



A hierarchy of hydrodynamic models for silicon carbide semiconductors

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Abstract

The electro-thermal transport in silicon carbide semiconductors can be described by an extended hydrodynamic model, obtained by taking moments from kinetic equations, and using the Maximum Entropy Principle. By performing appropriate scaling, one can obtain reduced transport models such as the Energy transport and the drift-diffusion ones, where the transport coefficients are explicitly determined.

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1. Introduction

Silicon carbide (SiC) is a wide-bandgap semiconductor considered to be one of the major enabling materials for advanced high power and high temperature electronics applications. In addition to its wide bandgap, SiC also has a high critical electric field strength and a high saturation drift velocity, making it able to sustain higher voltages with lower conduction loss. SiC-based electronics are now superior for power conversion than current silicon-based electronics, especially for high temperature, high-power, and high-frequency applications. Although the performances of SiC 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 necessary in order to predict the behaviour of such devices.

The Bloch-Boltzmann-Peierls kinetic equations (BBP) for the coupled system formed by the electrons and the phonons, together with the Poisson equation, is the natural framework for describing electro-thermal transport phenomena. To solve the BBP equations is not an easy task also from the numerical point of view, because they form a set of partial integro-differential equations. Particle-based solvers [1–6] of the BBP system can be proposed but with a huge computational effort. For engineering purposes, one has to introduce hydrodynamic models, which are obtained by taking the moments of the BBP equations and by using a suitable truncation procedure. This problem can be solved with the help of the variational method known as Maximum Entropy Principle (MEP) [7,8], which allows the determination of the nonequilibrium distribution function, and consequently, of the constitutive relations. Recently, this methodology has been applied to SiC [9] obtaining a closed set of balance equations of hyperbolic-type. The aim of this paper is to obtain, from this hydrodynamic model, simpler transport models, such as the energy transport and the drift-diffusion ones which are useful to devise efficient numerical schemes [10].

2. Kinetic and hydrodynamic equations

The main contribution to the charge transport phenomenon in semiconductors, is due to the electrons which occupy states around the lowest minima of the lowest conduction bands. The neighbors of these minima are called valleys which are analytically approximated by a parabolic dispersion relation. The band structure depends on the crystal. In the following we have considered the 4H-SiC polytype (having a hexagonal lattice) which is the least anisotropic among the SiC polytypes. Different band structures can be found in the literature, and we have used that in [11]. 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.

Let $f_A(t, \mathbf{x}, \mathbf{k})$ be the probability density to find an electron in the A -th valley, at time t , position $\mathbf{x} = (x_1, x_2, x_3)$, with wave vector $\mathbf{k} = (k_1, k_2, k_3)$ and energy $\varepsilon_A(\mathbf{k})$, $g_\eta = g_\eta(t, \mathbf{x}, \mathbf{q})$ the probability density to find a phonon of type η at time t , position \mathbf{x} with wave vector $\mathbf{q} = (q_1, q_2, q_3)$ and energy $\hbar\omega_\eta(\mathbf{q})$. These probability densities obey to the Bloch-Boltzmann-Peierls

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kinetics equations [12]

$$(1) \quad \frac{\partial f_A}{\partial t} + \mathbf{v}_A(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f_A - \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f_A = \mathcal{C}^{im}[f_A] + \sum_{\eta} \mathcal{C}[f_A, g_{\eta}] + \sum_{\eta} \sum_{B \neq A} \mathcal{C}_{AB}[f_A, f_B, g_{\eta}]$$

$$(2) \quad \frac{\partial g_{\eta}}{\partial t} + \mathbf{u}_{\eta}(\mathbf{q}) \cdot \nabla_{\mathbf{x}} g_{\eta} = \sum_A \mathcal{D}[f_A, g_{\eta}] + \sum_{A \neq B} \sum_B \mathcal{D}_{AB}[f_A, f_B, g_{\eta}]$$

where e is the absolute value of the electron charge, \mathbf{v}, \mathbf{u} the electron and phonon group velocity respectively

$$(3) \quad \mathbf{v}_A = \frac{\hbar \mathbf{k}}{m_A^*}, \quad \mathbf{u}_{\eta}(\mathbf{q}) = \nabla_{\mathbf{q}} \omega_{\eta}$$

and m_A^* is the effective mass of the A -th valley. The right-hand-sides of eqs.(1),(2) are the collisional operators, governing the collisions suffered by the electron/phonon in the semiconductor. In particular we have considered scattering of electrons with ionized impurities (*im*), intravalley acoustic phonons (*ac*), intravalley polar optical phonons (*p*), intervalley non-polar phonons (*n*) [9]. The previous BBP equations must be coupled to the Poisson equation for the self-consistent electric field \mathbf{E} , i.e.

