Hydrodynamic Model for Silicon Carbide Semiconductors including crystal heating

O Muscato and V Di Stefano

Dipartimento di Matematica e Informatica, Università degli Studi di Catania, Viale A. Doria 6, 95125 Catania – Italy

E-mail: muscato@dmi.unict.it, vdistefano@dmi.unict.it

Abstract. A hydrodynamic model describing the electron transport in silicon carbide semiconductors, coupled with the heating of the crystal lattice is presented. It has been obtained by taking the moments of the coupled Boltzmann equations for the electrons and phonons, and by using the Maximum Entropy Principle in order to determine the transport coefficients and the constitutive equations. Simulation results in the bulk case are shown.

1. Introduction

Power semiconductor devices have attracted increasing attention as key components in a variety of power conversion units. Because of the mature technology of Si power devices currently employed in most applications, it is now difficult to achieve innovative breakthroughs in this field. Newly emerging semiconductors such as Silicon Carbide (SiC) are attractive for advanced power devices, owing to their superior physical properties such as their exceptional wide bandgap (three times more than Si), a high thermal conductivity (twice or triple that of Si), and a very high field breakdown (five times more than Si). Although these performances are very promising, SiC devices may suffer from severe self-heating effects which impose a limitation on both the output power and the power density of the devices. Self heating results in a higher lattice temperature in the transistor channel which can significantly deteriorate the current-voltage characteristics because of the reduction in the device parameters such as mobility and electron saturation velocity. For these reasons, electro-thermal simulations are mandatory in order to predict the behaviour of such devices.

If we want to go beyond the drift-diffusion equation scheme, valid in the linear irreversible thermodynamic regime, it is mandatory to explore the microscopic details of self-heating process.

The natural framework to deal with electro-thermal transport is given by a set of Boltzmann-like equations (called Bloch-Boltzmann-Peierls equation, hereafter BBP) which describe, from the kinetic point of view, the transport of electrons and phonons, coupled to the Poisson equation [1]. To solve numerically this system is an hard task, because it forms a set of partial integro-differential equations. One possibility is to develop, for such material, an Electro-thermal Monte Carlo (ETMC) scheme at expenses of huge computational efforts [2–11]. Another alternative is to take the moments of the BBPs obtaining a set of hydrodynamic-like equations. The main drawback is how to model the constitutive equations for the higher-order moments (i.e. the fluxes) as well as for the production terms, i.e., moments of the collisional operator. These problems have successfully been tackled for Si by means of the Maximum Entropy Principle

(hereafter MEP) of extended thermodynamics [12]. Such an approach has successfully been used for simulating the electron transport [13–18] and the electro-thermal one in silicon devices [19–22]. Constructing such macroscopic model for SiC is the main aim of the present paper.

2. The Extended Hydrodynamic model

Over 200 crystal varieties of SiC, which are different by their atomic arrangement, are known. The 4H-SiC has a hexagonal lattice, and we have considered the valleys around the minima at the symmetry point M of the two lowest conduction bands. Due to the crystal symmetries, for each conduction band there are three equivalent valleys [23]. Then, for each of the two conduction bands, a Boltzmann-like kinetic equation for the unknown distribution function f_A must be considered. The phonon branches which mainly contribute to the transport phenomena in 4H-SiC are the polar and non-polar optical ones (in the Einstein approximation) and the acoustic one (in the Debye approximation). Again, for each η-th phonon branch, a Boltzmann-like kinetic equation for the unknown distribution function g_η must be added.

The BBP equations for phonons and electrons are coupled by the respective collisional operators, which depend on the scattering mechanisms. Here we have considered the electron scattering with ionized impurities (intravalley, Brooks and Herring model), acoustic (intravalley, elastic approximation), polar optical (intravalley, inelastic) and non-polar optical (*intervalley*, inelastic) phonons. The main complicacy introduced in such material is due to the *intervalley* scattering, which leaves the electron into a different valley after the collision with a phonon.

