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RAMADA HOTEL - GIARDINI NAXOS (MESSINA)

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A new hydrodynamic model for hot carriers in silicon based on the maximum entropy principle

Un nuovo modello idrodinamico per i portatori caldi nel silicio basato sul principio di massima entropia

Paolo Falsaperla
Dipartimento di Fisica, Universitá di Catania
Corso Italia 57, 95129 Catania, Italy
Falsaperla@ct.infn.it

Massimo Trovato
Dipartimento di Matematica, Universitá di Catania
viale A. Doria 6, 95125 Catania, Italy
Trovato@dipmat.unict.it

In the recent years the Boltzmann transport equation (BTE) has become a useful tool to model different problems in the field of many-body systems. The knowledge, in the phase space, of the evolution of the distribution function, as a solution of BTE, provides all the necessary information to describe the nonequilibrium properties of the physical systems considered. In the case of highly nonlinear processes, that lead the physical system very far from equilibrium, the determination of an analytical solution for the BTE (non considering drastic and reductive approximations), has proved to be still an unsolved mathematical problem. Its resolution has urged the search for various numerical approaches capable of adequately describing these physical features. These methods have turned out to be particularly suitable for the analysis of transport properties of hot electrons in submicrometric devices when the active regions are very small and the fields and electric gradients applied ($E \approx 10^5$ V/cm, $|E|/|\vec{\nabla} E| \approx 100$ Å) are very large.

In this paper we describe the transport properties of hot electrons in silicon, through a completely closed hydrodynamic model, without any free parameter. Starting from the maximum entropy principle (MEP) we obtain an analytic expression for the nonequilibrium distribution function of carriers, determining the microstate corresponding to the given macroscopic data. In this case the microscopic status is obtained from the solution of the variational problem of maximizing the entropy of the system under the constraints corresponding to the value of some mean quantities (density n, velocity v_i, energy density W, traceless momentum flux density $\Sigma_{\langle ij \rangle}$, energy flux density 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 hydrodynamic model for the mean quantities used as constraints, in which all the constitutive functions appearing in the fluxes and collisional productions are explicitly calculated [1-2]. We note here that, unlike of this model, hydrodynamic simulations have always suffered from questionable assumptions, such as relaxation times and 'ad hoc' expressions for the transport coefficients. Moreover, these expressions contain free parameters (which have an unknown dependence on the geometry and working conditions of the devices) that are usually fixed on the basis of Monte Carlo (MC) simulations or experimental data. The MEP has been successfully used in a large number

of missing-information problems in diverse fields [3-5] but, despite this success, has caused widespread controversy, mainly focused on the choice of the constraints and on their effective use in the characterization of dynamic systems [6]. In fact, the mere determination of the distribution function of maximum entropy does not allow us to obtain any information on the dynamical evolution of a system, nor such information can be introduced as further constraint conditions. In this paper we obtain a dynamical description of the system by determining a hierarchy of evolution equations for the macroscopic quantities used as *constraints*. Assuming the set $F_A = \{n, nv_i, W, \Sigma_{(ij)}, S_i\}$ as constraint, being the distribution function known and calculating explicitly the corresponding collisional productions, we can adequately describe the dynamical evolution of the system, thus including the *kinetic details of the collisional interactions* in the evolution equations for the constraints.

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 $m^* = 0.32\, m_e$ and a band energy $\varepsilon(\vec{k}) = \hbar^2 k^2/2m^*$. In the same energy range, the main scattering phenomena are due to electron-phonon interactions, which produce intervalley and intravalley transitions [7]. We will consider intervalley transitions caused both by f type and g type phonons. The scattering probability per unit time for intervalley transitions of an electron from state $\vec{k}$ to state $\vec{k'}$ can be expressed as

$$S_\eta(\vec{k},\vec{k'}) = Z_\eta \frac{\pi \Delta_\eta^2}{V \rho \omega_\eta} \left[\begin{array}{c} N_\eta \\ N_\eta + 1 \end{array} \right] \delta[\varepsilon(\vec{k'}) - \varepsilon(\vec{k}) \mp \hbar\omega_\eta] \,, \tag{1}$$