$$(4) \quad \Delta_{\mathbf{x}}(\epsilon_s \epsilon_0 \phi) = e [n(t, \mathbf{x}) - N_D(\mathbf{x}) + N_A(\mathbf{x})] \quad , \quad \mathbf{E} = -\nabla_{\mathbf{x}} \phi$$

where $\phi(t, \mathbf{x})$ is the electric potential, N_D and N_A , respectively are the donor and acceptor densities, and n the total electron density.

By multiplying the kinetic equations (1),(2) by suitable weight functions, one can obtain balance equations for the macroscopic quantities associated to the flow of the electrons and phonons. For the electron flow, by introducing the weight functions

$$\psi_{\gamma}(\mathbf{k}) = (1, \mathbf{v}_A, \varepsilon_A, \varepsilon_A \mathbf{v}_A)$$

one obtains a 8-moments model, with the following balance equations for the A -th valley

$$(5) \quad \frac{\partial n_A}{\partial t} + \frac{\partial(n_A V_A^i)}{\partial x^i} = n_A C_{n_A}$$

$$(6) \quad \frac{\partial(n_A V_A^i)}{\partial t} + \frac{\partial(n_A U_A^{ij})}{\partial x^j} + e n_A E_j G_A^{ij} = n_A C_{V_A}^i$$

$$(7) \quad \frac{\partial(n_A W_A)}{\partial t} + \frac{\partial(n_A S_A^i)}{\partial x^i} + e n_A V_A^i E_i = n_A C_{W_A}$$

$$(8) \quad \frac{\partial(n_A S_A^i)}{\partial t} + \frac{\partial(n_A F_A^{ij})}{\partial x^j} + e E_j n_A H_A^{ij} = n_A C_{S_A}^i$$

where n_A is the electron density, V_A^i the average electron velocity, W_A the average electron energy, S_A^i the average electron energy flux, $U_A^{ij}, G_A^{ij}, F_A^{ij}, H_A^{ij}$ the higher-order fluxes, $C_{n_A}, C_{V_A}^i, C_{W_A}, C_{S_A}^i$ the production terms. For the assigned weight function $\psi_\gamma(\mathbf{k})$ and the corresponding moment, the production term represents the rate of change of the function ψ due to the scattering mechanism (electron/phonon or electron/impurity) taking place in the position \mathbf{x} .

Now we have to introduce balance equations for the phonon population. The **polar optical phonons** in the Einstein approximation have zero group velocity (3)₂, and since they are created/destroyed in an intravalley process, then the transport equation (2) reduces to

$$(9) \quad \frac{\partial g_p}{\partial t} = \sum_A \mathcal{D}[f_A, g_p] \quad .$$

Since the phonon energy does not depend on the phonon momentum, it has no sense to consider a balance equation for this quantity and we shall consider just a one moment model (the energy), which is obtained by multiplying for $\hbar\omega_p$ and integrating over \mathbf{q} , i.e.

$$(10) \quad \frac{\partial W_p}{\partial t} = \sum_A P_p(f_A)$$

where W_p is the energy density of polar optical phonons, $P_p(f_A)$ the polar optical energy density production due to the scattering with the electrons in the A valley.

The **non-polar optical** Phonons are produced in an intervalley process, and due to the zero group velocity argument, from eq.(2) we have

$$(11) \quad \frac{\partial g_n}{\partial t} = \sum_A \sum_{B \neq A} \mathcal{D}[f_A, f_B, g_n]$$

and, as in the previous case, we shall consider just one moment model

$$(12) \quad \frac{\partial W_n}{\partial t} = \sum_A P_n(f_A)$$

where W_n is the energy density of non-polar optical phonons, $P_n(f_A)$ the non-polar optical energy density production due to the scattering with the electrons in the A valley.