By multiplying the BBP kinetic equation describing the electron flow by suitable weight functions, one can obtain balance equations for the macroscopic quantities associated to the electron flow (called moments) in the A-th valley [24]

$$\frac{\partial n_A}{\partial t}+\frac{\partial (n_A V_A^i)}{\partial x^i}=n_A C_{n_A} \quad , \quad \frac{\partial (n_A V_A^i)}{\partial t}+\frac{\partial (n_A U_A^{ij})}{\partial x^j}+\frac{e n_A}{m_A^*}E_i=n_A C_{V_A}^i \tag{1}$$

$$\frac{\partial (n_A W_A)}{\partial t}+\frac{\partial (n_A S_A^i)}{\partial x^i}+e n_A V_A^i E_i=n_A C_{W_A} \tag{2}$$

$$\frac{\partial (n_A S_A^i)}{\partial t}+\frac{\partial (n_A F_A^{ij})}{\partial x^j}+e n_A E_j U_A^{ij}+\frac{e n_A W_A}{m_A^*}E^i=n_A C_{S_A}^i \tag{3}$$

where n_A, V_A^i, W_A, S_A^i are the electron density, average velocity, average energy and average energy-flux respectively, and $C_{n_A}, C_{V_A}^i, C_{W_A}, C_{S_A}^i$ the corresponding productions; U_A^{ij} and F_A^{ij} are the higher-order fluxes, and E_j the electric field. Similarly, one obtains the balance equations for the phonons

$$\frac{\partial W_p}{\partial t}=\sum_A P_p(f_A) \quad , \quad \frac{\partial W_n}{\partial t}=\sum_{AB} P_n(f_A,f_B) \tag{4}$$

$$\frac{\partial W_{ac}}{\partial t}+\frac{\partial Q^i}{\partial x^i}=\sum_A P_{ac}(f_A) \quad , \quad \frac{\partial Q^i}{\partial t}+v_s^2\frac{\partial N^{ij}}{\partial x^j}=v_s^2\sum_A P_{ac}^i(f_A) \tag{5}$$

where v_s is the sound velocity, W_{ac}, W_p, W_n are the energy densities for the acoustic, polar optical, non-polar optical phonons respectively, P_{ac}^i, P_p, P_n the corresponding productions, and Q^i the acoustic phonon energy-flux density. In the above system of PDEs, we have to determine the higher-order fluxes (i.e., $U_A^{ij}, F_A^{ij}, N^{ij}$) as well as the production terms (i.e., the right-hand-side). According to the Maximum Entropy Principle, if a certain number of moments is known, then the distribution functions which can be used for evaluating the unknown moments are those that extremize the entropy functional, under the constraint that those functions reproduce the known moments. By performing a suitable expansion around the thermal equilibrium, we

obtain a hyperbolic system of PDEs, where the higher-order fluxes and the production terms are determined functions of the moments $n_A, V_A^i, W_A^i, S_A^i, W_p, W_n, W_{ac}, Q^i$. We observe that, in this scheme, no Fourier law relating the electron/phonon heat flow to the temperature gradient has been invoked because the energy-fluxes S_A^i, Q^i are considered as new variables.

