SIMULATION OF SEMICONDUCTOR DEVICES AND PROCESSES Vol. 3
Edited by G. Baccarani, M. Rudan - Bologna (Italy) September 26-28, 1988 - Tecnoprint

A New Coupling Scheme for a Self-consistent Poisson and Monte Carlo Device Simulator

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This paper describes a new and efficient coupling scheme between Poisson equation and Monte Carlo transport, embodied in a self-consistent device simulator suitable for general silicon structures. The simulator has been used to characterize non-equilibrium transport in deep submicron nMOSFETs where substantial effects are noticeable at room temperature.

Recent experimental work on silicon MOSFETs [1,2] indicates that non-equilibrium transport effects, not described by the conventional drift-diffusion (DD) model, become important in determining the intrinsic characteristics of very small devices. The Monte Carlo (MC) technique, first applied to the charge transport in semiconductors by Kurosawa [3], represents an alternative description of current transport that overcomes this problem and has consequently attracted a lot of attention in the last few years.

The major drawback of the MC approach comes from the intensive computational requirements that become particularly severe if the carrier distributions obtained from the MC calculations are to be made self-consistent with the electrostatic potential, given by Poisson equation, by means of an iterative procedure.

When a significant fraction of the electron population is under non-equilibrium conditions, the MC carrier distributions must be computed self-consistenly with the electrostatic potential as demonstrated in fig.1 which shows a comparison between the MOSFET surface densities given by the DD model, non self-consistent and self-consistent MC, respectively. As can be seen, the DD model predicts a much higher carrier concentration at the surface because electron heating is neglected. Furthermore, the MC concentrations obtained using the DD potential (i.e. in a non self-consistent manner) are significantly different from the self-consistent solution. Thus, non self-consistent approaches [4], though much simpler and faster than complete solutions, can only be used when most of the electron population is reasonably well described by the DD model.

In this work we describe an efficient scheme to couple MC and Poisson calculations in order to obtain self-consistent solutions. Our approach starts from an initial guess generated by a DD simulator and iteratively solves the transport equation (by MC) and Poisson equation until convergence is reached. A flowchart illustrating this procedure -the well known Gummel method- is shown in fig.2. The standard way to implement this scheme is that of substituting the updated MC carrier density n_{MC} in the Poisson equation,

$$\nabla \cdot (\epsilon \nabla \psi) = \rho = q(p - n_{MC} + N_{DA}) \tag{1}$$

where N_{DA} is the net doping concentration, ϵ the dielectric permittivity, and p the hole concentration, neglected in the region of interest. Unfortunately, this simple scheme cannot be applied to cases with high carrier concentrations (as a silicon MOSFET) because the unavoidable noise inherent to the MC solutions inhibits the stability of the algorithm. One way to overcome this problem is that of solving Poisson equation at a frequency higher than the electron plasma frequency [5] -i.e. $\approx (1fs)^{-1}$- but, though reasonably safe, such a method implies extremely large computation time. The

alternative solution of this work is to use, as output of the MC, the electron quasi-fermi level ϕ_n defined as

$$\phi_n(\vec{x}) = \psi(\vec{x}) - k_B T_L ln \frac{n_{MC}(\vec{x})}{n_i} \tag{2}$$

where T_L is the lattice temperature, k_B the Boltzmann constant, n_i the intrinsic concentration and $\vec{x}$ denotes the dependence on position. In terms of ϕ_n the electron concentration n can be written as

$$n(\vec{x}) = n_i exp\left[\frac{\psi(\vec{x}) - \phi_n(\vec{x})}{k_B T_L}\right] \tag{3}$$

and Poisson equation becomes non linear in ψ while ϕ_n is kept fixed. This scheme guarantees stability because even large variations in the MC carrier densities lead to very small variations in the potential. In particular the regions where the electrons are cold (MOSFET source and drain) reach convergence in very few iteration steps. As for the channel the convergence rate of a high energy point is examined in fig.3 where the x and y axes represent the potential and the quasi-fermi level which define the status of a grid node. Each vertical line corresponds to a Poisson solution -where the potential is changed and the quasi-fermi level is kept fixed- while each horizontal line represents a MC solution. The staircase-like behavior of the point electrical parameters (ψ and ϕ_n) requires a large number of iterations to reach convergence because the actual solution is far from the initial guess (i.e, the DD solution). Thus the coupling with nonlinear Poisson equation guarantees stability but features slow convergence in the regions where the electrons are hot.