The **acoustic phonons**, in the Debye approximation, have $\omega_{ac}(\mathbf{q}) = v_s|\mathbf{q}|$, where v_s is the sound speed, and hence they have not vanishing

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group velocity \mathbf{u}_{ac} . We have chosen a 2-moments model which comprises the energy ($\hbar\omega_{ac}$) and the energy-flux ($\hbar\omega_{ac}\mathbf{u}_{ac}$). The weight functions are:

$$\varphi_{\beta}(\mathbf{q}) = (\hbar v_s |\mathbf{q}|, \hbar v_s^2 q^i)$$

and the corresponding balance equations read

$$(13) \quad \frac{\partial W_{ac}}{\partial t} + \frac{\partial Q^i}{\partial x^i} = \sum_A P_{ac}(f_A)$$

$$(14) \quad \frac{\partial Q^i}{\partial t} + v_s^2 \frac{\partial N^{ij}}{\partial x^j} = v_s^2 \sum_A P_{ac}^i(f_A)$$

where W_{ac} is the acoustic phonon energy density, Q^i the acoustic phonon energy-flux density, N^{ij} the acoustic phonon flux of energy-flux density, P_{ac} the total production of acoustic phonon energy density, P_{ac}^i the total production of acoustic phonon energy-flux density.

3. Constitutive equations

At this point we notice that the number of unknowns exceeds the number of equations, the production terms are unknown, and closure relations must be introduced. The MEP gives a systematic way for obtaining constitutive relations, as successfully done in silicon based semiconductors [13–20], as well as for nanometric structures [21–25]. We assume that the electron gas is sufficiently dilute, then the entropy density can be taken as the classical limit of the expression arising in the Fermi statistics, i.e.

$$(15) \quad S_e = -\frac{2k_B}{(2\pi)^3} \sum_A \int (f_A \log f_A - f_A) d\mathbf{k} \quad ,$$

whereas phonons are Bose particles, and the corresponding entropy density for the η -th branch is

$$(16) \quad S_{\eta} = \frac{1}{(2\pi)^3} \int [(1 + g_{\eta}) \log (1 + g_{\eta}) - g_{\eta} \log (g_{\eta})] d\mathbf{q}$$

then, the total entropy density writes

$$S_{tot} = S_e + S_{ac} + S_p + S_n \quad .$$

According to the MEP, if a given number of moments $M_A^\gamma, M_{ac}^\beta, M_p, M_n$ are known, the distribution functions $\hat{f}_A, \hat{g}_{ac}, \hat{g}_p, \hat{g}_n$ which can be used to evaluate the unknown moments, correspond to the extremum of the total entropy density under the constraint that they yield the known moments, i.e.

$$(17) \quad M_A^\gamma = \frac{2}{(2\pi)^3} \int_{\mathbb{R}^3} \psi_\gamma(\mathbf{k}) \hat{f}_A d\mathbf{k} \quad , \quad M_{ac}^\beta = \frac{3}{(2\pi)^3} \int_{\mathbb{B}} \varphi_\beta(\mathbf{q}) \hat{g}_{ac} d\mathbf{q}$$

$$(18) \quad M_p = \frac{1}{(2\pi)^3} \int_{\mathbb{B}} \hat{g}_p d\mathbf{q} \quad , \quad M_n = \frac{1}{(2\pi)^3} \int_{\mathbb{B}} \hat{g}_n d\mathbf{q}$$

By introducing a set of Lagrange multipliers $\lambda_\gamma, \Lambda_\beta, \Upsilon_p, \Upsilon_n$, the problem to maximize S_{tot} under the constraints (17),(18) is equivalent to maximize

$$S' = S_{tot} - \sum_{\gamma,A} \lambda_\gamma \left[\frac{2}{(2\pi)^3} \int_{\mathbb{R}^3} \psi_\gamma \hat{f}_A d\mathbf{k} - M_A^\gamma \right] - \sum_{\beta} \Lambda_\beta \left[\frac{1}{(2\pi)^3} \int_{\mathbb{B}} \varphi_\beta \hat{g}_{ac} d\mathbf{q} - M_{ac}^\beta \right] \\ - \Upsilon_p \left[\frac{1}{(2\pi)^3} \int_{\mathbb{B}} \hat{g}_p d\mathbf{q} - M_p \right] - \Upsilon_n \left[\frac{1}{(2\pi)^3} \int_{\mathbb{B}} \hat{g}_n d\mathbf{q} - M_n \right]$$

