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A Hydrodynamic Model for Transport in Semiconductors without Free Parameters

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We derive, using the Entropy Maximum Principle, an expression for the distribution function of carriers as a function of a set of macroscopic quantities (density, velocity, energy, deviatoric stress, energy flux). Given the distribution function, we obtain, for these macroscopic quantities, a hydrodynamic model in which all the constitutive functions (fluxes and collisional productions) are explicitely computed starting from their kinetic expressions. We have applied our model to the simulation of some one-dimensional submicron devices in a temperature range of 77–300 K, obtaining results comparable with Monte Carlo. Computation times are of order of few seconds for a picosecond of simulation.

Keywords: Entropy maximum principle, electron transport, submicron devices

1. INTRODUCTION

Modeling of modern semiconductor devices is currently performed by means of two distinct approaches, kinetic models and Fluid Dynamic (FD) models. The most accurate kinetic description is given by Monte Carlo methods, which can take into account explicitely both the band structure and the various scattering phenomena [1, 2]. Other kinetic approaches are based on the choice of particular forms of the non-equilibrium distribution function of carriers. Common examples are the simple shifted Maxwellian [3] or an expansion of the distribution in spherical harmonics [4]. The cylindrical symmetry constraint in momentum space and the reduced number of terms of the expansion that can be practically used do not permit, however, to describe transport properties of carriers in conditions very far from equilibrium [5]. The FD models are obtained considering a set of moments of the Boltzmann Transport Equation (BTE). These models need the knowledge of *constitutive functions* (fluxes and collisional productions) present in the hierarchy of equations, that are usually fixed on a phenomenological basis, introducing parameters, such as e.g. relaxation times and transport coefficients, which have an unknown dependence on the geometry and working conditions of the simulated devices. The presence of these *free parameters* [6] has always been

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a limit to a practical use of FD models, because, in general, they are determined in each case on the basis of MC simulations or experimental data.

We have developed a HydroDynamic (HD) model for the simulation of transport phenomena in semiconductors, based on the Entropy Maximum Principle (EMP). Following this principle, we find the distribution that makes best use of the 'information' deriving from the knowledge of a given set of moments. This distribution turns out to be a strongly non-linear function of the moments. Given the distribution, we determine the unknown constitutive functions appearing in the hierarchy of the equations that describes the time evolution of the moments. We point out that the computation of collisional productions is then based on the sole knowledge of the scattering kernels and the physical quantities they contain. Our HD model is then fully closed, and, contrarily to other HD models, does not contain any *free parameter*. On the other hand, the distribution function we obtain has no particular symmetry restrictions and is fully suitable for three-dimensional models. Its strong non-linearity is also capable of describing transport phenomena even in conditions far from thermodynamic equilibrium, as those present in submicron devices with very high electric fields and field gradients ($E \simeq 10^5$ V/cm, $E/(dE/dx) \simeq 100$Å).

2. PHYSICAL CHARACTERISTICS OF THE MODEL

We consider here a HD model for transport phenomena in silicon. Our main purpose in the development of this model, has been to test how accurately our distribution function describes strong non-equilibrium conditions. Therefore we have used a simplified band structure. As is well known, electrons contributing to transport are mainly those belonging to the six equivalent X valleys which, up to an energy of about 0.5 eV, can be considered approximately parabolic. Electrons can then be described by a density of states effective mass $m^* = 0.32\, m_e$. In the same energy range, the main scattering phenomena are due to electron-phonon interactions, and we will consider intervalley transitions caused both by f type and g type phonons; for intravalley transitions we will consider scattering with acoustic phonons, which will be regarded as approximately elastic. For the evaluation of the scattering terms we have used the parameters reported in [2]. We will show (by a comparison with MC simulations performed under the same physical approximations) that in this way it is possible to describe accurately some simple Si devices even in conditions very far from thermodynamic equilibrium. An extension of the model toward a non parabolic band structure (for Si or other semiconductors) and the inclusion of further scattering terms (ionized impurities, polar optical phonons, ...) do not present, however, conceptual difficulties, and they are at present in development.

