIMOS mobility results.

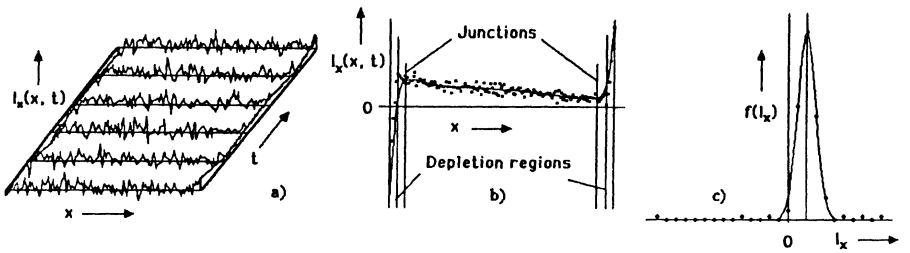

Fig. 4

Table 1.

Scattering type	Scattering rate [ps^{-1}]	Mobility [m^2/Vs] MicroMOS	MINIMOS
Lattice scattering	0.368	1.489	
Intervalley scattering	0.543	0.902	
Impurity scattering	1.665	0.329	
Electron - electron scattering	7.150	0.077	
Electron - hole scattering	0.223	2.461	
Interface state scattering	0.481	1.140	
Elastic surface scattering	0.332	1.648	
Specular surface scattering	0.407	1.348	
Resulting mobility		0.048	0.034

References

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9 The ratio of the elastic and specular surface scattering are determined by the *Fuchs parameter* [4] and by random numbers.

10 For the estimation of the *drain current* components and their *RMS noise*; regression analysis of the *number of carriers, electrons entering to drain, the average time spent in the active region*, etc.; *distribution of electrons* over different ellipsoids; the *electron temperature* vs. time spent in the structure, or vs. x ; *statistics of scattering rates*; estimation of *mobility components*, etc.