Hence, we shall obtain the following distribution functions:

- for the electrons

$$(19) \quad \hat{f}_A = \exp \left[- \left(\frac{1}{k_B} \lambda^A + \lambda_V^A \cdot \mathbf{v}_A + \lambda_W^A \varepsilon_A + \lambda_S^A \cdot \mathbf{v}_A \varepsilon_A \right) \right]$$

- for the acoustic phonons

$$(20) \quad \hat{g}_{ac} = \frac{1}{\exp[\varphi_0 \Lambda_0 + \varphi_i \Lambda_i] - 1}$$

- for the polar optical phonons

$$(21) \quad \hat{g}_p = \frac{1}{\exp[\hbar\omega_p \Upsilon_p] - 1}$$

- for the non-polar optical phonons

$$(22) \quad \hat{g}_n = \frac{1}{\exp[\hbar\omega_n \Upsilon_n] - 1}$$

By inserting the previous equations in (17)-(18), we obtain

$$M_A^\gamma = M_A^\gamma(\lambda_\gamma) \quad , \quad M_{ac}^\beta = M_{ac}^\beta(\Lambda_\beta) \quad , \quad M_p = M_p(\Upsilon_p) \quad , \quad M_n = M_n(\Upsilon_n)$$

which define implicitly the Lagrange multipliers. To invert the above relations, we shall perform an expansion around the thermal equilibrium. In

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fact, at equilibrium, \hat{f}_A, \hat{g}_η must reduce to the Fermi-Dirac and the Bose-Einstein respectively. This means

$$(23) \quad \lambda_V^A|_E = \lambda_S^A|_E = \Lambda|_E = 0, \quad \Lambda_0|_E = \frac{1}{k_B T_L}, \quad \lambda_W^A|_E = \frac{1}{k_B T_L}$$

where T_L is the equilibrium lattice temperature. Then we consider the vanishing Lagrange multipliers of higher order respect to equilibrium, by introducing the smallness parameter τ

$$(24) \quad \lambda_V^A = \tau \hat{\lambda}_V^A, \quad \lambda_S^A = \tau \hat{\lambda}_S^A, \quad \Lambda_i = \tau \hat{\Lambda}_i.$$

Then, the electron distribution function up to the first order in τ is

$$(25) \quad \hat{f}_A = \exp\left(-\frac{\lambda^A}{k_B} - \lambda_W^A \varepsilon_A\right) \left\{1 - \tau \left(\hat{\lambda}_V^A v_A^i + \hat{\lambda}_S^A v_A^i \varepsilon_A\right)\right\} + \mathcal{O}(\tau^2)$$

and the closures for the high-order fluxes

$$(26) \quad U_A^{ij} = \frac{2}{3m_A^*} W_A \delta^{ij}, \quad F_A^{ij} = \frac{10}{9m_A^*} W_A^2 \delta^{ij}.$$

The acoustic phonon distribution function writes

$$(27) \quad \hat{g}_{ac} = g^{(0)} + \tau g^{(1)} + \mathcal{O}(\tau^2)$$

where

$$(28) \quad g^{(0)} = \frac{1}{\exp(\Lambda_0 \hbar v_s |\mathbf{q}|) - 1}$$

$$(29) \quad g^{(1)} = -\hbar v_s^2 q^i \hat{\Lambda}_i g^+, \quad g^+ = \frac{\exp(\Lambda_0 \hbar v_s |\mathbf{q}|)}{[\exp(\Lambda_0 \hbar v_s |\mathbf{q}|) - 1]^2}.$$

and the closure for the high-order flux

$$(30) \quad N^{ij} = \frac{1}{3} W_{ac} \delta^{ij}.$$

Explicit expressions for the production terms are also obtained [9].