with $\eta = g_1, g_2, g_3, f_1, f_2, f_3$. Here Z_η is the number of possible final equivalent valleys ($Z_\eta = 1$ for $\eta = g_1, g_2, g_3$ and $Z_\eta = 4$ for $\eta = f_1, f_2, f_3$), Δ_η is the coupling constant, V is the crystal volume, ρ is the Si density, ω_η is the phonon angular frequency, $N_\eta = 1/[\exp(\hbar\omega_\eta/K_B T_0) - 1]$ is the phonon occupation number (with T_0 the lattice temperature), while the upper and the lower option in the expression corresponds to absorption and emission, respectively. For intravalley transitions we will consider scattering with acoustic phonons, which will be regarded as approximately elastic. We can express the sum of the intravalley transitions probabilities as

$$S_{ac}(\vec{k},\vec{k'}) = \frac{2\pi K_B T_0 E_l^2}{V \hbar \rho U_l^2} \delta[\varepsilon(\vec{k'}) - \varepsilon(\vec{k})] \,, \tag{2}$$

being K_B the Boltzmann constant, U_l the longitudinal sound velocity, E_l the deformation potential for longitudinal acoustic phonons. For the values of all the costants appearing in the scattering terms (1),(2) we have used the parameters reported in [7]. We can pass from the BTE to the hydrodynamic equations of the first thirteen moments considering the following *kinetic quantities* $\psi_A(\vec{k}) = \{1,\ \hbar k_i/m^*,\ \hbar^2 k^2/2m^*,\ \hbar^2 k_{<i} k_{j>}/m^*,\ \hbar^3 k^2 k_i/2(m^*)^2\}$. 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

$$\frac{\partial F_A}{\partial t} + \frac{\partial F_{Ak}}{\partial x_k} = R_A + P_A + \tilde{P}_A. \tag{3}$$

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

$$F_A = \int \psi_A(\vec{k})\, \mathcal{F}(\vec{k},\vec{r},t)\, d\vec{k}, \quad F_{Ak} = \frac{\hbar}{m^*} \int \psi_A(\vec{k})\, k_k \mathcal{F}(\vec{k},\vec{r},t)\, d\vec{k} \qquad (4)$$

$$P_A = \sum_\eta \int \psi_A(\vec{k})\, Q_\eta(\mathcal{F})\, d\vec{k} \quad , \quad \tilde{P}_A = \int \psi_A(\vec{k})\, Q_{ac}(\mathcal{F})\, d\vec{k}.$$

F_{Ak} denotes the fluxes and $\{P_A,\ \tilde{P}_A\}$ the collisional productions associated with the intravalley and intervalley transitions, with

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

The set of balance equations (3) 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. This problem can be solved with the help the variational method known as *entropy maximum principle* [8] which allows the determination of the non-equilibrium distribution function of hot carriers and consequently permits to find a closure for the *constitutive functions*. We start from the known expression of entropy density $h = -C \int \mathcal{F} \log(\mathcal{F}) d\vec{k}$ (where C is a constant) assuming that $\mathcal{F}(\vec{k},\vec{r},t)$ depends on $\vec{r}$ and t only through the fields $F_A(\vec{r},t)$ and then we determine the distribution function, of the form $\mathcal{F}(\vec{r},\vec{k},t) = \mathcal{F}[F_A(\vec{r},t),\vec{k}]$ that maximizes h under the constraints that the moments F_A are expressed by the relations $(4)_1$. Following this procedure, we maximize the functional $h' = h - \sum_{A=1}^{13} \Lambda_A \left[\int \psi_A(\vec{k})\, \mathcal{F}(\vec{r},\vec{k},t)\, d\vec{k} - F_A \right]$ imposing $\delta h' = 0$. The quantities Λ_A are the *Lagrange multipliers* associated with the constraint equations $(4)_1$. As is well known, the distribution function obtained with this procedure [9] assumes the following form

$$\mathcal{F} = \exp(-\Sigma), \qquad \Sigma = \sum_{A=1}^{13} \psi_A\, \Lambda_A. \qquad (5)$$

To obtain an explicit expression of $\mathcal{F}$ we have yet to express the multipliers Λ_A as function of the constraints, i.e. the moments F_A. By inserting Eq. (5) into the definition of fields $(4)_1$ we have $F_A = F_A(\Lambda_B)$, and so, to determine $\mathcal{F}$, we must invert this latter relations 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 $\mathcal{F}$ [2,9]. We have followed the latter approach, expanding $\mathcal{F}$ around an equilibrium configuration defined by a local Maxwellian. In this way we can express $\mathcal{F}$ as a strongly non-linear function of F_A. The analytical closure so obtained has been applied to the case of some n^+nn^+ submicron silicon devices, with results comparable to similar MC simulations [1,2,10]. Computation times are of order of few seconds for a picosecond of simulation on a workstation.

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