Hydrodynamic model for hot carriers in silicon based on the maximum entropy formalism

M. Trovato[a], P. Falsaperla[b]

[a]Dipartimento di Matematica, Università di Catania
Viale A. Doria 6, I-95125 Catania, Italy
[b]Dipartimento di Fisica, Università di Catania
Corso Italia 57, I-95129 Catania, Italy

Abstract

We describe the transport properties of hot electrons in silicon through a completely closed hydrodynamic (HD) model, without any free parameter. We apply our model to the simulation of some n^+nn^+ devices at temperatures of 300K and 77K. Results are very accurate and the computation times are of few seconds for a picosecond of simulation.

1. Introduction

In this paper starting from the maximum entropy principle (MEP) [1, 2] we obtain an analytic expression for the nonequilibrium distribution function of carriers in silicon, determining the microstate corresponding to the given macroscopic data. We solve then the variational problem of maximizing the entropy of the system under the constraints corresponding to the value of some mean quantities F_A (density n, velocity v_i, energy W, traceless part of momentum flux $\Sigma_{\langle ij \rangle}$, energy flux S_i) which define the macroscopic status. Given the distribution function and considering the collisional interactions of carriers with phonons of the acoustic and optical branches, we can determine a hierarchy of evolution equations for the F_A. In this hydrodynamic model all the constitutive functions appearing in the fluxes and collisional productions are explicitly calculated [3, 4], thus including the *kinetic details of the collisional interactions* in the evolution equations for the constraints.

2. The hydrodynamic 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

Device	Temp. (K)	N^+ (cm^{-3})	N (cm^{-3})	chan. (μm)	x_s (μm)	bias (V)
A	300	10^{19}	10^{17}	~ 0.3	0.01 - 0.06	1 - 2
B	77	10^{17}	10^{15}	~ 0.4	0.06	1

Table 1: Devices parameters.

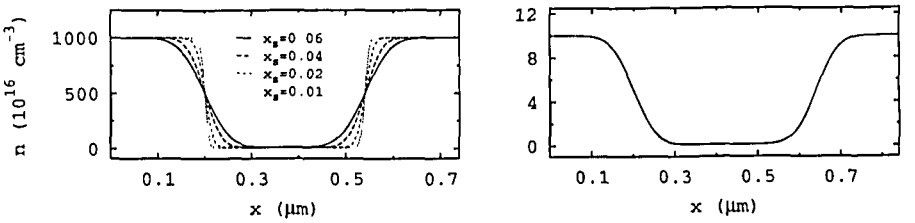

Figure 1: Doping profiles of devices A and of device B. The profiles are smoothed at the junction points by an erfc function [4] scaled by the parameter x_s.

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. In the same energy range, the main scattering phenomena are due to electron-phonon interactions, which produce intervalley and intravalley transitions [5]. We will consider intervalley transitions caused both by f type and g type phonons. We can pass from the Boltzmann Transport Equation (BTE) to the hydrodynamic equations of the first thirteen moments considering the following *kinetic quantities* $\psi_A(\vec{k}) = \{1,\ \hbar k_i/m^*,\ \hbar^2k^2/2m^*,\ \hbar^2k_{<i}k_{j>}/m^*,\ \hbar^3k^2k_i/2(m^*)^2\}$. Multiplying the BTE by $\psi_A(\vec{k})$ and integrating in $\vec{k}$ space we obtain the balance equations for the *moments of the distribution function* F_A. The generic balance equation is

$$\frac{\partial F_A}{\partial t} + \frac{\partial F_{Ak}}{\partial x_k} = R_A + P_A + \tilde{P}_A. \tag{1}$$

Where R_A denotes the production term due to the electric field,

$$F_A = \int \psi_A(\vec{k})\,\mathcal{F}(\vec{k},\vec{r},t)\,d\vec{k}, \quad F_{Ak} = \frac{\hbar}{m^*}\int \psi_A(\vec{k})\,k_k\mathcal{F}(\vec{k},\vec{r},t)\,d\vec{k}$$
$$P_A = \sum_\eta \int \psi_A(\vec{k})\,Q_\eta(\mathcal{F})\,d\vec{k} \quad , \quad \tilde{P}_A = \int \psi_A(\vec{k})\,Q_{ac}(\mathcal{F})\,d\vec{k}.$$

F_{Ak} denotes the fluxes and $\{P_A,\ \tilde{P}_A\}$ are the collisional productions associated with the intervalley and intravalley transitions. The production terms Q_η and Q_{ac} are function of the respective scattering probabilities S_η and S_{ac} [5] and can be expressed through the general relation

$$Q(\mathcal{F}) = \frac{V}{(2\pi)^3}\left\{\int d\vec{k}'\,S(\vec{k}',\vec{k})\,\mathcal{F}(\vec{k}',\vec{r},t) - \int d\vec{k}'\,S(\vec{k},\vec{k}')\,\mathcal{F}(\vec{k},\vec{r},t)\right\}$$

The set of balance equations (1) contains several unknown functions, i.e. the fluxes of the equations for $\Sigma_{<ij>}$ and S_i, and the collisional productions $\{P_A,\ \tilde{P}_A\}$. The system can then be *closed* if the unknown constitutive functions $H_A = \{P_A,\ \tilde{P}_A,\ F_{Ak}\}$ can be expressed by means of the fields F_A. We have solved this problem expanding the distribution function around the local equilibrium configuration and applying the MEP[4] [1].