From the knowledge of the phonon energy densities, one can introduce the respective temperatures

$$(31) \quad dW_p = c_p dT_p, \quad dW_n = c_n dT_n, \quad dW_{ac} = c_{ac} dT_{ac}$$

where c_p, c_n, c_{ac} are the corresponding volumetric specific heats. Consequently, we define the lattice temperature T_L as

$$(32) \quad T_L = \frac{c_{ac} T_{ac} + c_p T_p + c_n T_n}{c_{ac} + c_p + c_n}.$$

4. Hydrodynamic limits

Our system in the unknowns $(n_A, V_A^i, W_A, S_A^i, T_{ac}, Q^i, T_p, T_n)$ in the parabolic band approximation, writes

$$(33) \quad \frac{\partial n_A}{\partial t} + \frac{\partial(n_A V_A^i)}{\partial x^i} = n_A C_{n_A}$$

$$(34) \quad \frac{\partial(n_A V_A^i)}{\partial t} + \frac{2}{3m_A^*} \frac{\partial(n_A W_A)}{\partial x^i} + \frac{en_A}{m_A^*} E_i = n_A C_{V_A^i}$$

$$(35) \quad \frac{\partial(n_A W_A)}{\partial t} + \frac{\partial(n_A S_A^i)}{\partial x^i} + en_A V_A^i E_i = n_A C_{W_A}$$

$$(36) \quad \frac{\partial(n_A S_A^i)}{\partial t} + \frac{10}{9m_A^*} \frac{\partial(n_A W_A^2)}{\partial x^i} + \frac{5}{3m_A^*} e n_A W_A E_i = n_A C_{S_A^i}$$

$$(37) \quad c_{ac} \frac{\partial T_{ac}}{\partial t} + \frac{\partial Q^i}{\partial x^i} = \sum_A P_{ac}(f_A)$$

$$(38) \quad \frac{\partial Q^i}{\partial t} + \frac{1}{3} v_s^2 c_{ac} \frac{\partial T_{ac}}{\partial x^i} = v_s^2 \sum_A P_{ac}^i(f_A)$$

$$(39) \quad c_p \frac{\partial T_p}{\partial t} = \sum_A P_p(f_A)$$

$$(40) \quad c_n \frac{\partial T_n}{\partial t} = \sum_A P_n(f_A)$$

where the Poisson equation (4) must be added. The main advantage of this model is that the transport coefficients are explicitly determined, and no additional tuning is needed. This system is of hyperbolic type.

Simplified transport models can be obtained from the above system by assuming reasonable scaling. By using the smallness parameter τ which measures the deviation from thermal equilibrium, we assume the following scaling

$$(41) \quad t = \frac{\hat{t}}{\tau^2}, \quad x = \frac{\hat{x}}{\tau}, \quad E = \tau \hat{E}, \quad V^i = \tau \hat{V}^i, \quad S^i = \tau \hat{S}^i, \quad Q^i = \tau \hat{Q}^i$$

where the first relation means a long time scaling, the second one a diffusive scaling, and the others are consistent with the hypothesis of small deviation from thermal equilibrium.

By equating to zero the coefficients of the various powers in τ , and omit-

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ting the hat, we obtain the so-called **Energy Transport model** (ETM)

$$(42) \quad \frac{\partial n_A}{\partial t} + \frac{\partial(n_A V_A^i)}{\partial x^i} = n_A C_{n_A}$$

$$(43) \quad \frac{\partial(n_A W_A)}{\partial t} + \frac{\partial(n_A S_A^i)}{\partial x^i} + n_A e V_A^i E_i = n_A C_{W_A}$$

$$(44) \quad c_{ac} \frac{\partial T_{ac}}{\partial t} + \frac{\partial Q^i}{\partial x^i} = \sum_A P_{ac}(f_A)$$

$$(45) \quad c_p \frac{\partial T_p}{\partial t} = \sum_A P_p(f_A) \quad , \quad c_n \frac{\partial T_n}{\partial t} = \sum_A P_n(f_A)$$

with a reduced set of unknowns $(n_A, W_A, T_{ac}, T_p, T_n)$, and the constitutive equations

$$(46) \quad \frac{2}{3} \frac{\partial(n_A W_A)}{\partial x^i} + n_A e E^i = -\Delta_Q(W_A, W_{ac}) Q^i + \Sigma_S S_A^i$$

$$(47) \quad \frac{10}{9} \frac{\partial(n_A W_A^2)}{\partial x^i} + \frac{5}{3} n_A e W_A E_i = \Phi_V V_A^i + \Psi_S S_A^i$$

$$(48) \quad \frac{1}{3} c_{ac} \frac{\partial T_{ac}}{\partial x^i} = \sum_A (\Delta_Q(W_A, W_{ac}) Q^i + \Delta_V(W_A, W_{ac}) V_A^i + \Delta_S(W_A, W_{ac}) S_A^i) \quad .$$