To increase the convergence rate, we introduce the electron temperature T_e instead of that of the lattice in eq.(3) so that the greater is T_e, the larger becomes the change in potential allowed by the Poisson solver. Starting from the average electron energy E_{av} given by the MC calculation, the electron temperature T_e is computed as

$$E_{av}(\vec{x}) = \frac{3}{2}\frac{k_B T_e(\vec{x})}{q} \tag{4}$$

Therefore eqs.(2) and (3) become

$$\phi_n(\vec{x}) = \psi(\vec{x}) - k_B T_e(\vec{x}) ln \frac{n_{MC}(\vec{x})}{n_i} \tag{5}$$

and

$$n(\vec{x}) = n_i exp\left[\frac{\psi(\vec{x}) - \phi_n(\vec{x})}{k_B T_e(\vec{x})}\right] \tag{6}$$

Because $T_e \approx T_L$ for the points inside the source and drain regions, the stability of the solution is guaranteed, while the convergence rate is much faster in the other parts of the device. In fig.4 the covergence rate given by the pure nonlinear coupling scheme and that making use of the electronic temperature are compared. The new scheme -where a Poisson solution is represented by a diagonal line because the quasi-fermi level has been computed using T_L- is more than four times faster, while yielding the same solution.

Considering, as an example, the case of a quarter micron MOSFET, the L-2 norm of the relative error in the electrostatic potential as a function of the number of self-consistent iterations is shown in fig.5. The error first decreases rapidly but eventually is limited by the statistical noise of the MC procedure. Within the accuracy of the MC calculations, we find that a reasonable stopping criteria is about 0.5 mV in this norm. For the examples we have tried, this tolerance is achieved after about 10 iterations.

A simulator embodying the above concept has been used to analyze deep submicron MOS devices at $T = 300K$ and gate lengths varying from 0.15-0.75 μm. Consistent with recent experimental reports, non equilibrium effects do not seem to be observable in the computed g_m down to $L_{gate} \approx 0.25\mu m$; at $0.15\mu m$ the MC g_m is two times the DD result. As an example, fig.6 shows the average electron velocities in the channel for the 0.15 μm device computed using MC and DD. The device exhibits MC velocities in excess of that predicted by DD throughout the entire channel. In particular the different velocities at the source end of the FET cause the difference in g_m because of enhanced current injection. For the $0.25\mu m$ device, on the other hand, the MC and DD velocities differ for most of the channel but are nearly identical at the source end, leading to the same g_m. The above results indicate the need for a self-consistent, non-equilibrium treatment of carrier transport for deep submicron MOSFETs ($L_{gate} \leq 0.25\mu m$).

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[2] M. C. Jeng, *et al.*, IEDM Tech. Dig., p.710, 1987.

[3] T. Kurosawa, J. Phys. Soc. Jpn., Suppl.21, pp.424-426, 1966.

[4] E. Sangiorgi, *et al.*, IEEE Trans. on CAD, vol. CAD-7, pp.259-271, 1988.

[5] S. E. Laux and M. V. Fischetti, Second Workshop on Numerical Modeling of Processes and Devices for Integrated Circuits- NUPAD II, San Diego, Ca., May 1988.

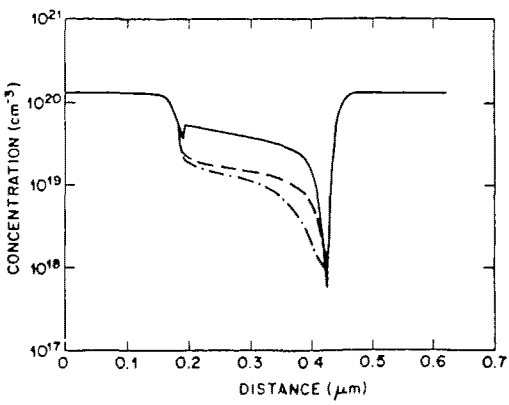

Fig.1 Electron surface concentration for a MOSFET with a gate mask length $L_{gate} = 0.25\mu m$ at $V_{GS} = 1.5V$, $V_{DS} = 2.0V$ in the DD (solid), non self-consistent MC (dashed-dotted) and self-consistent MC (dashed) case.