3. MAXIMIZATION OF ENTROPY

Let f be the the distribution function of electrons in phase space. The entropy density is defined by

$$h = -C \int f \log(f)\, d\vec{k}, \tag{1}$$

where C is a constant. Given a set of kinetic quantities $\psi_A(\vec{k})$, we can calculate the corresponding moments F_A of the f by means of

$$F_A = \int \psi_A(\vec{k}) f\, d\vec{k}. \tag{2}$$

We search the distribution f that maximizes the entropy density (1), under the constraints given by the relations (2). For this problem we have considered the set of kinetic quantities [7]:

$$\psi_A(\vec{k}) = \left\{ 1, \frac{\hbar}{m^*} k_i, \frac{\hbar^2}{2m^*} k^2, \frac{\hbar^2}{m^*} k_{\langle i} k_{j\rangle}, \frac{\hbar^3}{2(m^*)^2} k^2 k_i \right\}$$

and the corresponding moments: density of carriers (n), flux of carriers (nv_i), total energy density (W), traceless part of momentum flux density ($\Sigma_{\langle ij\rangle}$), energy flux density ($S_i$), being

$$W = \tfrac{3}{2}p + \tfrac{1}{2}nm^*v^2,$$
$$\Sigma_{\langle ij\rangle} = \sigma_{\langle ij\rangle} + nm^*v_{\langle i}v_{j\rangle},$$
$$S_i = q_i + \sigma_{\langle ij\rangle}v_j + \tfrac{5}{2}pv_i + \tfrac{1}{2}nm^*v^2v_i$$

where v_i is the mean velocity, $p = nK_BT$ is the pressure, $\sigma_{\langle ij\rangle}$ is the non convective part of tensor $\Sigma_{\langle ij\rangle}$ and q_i is the heat flux. Application of the EMP requires then the maximization of the functional

$$h' = h - \sum_{A=1}^{13}\lambda_A\left[\int \psi_A(\vec{k})f\,d\vec{k} - F_A\right],$$

where λ_A's are Lagrange multipliers. The resulting distribution will have the functional form:

$$f = \exp(-\Pi), \qquad \Pi = \sum_A \psi_A(\vec{k})\lambda_A. \qquad (3)$$

From (2) we have that $F_A = F_A(\lambda_B)$, and so, to determine f, we must invert (2) obtaining $\lambda_A = \lambda_A(F_B)$. This inversion is extremely difficult and can be obtained only by numerical integration or by a series expansion of f [8]. We have followed the latter approach, expanding f to third order in $\tilde{F}_A = \{v, \sigma, q\}$ around an equilibrium configuration defined by a local Maxwellian f_M. Introducing this expression into (2) all the quadratures can be done analitically, and the resulting relations can be inverted. In this way we express f as

$$f(\vec{r}, t, \vec{k}) \equiv f(\tilde{F}_A(\vec{r}, t), \vec{k}),$$

which is a strongly non-linear function of $\tilde{F}_A$.

4. THE HYDRODYNAMIC MODEL

The model resulting from the procedure described in the previous section is fully three-dimensional, but we show here one-dimensional results. The only independent variables are in this case $F_A = \{n, nv_x = nv, W, \Sigma_{\langle xx\rangle} = \Sigma, S_x = S\}$, satisfying the following balance equations

$$\frac{\partial n}{\partial t} + \frac{\partial nv}{\partial x} = 0,$$

$$\frac{\partial nv}{\partial t} + \frac{1}{m^*}\frac{\partial(\Sigma + (2/3)W)}{\partial x} = -\frac{neE}{m^*} + P_{nv},$$

$$\frac{\partial W}{\partial t} + \frac{\partial S}{\partial x} = -nveE + P_w,$$

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial\left(\frac{2}{3}nm^*v^3 + \frac{4}{3}pv + \frac{7}{3}\sigma v + \frac{8}{15}q + G_\Sigma\right)}{\partial x} = -\tfrac{4}{3}nveE + P_\Sigma,$$

$$\frac{\partial S}{\partial t} + \frac{\partial\left(\frac{1}{2}nm^*v^4 + \frac{16}{5}qv + 4pv^2 + \frac{5}{2}\sigma v^2 + G_s\right)}{\partial x} = -eE\left(\tfrac{3}{2}nv^2 + \tfrac{5}{2}\frac{p}{m^*} + \frac{\sigma}{m^*}\right) + P_s,$$

where $E_x = E$ is the electric field, $G_A = \{G_\Sigma, G_S\}$ are terms of the fluxes dependendig on higher order moments and $P_A = \{P_{nv}, P_W, P_\Sigma, P_S\}$ are the collisional productions. Such unknown constitutive functions have been determined by integration of their kinetic expression using the distribution function given by the EMP. The fluxes and the collisional productions are very complex functions of $\tilde{F}_A$ which we do not show here.