The equation (48) gives:

$$(49) \quad Q^i = -\frac{1}{3} \tau_Q c_{ac} \frac{\partial T_{ac}}{\partial x^i} + \tau_Q \sum_A (\Delta_V(W_A, W_{ac}) V_A^i + \Delta_S(W_A, W_{ac}) S_A^i)$$

$$\tau_Q = -\frac{1}{\sum_A \Delta_Q(W_A, W_{ac})}$$

which is the usual Fourier law with an extra convective term, due to the electron flow. The conductivity, i.e. the coefficient of $\partial T_{ac}/\partial x^i$, is similar to that obtained by kinetic considerations [26]. If we introduce the particle flux $J_A^i = n_A V_A^i$, and the electron energy-flux $J_{W_A}^i = n_A S_A^i$, by solving the system (46)-(48) we obtain

$$(50) \quad J_A^i = a_{11} \frac{\partial \phi}{\partial x^i} + a_{12} \frac{\partial n_A}{\partial x^i} + a_{13} \frac{\partial W_A}{\partial x^i} + a_{14} \frac{\partial T_{ac}}{\partial x^i}$$

$$(51) \quad J_{W_A}^i = a_{21} \frac{\partial \phi}{\partial x^i} + a_{22} \frac{\partial n_A}{\partial x^i} + a_{23} \frac{\partial W_A}{\partial x^i} + a_{24} \frac{\partial T_{ac}}{\partial x^i}$$

$$(52) \quad Q^i = a_{31} \frac{\partial \phi}{\partial x^i} + a_{32} \frac{\partial n_A}{\partial x^i} + a_{33} \frac{\partial W_A}{\partial x^i} + a_{34} \frac{\partial T_{ac}}{\partial x^i}$$

where the coefficients $a_{ij} = a_{ij}(n_A, W_A, T_{ac}, T_p, T_n)$ are known functions. The previous equations can be interpreted as constitutive linear equations between the fluxes $J_\alpha = (J_A^i, J_{W_A}^i, Q^i)$, and the quantities

$$X_\beta = \left(\frac{\partial \phi}{\partial x^i}, \frac{\partial n_A}{\partial x^i}, \frac{\partial W_A}{\partial x^i}, \frac{\partial T_{ac}}{\partial x^i} \right) .$$

This result is similar to the linear flux-force relations introduced in the framework of the Linear Irreversible Thermodynamics (LIT). In this context, in order to introduce the thermodynamic forces, one must invoke the *Local Equilibrium Hypothesis* [7] (and consequently the Gibbs relation), which we have not introduced in our theory.

Moreover the well known **drift-diffusion** model can be retrieved. Since in the parabolic approximation one can write

$$(53) \quad W_A = \frac{1}{2} m_A^* V_A^2 + \frac{3}{2} k_B T_A^{(e)}$$

where $T_A^{(e)}$ is the electron temperature, if we assume that the electrons and phonons have the same temperature, i.e.

$$(54) \quad T_A^{(e)} = T_n = T_p = T_{ac} = T_L$$

and by approximating

$$(55) \quad W_A \simeq \frac{3}{2} k_B T_L$$

then eq.(50) reduces to

$$(56) \quad J_A^i = n_A \mu_n^A \frac{\partial \phi}{\partial x^i} - D_n^A \frac{\partial n_A}{\partial x^i} - S_n^A \frac{\partial T_L}{\partial x^i}$$

with

$$(57) \quad \mu_n^A = \frac{1}{n_A} a_{11} \quad , \quad D_n^A = -a_{12} \quad , \quad S_n^A = - \left(\frac{3}{2} k_B a_{13} + a_{14} \right) .$$

The equation (56) is the closure equation used in the drift-diffusion model, where μ_n^A is the low-field mobility, D_n^A the diffusivity and S_n^A the Soret coefficient for the A -th valley. Moreover, it is possible to verify that the Einstein relation holds [26], i.e.

$$(58) \quad D_n^A = \mu_n^A \frac{k_B T_L}{e} .$$

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Finally we have evaluated with our model the low-field mobility

$$(59) \quad \mu_n = \frac{\sum_A n_A \mu_n^A}{\sum_A n_A}$$

versus the lattice temperature T_L , and compared the obtained results with the experimental data in [27]. In figure 1 we plot the results, showing a good agreement.