3. The bulk case

The bulk case is represented by a SiC semiconductor with a uniform doping. If homogeneous initial conditions are taken, the above moment system reduces to a system of ordinary differential equations with the time as the only independent variable, and an electric field frozen into the sample. The parameters used in the simulation have been taken form [23]. For the initial conditions, we have taken the corresponding equilibrium values. In figure 1 we plot the electron density for the two conduction bands versus the simulation time, for an electric field of 450 kV/cm. The inversion of two electron populations begins at long times. In figure 2 we plot the electron velocity for the two conduction bands and their average (weighed with their densities). The velocity overshoot phenomenon is clearly observed. Finally, in figures 3, 4 the average electron energies and phonon temperatures are shown, respectively. The lattice temperature is defined as $T_L = (c_{ac}T_{ac} + c_pT_p + c_nT_n)/(c_{ac} + c_p + c_n)$ where c_{ac}, c_p, c_n are the volumetric specific heat for the respective phonon branches. Since the (bulk) semiconductor is supposed to be infinite without any boundary condition, and the lattice is not considered as a thermal reservoir, the heat produced by Joule effect inside the device cannot be dissipated and we expect a general overheating of the sample. The overheating of the sample has been predicted as function of the simulation time, and the contribution to the heat transport of the different phonon branches has been highlighted. The figure 4 shows a significant variation of the lattice temperature for a simulation time of $\simeq 100$ ps. Since the transfer of energy from the electrons to phonons occurs in a time scale of $\simeq 0.3$ ps., the energy transfer from the electrons to phonons can be assumed to occur instantaneously, when compared to the heat transport time scale. For this reason, in the simulation, one can use for the phonon flow a time step 100 times larger than the time step used for solving the electron flow (1)-(3), saving CPU time.

The simulation of real devices, where hot electron effects can play an important role in the energy dissipation phenomenon, using this hydrodynamic model will be the subject of the next researches.

Acknowledgments

This work has been supported by the research project AMBITION POWER (MIUR PON Ricerca e Competitività 2007-2013 Regioni Convergenza).

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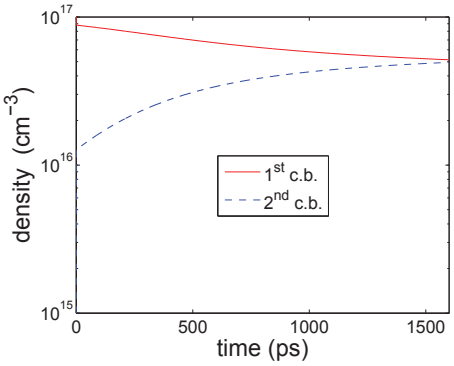

Figure 1. The electron density for the 1st, 2nd conduction band versus the simulation time.

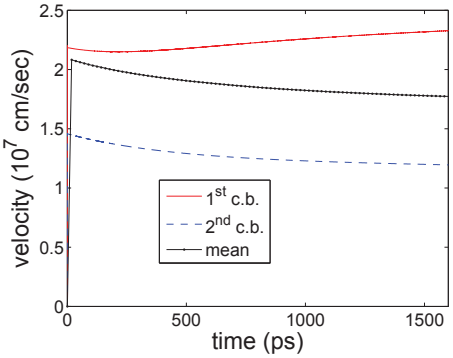

Figure 2. The electron velocity for the 1st, 2nd conduction band versus the simulation time, and their average.

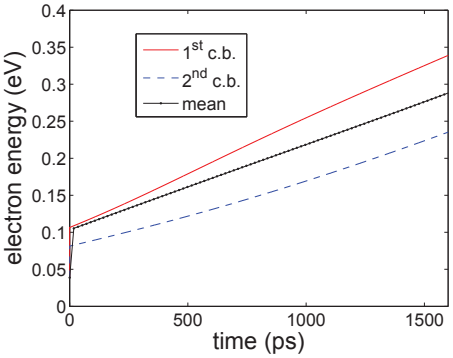

Figure 3. The electron energy for the 1st, 2nd conduction band versus the simulation time, and their average.

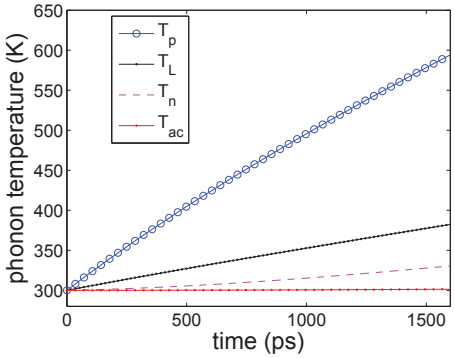

Figure 4. The phonon temperatures versus the simulation time, and the lattice temperature T_L.

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