5. DEVICE SIMULATIONS

As test case, we have considered four unipolar and one-dimensional devices n^+nn^+ (labelled A, B, C, D) at different temperatures, doping and applied biases, as summarized in Table I. All the results are compared with a MC model using the same physical approximations.

In Figure (1) we report the results of a series of simulations for device A. We see that for devices with such high fields and field gradients a strongly

TABLE I Devices parameters

Dev.	Temp. (K)	Bias (V)	$N^+(cm^{-3})$	N (cm^{-3})	Chan. (μm)
A	300	2	10^{19}	10^{17}	0.25
B	150	1	10^{18}	10^{16}	0.25
C	77	1	10^{17}	10^{15}	0.45
D	300	1	10^{18}	10^{16}	0.3

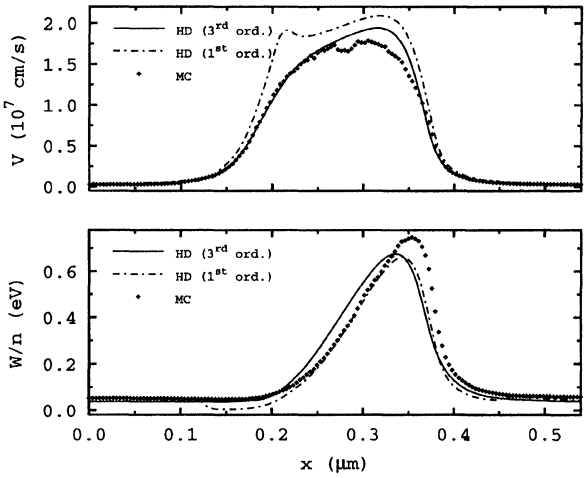

FIGURE 1 Velocity and total energy as a function of position for device A. We show a comparison with MC data and results for the HD model with production terms computed at different orders of the expansion. Differences in the values of energy in the highly doped regions are due to the correlation energy of electrons, included in MC model.

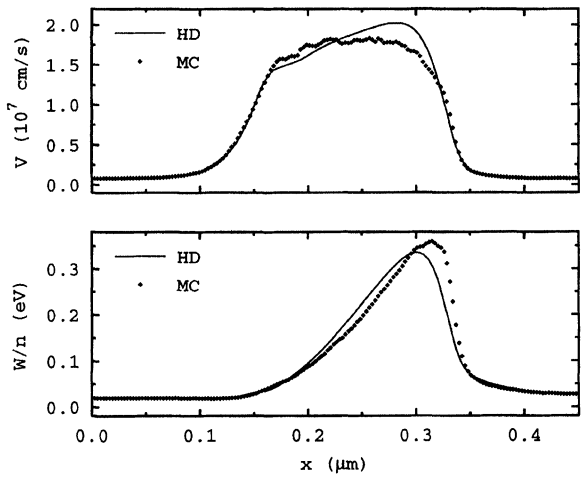

FIGURE 2 Velocity and total energy for device B. Results from a MC simulation and the HD model.

non linear description is necessary to obtain a good agreement with MC simulations. In Figures (2), (3) we report two examples of computations at lower temperatures (with production term evaluated at third order). Note that MC data for the 77 K simulation show evident oscillations on both velocity and energy. This phenomenon is probably due to single-phonon interactions, and is partially reproduced by our model. Note also the ballist pick, characteristic of low-temperature devices. Figure (4) shows velocity, energy, traceless stress and heat flux for device D. Current densities for devices A, B, C and electric fields for devices A, B, D are shown in Figures (5), (6). Computation times for the present results have been in a range of $1 \div 10$ sec for a ps of simulation.

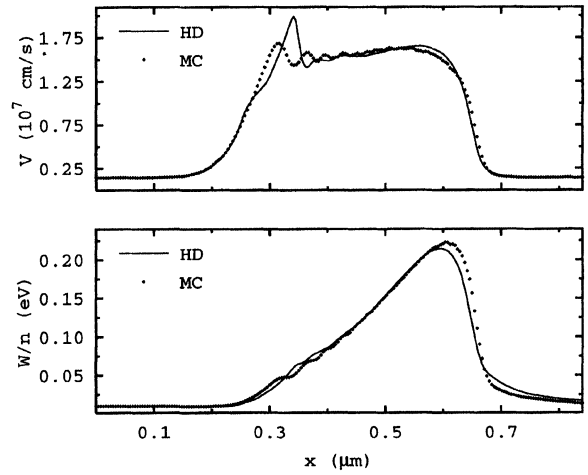

FIGURE 3 Velocity and total energy for device C. Results from a MC simulation and the HD model.