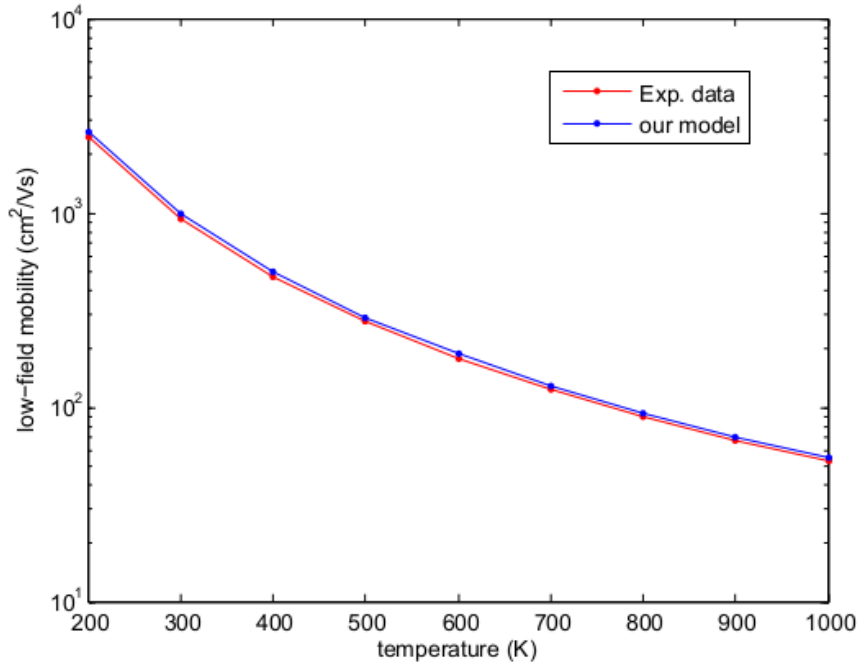


Figure 1. Low-field mobility versus temperature

5. Conclusions

The electro-thermal phenomena in SiC semiconductors can be described by an extended hydrodynamic model. Closure relations for the higher order moments and production terms, involving the electron-phonon scattering, have been obtained by means of the MEP. By introducing a diffusive scaling, an Energy Transport model has been derived, where the transport coefficients do not contain any fitting parameters, but only the physical

constants like the coupling ones and the phonon energies that are present in the transition rate probabilities of the scatterings between the electrons and phonons. In the limit case when the electrons and phonons have the same temperature, the ETM reduces to the standard non-isothermal Drift Diffusion model. The low-field mobility we have obtained in this case, shows a good agreement with the experimental data. The simulation of real devices using this Energy Transport Model will be the topic of future researches.

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REFERENCES

1. O. Muscato, W. Wagner, and V. Di Stefano, Numerical study of the systematic error in Monte Carlo schemes for semiconductors, *ESAIM: M2AN*, vol. 44, no. 5, pp. 1049–1068, 2010.
2. O. Muscato, W. Wagner, and V. Di Stefano, Properties of the steady state distribution of electrons in semiconductors, *Kinetic and Related Models*, vol. 4, no. 3, pp. 809–829, 2011.
3. O. Muscato, V. Di Stefano, and W. Wagner, A variance-reduced electrothermal Monte Carlo method for semiconductor device simulation, *Comput. Math. with Appl.*, vol. 65, no. 3, pp. 520–527, 2013.
4. T. Sadi, R. Kelsall, N. Pilgrim, J.-L. Thobel, and F. Dessene, Monte carlo study of self-heating in nanoscale devices, *J. Comp. Electr.*, vol. 11, no. 1, pp. 118–128, 2012.
5. O. Muscato and W. Wagner, A class of stochastic algorithms for the wigner equation, *SIAM J. Sci. Comput.*, vol. 38, no. 3, pp. A1438–A1507, 2016.
6. A. Majorana, G. Mascali, and V. Romano, Charge transport and mobility in monolayer graphene, *J. Math. Industry*, vol. 7, p. 4, 2017.
7. G. Lebon, D. Jou, and J. Casas-Vázquez, *Understanding Non-equilibrium Thermodynamics*. Springer-Verlag, 2008.
8. I. Mueller and T. Ruggeri, *Rational Extended Thermodynamics*. Springer-Verlag, 1998.
9. O. Muscato and V. D. Stefano, Electrothermal transport in silicon carbide semiconductors via a hydrodynamic model, *SIAM J. APPL. MATH.*, vol. 75, no. 4, pp. 1941–1964, 2015.