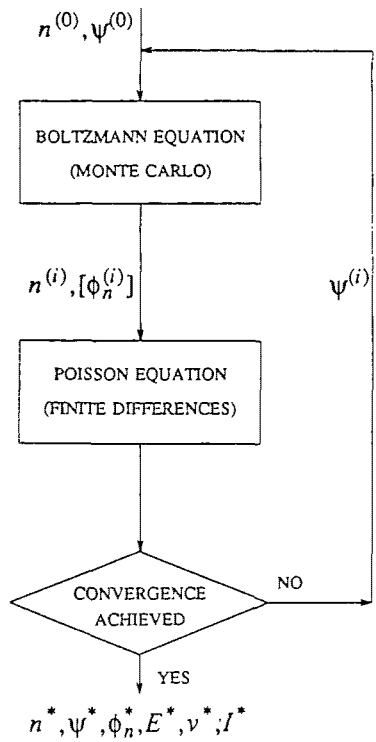

Fig.2 Flow chart of the Monte Carlo program.

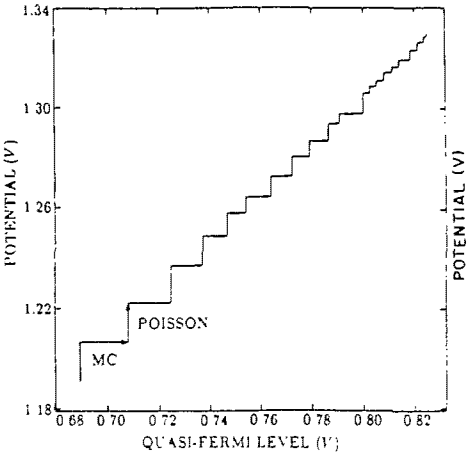

Fig.3 Non linear Poisson coupling: convergence rate of a point in the channel where the electrons are hot.

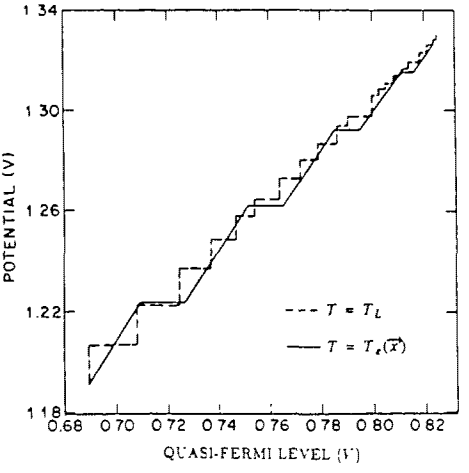

Fig.4 Converge rates of the point in fig.3 when using the lattice temperature T_L (dashed line) or the electronic temperature T_e (solid line) in the non linear Poisson equation.

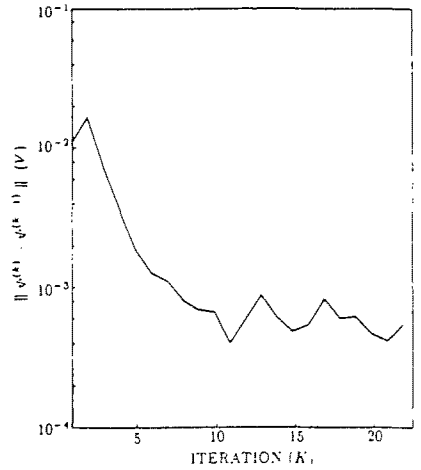

Fig.5 The L-2 norm of the relative error in the electrostatic potential as a function of the number of iterations.

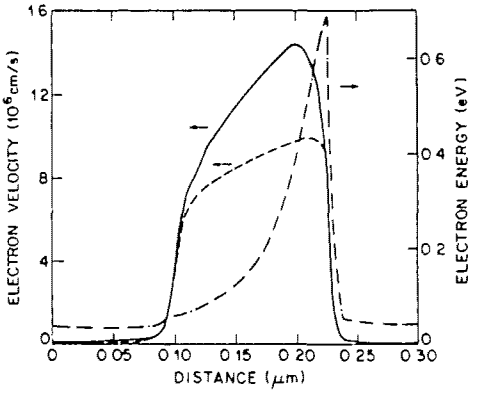

Fig.6 Average electron velocity in the MC (solid) and DD (dashed) case and surface electron energy in the MC solution (dashed-dotted) for $L_{gate} = 0.15\mu m$, $V_{GS} = 1.5V$, $V_{DS} = 2.0V$.