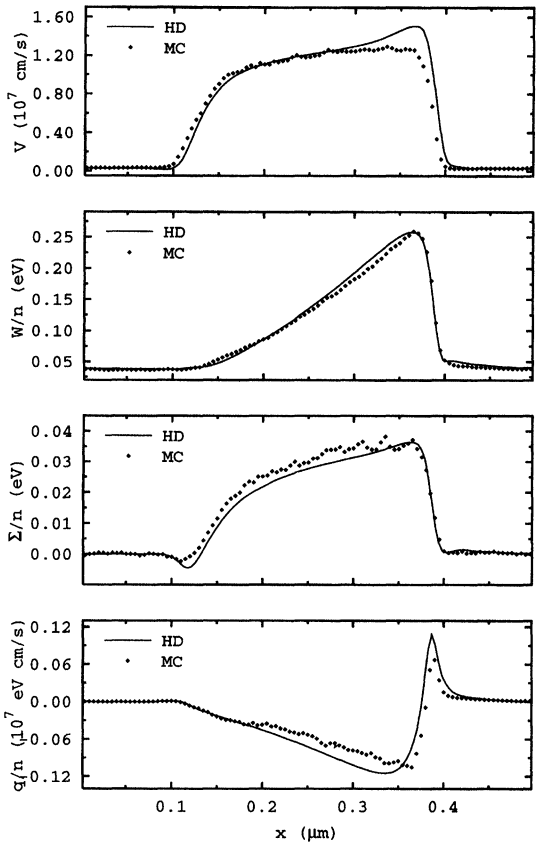

FIGURE 4 Velocity, total energy, traceless stress and heat flux for device D from a MC simulation and the HD model.

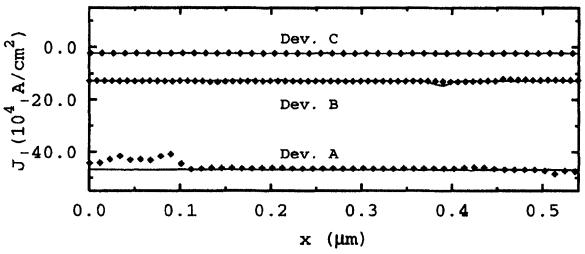

FIGURE 5 Current densities J for devices A, B and C, from MC (points) and HD (lines).

6. CONCLUSIONS

We have shown that the EMP allows to create a closed HD model to describe transport phenomena in Si in strong non-equilibrium conditions. We point out that an effective use of the EMP depends both on the choice of a set of 'constraints' (moments of the distribution function) and on the determination of a set of evolution equations for these 'constraints' that takes explicitely into account the underlying physical processes (the various scattering phenomena, in this case).

A better model of transport in semiconductors will require a more accurate description of band structure and the inclusion of further scattering terms. These extensions are now in development.

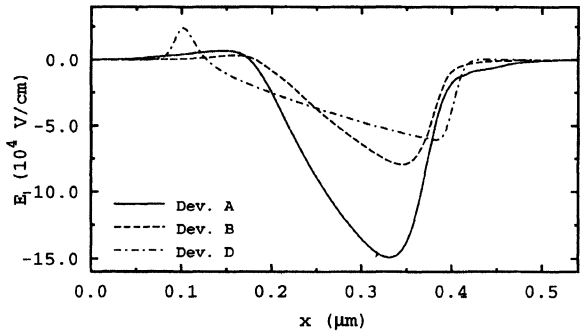

FIGURE 6 Electric fields for devices A, B and D, from the HD model.

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[7] Here and in the following symbol $A_{\langle ij \rangle}$ denotes the traceless part of a symmetric tensor A, i.e. $A_{\langle ij \rangle} = A_{ij} - (1/3)\delta_{ij}\mathrm{Tr}(A)$.
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Authors' Biographies

Paolo Falsaperla graduated in Physics in 1992 at University of Catania, Italy. He has worked on mathematical methods for atomic structures in high magnetic fields. His current interests include Monte Carlo simulation of noise and hydrodynamic models for semiconductor devices.

Massimo Trovato graduated in Physics in 1993 at University of Catania, Italy. He is currently working toward the Ph.D. degree in Physics at University of Catania. He has worked on the application of the Entropy Maximum Principle to transport problems. His current research interest is in the modeling and simulation of hot-carrier effects in submicrometer devices.