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10. A. Jüngel, Energy transport in semiconductor devices, *Math. Comput. Model. Dyn. Syst.*, vol. 16, pp. 1–22, 2010.
11. G. Pennington and N. Goldsman, Consistent calculation for n -type hexagonal SiC inversion layers, *J. Appl. Phys.*, vol. 95, no. 9, pp. 4223–4234, 2004.
12. J. Ziman, *Electrons and Phonons*. Clarendon Press, 1967.
13. O. Muscato and V. Di Stefano, Hydrodynamic modeling of the electro-thermal transport in silicon semiconductors, *J. Phys. A: Math. Theor.*, vol. 44, no. 10, p. 105501, 2011.
14. O. Muscato and V. Di Stefano, An energy transport model describing heat generation and conduction in silicon semiconductors, *J. Stat. Phys.*, vol. 144, no. 1, pp. 171–197, 2011.
15. O. Muscato and V. Di Stefano, Local equilibrium and off-equilibrium thermoelectric effects in silicon semiconductors, *J. Appl. Phys.*, vol. 110, no. 9, p. 093706, 2011.
16. O. Muscato and V. Di Stefano, Heat generation and transport in nanoscale semiconductor devices via Monte Carlo and hydrodynamic simulations, *COMPEL*, vol. 30, no. 2, pp. 519–537, 2011.
17. V. Di Stefano and O. Muscato, Seebeck effect in silicon semiconductors, *Acta Appl. Math.*, vol. 122, no. 1, pp. 225–238, 2012.
18. O. Muscato and V. Di Stefano, Electro-thermal behaviour of a sub-micron silicon diode, *Semicond. Sci. Tech.*, vol. 28, no. 2, p. 025021, 2013.
19. G. Mascali, A hydrodynamical model for silicon semiconductors including crystal heating, *Europ. J. Appl. Math.*, vol. 26, pp. 477–496, 2015.
20. G. Mascali, A new formula for silicon thermal conductivity based on a hierarchy of hydrodynamical models, *J. Stat. Phys.*, vol. 163, no. 5, pp. 1268–1284, 2016.
21. O. Muscato and V. Di Stefano, Hydrodynamic modeling of silicon quantum wires, *J. Comput. Electron.*, vol. 11, no. 1, pp. 45–55, 2012.
22. O. Muscato and V. Di Stefano, Hydrodynamic simulation of a $n^+ - n - n^+$ silicon nanowire, *Contin. Mech. Thermodyn.*, vol. 26, pp. 197–205, 2014.
23. O. Muscato and T. Castiglione, Electron transport in silicon nanowires having different cross-sections, *Comm. Appl. Ind. Math.*, vol. 7, no. 2, pp. 8–25, 2016.
24. O. Muscato and T. Castiglione, A hydrodynamic model for silicon nanowires based on the maximum entropy principle, *Entropy*, vol. 18, no. 10, p. 368, 2016.
25. M. Coco, G. Mascali, and V. Romano, Monte Carlo analysis of the

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- thermal effects in monolayer graphene, *J. Comp. Theor. Transp.*, vol. 45, no. 7, pp. 540–553, 2016.
26. M. Lundstrom, *Fundamentals of Carrier Transport*. Cambridge University Press, 2000.
 27. M. Roschke and F. Schwier, Electron mobility models for 4H, 6H, and 3C SiC, *IEEE Trans. Elec. Dev.*, vol. 48, no. 7, pp. 1442–1447, 2001.