[1] All the unknown constitutive functions of our model are explicitely reported in [4], where the collisional productions P_A are expressed by means of a set of functions $H_i^{\pm}$. Due to a transcription

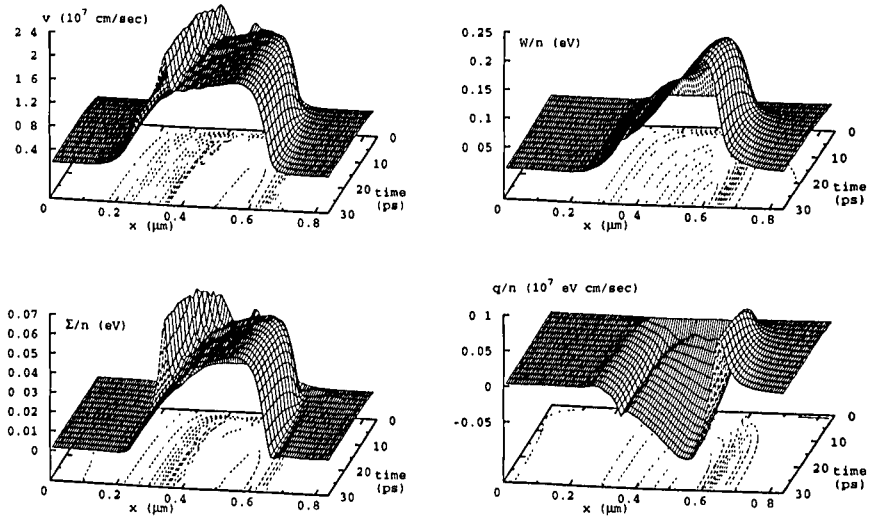

Figure 2: Quantities v, W, Σ (as defined in text) and heat flux q (see [4]) as functions of position and time in device B.

The analytical closure so obtained has been applied to the case of some n^+nn^+ submicron devices (see Table), with results comparable to MC simulations performed under the same physical approximation of our HD model. The HD simulations of devices A show an overshoot velocity pick around the second junction, which depends strongly on the electric field gradient. Differences between HD and MC data in the values of energy in the highly doped regions of devices A are due to the correlation energy of electrons, included in MC model. Note, in the 77K simulation, the ballistic pick of velocity after the first junction, and the oscillations of velocity and energy in the MC data, partially reproduced by the HD model. Computation times are of order of few seconds for a picosecond of simulation on a workstation.

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error, part of the definition of the $H_i^{\pm}$, appearing in [4] at the end of Section IV, is incorrect and should read instead:

$$H_1^{\pm} = \exp(\mp X_\eta) K_1(X_\eta), \qquad H_3^{\pm} = \pm X_\eta H_1^{\pm} + G^{\pm},$$

$$H_{2i+1}^{\pm} = \pm 2\, X_\eta H_{2i-1}^{\pm} \pm (i+1)! \left[\sum_{n=1}^{i-2} \frac{3\, X_\eta H_{2n+1}^{\pm}}{(n+3)!} \pm \frac{G^{\pm}}{2} \right], \qquad i = 2, \ldots, 6.$$

The correctness of functions $H^{\pm}$ is of fundamental importance to perform simulations based on our model.

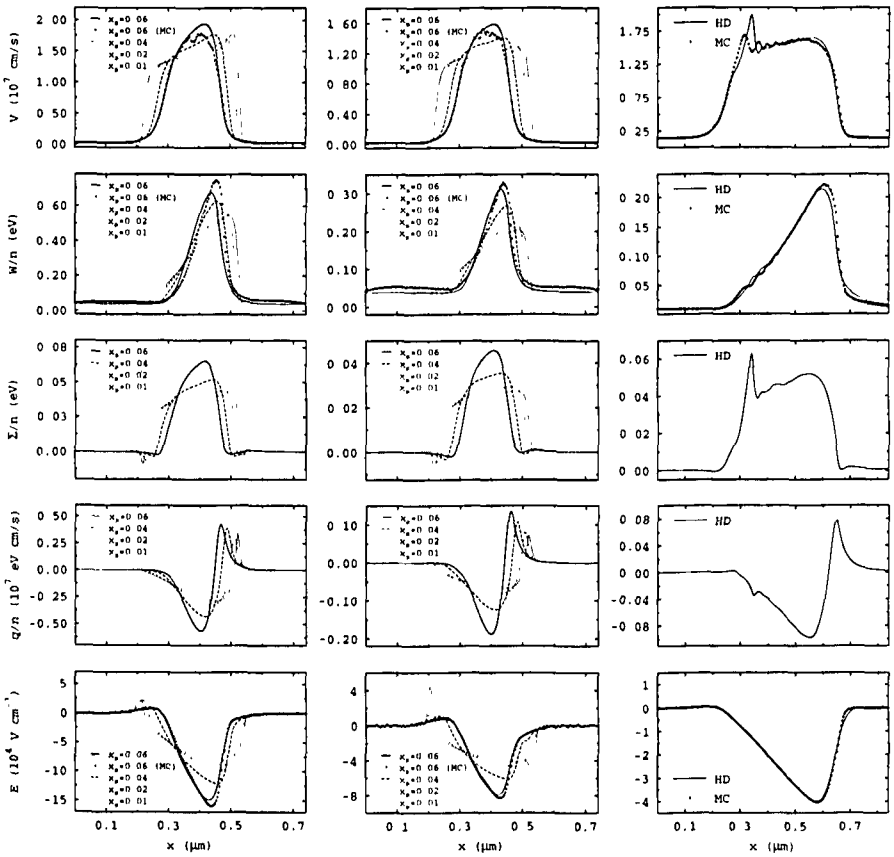

Figure 3: Value of quantities v, W, Σ, q and electric field E as function of position for devices A (with bias of 2V and 1V respectively in the first and second column) and B. Points are MC data, lines are from the present HD model.

References

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