An Extended Hydrodynamic model for Silicon Nano Wires

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***Abstract*—We present an extended hydrodynamic model describing the transport of electrons in the axial direction of a silicon nanowire. This model has been formulated by closing the moment system derived from the Boltzmann equations on the basis of the maximum entropy principle of Extended Thermodynamics, coupled to the Effective Mass and Poisson equations. Explicit closure relations for the high-order fluxes and the production terms are obtained without any fitting procedure, including scattering of electrons with acoustic and non polar optical phonons. By using this model, thermoelectric effects have been investigated.**

I. Introduction

By shrinking the dimension of electronic devices, effects of quantum confinement are observed Under reasonable hypotheses, transport in low-dimension semiconductors can be tackled using semiclassical tools. In fact, the main quantum transport phenomena in Silicon Nanowires (SiNW) transistors at room temperature, such as the source-to-drain tunneling, and the conductance fluctuation induced by the quantum interference, become significant only when the channel lengths are smaller than 10nm [1]. Therefore, for longer channels, semi-classical formulations based on the 1-D multisubband Boltzmann Transport Equation (MBTE) can give reliable simulation results when it is solved self-consistently with the 3-D Poisson and 2-D Schrödinger equations in order to obtain the self-consistent potential and subband energies and wavefunctions [2]. Another simplification comes from the use of the Effective Mass Approximation (EMA), which is supposed to be still a good solution in the confining direction in the presence of disorder, which is probably valid for semiconductor nanowires down to 5 nm in diameter, below which atomistic electronic structure models need to be employed. Solving the MBTE numerically is not an easy task, because it forms an integro-differential system in two dimensions in the phase-space and one in time, with a complicate collisional operator. A considerable simplification of the MBTE can be obtained employing the relaxation time approximation for the collisional operator [3], whereas the full solution of the MBTE can be obtained or by using the Monte Carlo (MC) method [4]-[7] or by using deterministic numerical solvers [8],[9] at expense of huge computational times. Another alternative is to obtain from the MBTE hydrodynamic models that are a good engineering-oriented approach. This can be achieved by taking moments of the MBTE, and by closing the obtained hierarchy of balance equations as well as modeling the production terms (i.e. the moments on the collisional operator).

II. The Extended Hydrodynamic Model

For a SiNW with linear extension along the z-direction, the MBTE for the electron distribution functions $f_\alpha(z, k_z, t)$ in each α-th subband writes [2]

$$\frac{\partial f_\alpha}{\partial t} + v_z(k_z)\frac{\partial f_\alpha}{\partial z} - \frac{e}{\hbar}\,\mathcal{E}_z\frac{\partial f_\alpha}{\partial k_z} = \sum_{\alpha'}\sum_{\eta}\mathcal{C}_\eta[f_\alpha, f_{\alpha'}] \quad (1)$$

where $\mathcal{E}_z$ is the electric field, $v_z = \frac{1}{\hbar}\frac{\partial E_\alpha}{\partial z}$ the electron group velocity, E_α the total energy, which, in the parabolic band approximation, writes

$$E_\alpha = \varepsilon_\alpha + \varepsilon_z + E_c \quad , \quad \varepsilon_z = \frac{\hbar^2 k_z^2}{2m^*}$$

where E_c is the conduction band edge energy, and ε_α the kinetic energy associated with the confinement. All the relevant 1D scattering mechanisms in Si, i.e. acoustic phonon scattering and nonpolar phonon scattering, are taken into account by the collisional integral $\mathcal{C}_\eta[f_\alpha, f_{\alpha'}]$. This transport equation must be coupled to the EMA-Poisson system. By multiplying the MBTE by the weight functions $\psi_A = \{1, v_z, \varepsilon_z, v_z\varepsilon_z\}$, and integrating in the k_z space, one obtains the following hydrodynamic-like equations

$$\frac{\partial\rho^\alpha}{\partial t}+\frac{\partial(\rho^\alpha V^\alpha)}{\partial z}=\rho^\alpha\sum_{\alpha'}C_\rho^{\alpha\alpha'}$$
$$\frac{\partial(\rho^\alpha V^\alpha)}{\partial t}+\frac{2}{m^*}\frac{\partial(\rho^\alpha W^\alpha)}{\partial z}+\frac{e}{m^*}\rho^\alpha\mathcal{E}_z=\rho^\alpha\sum_{\alpha'}C_V^{\alpha\alpha'}$$
$$\frac{\partial(\rho^\alpha W^\alpha)}{\partial t}+\frac{\partial(\rho^\alpha S^\alpha)}{\partial z}+\rho^\alpha e\mathcal{E}_z V^\alpha=\rho^\alpha\sum_{\alpha'}C_W^{\alpha\alpha'}$$
$$\frac{\partial(\rho^\alpha S^\alpha)}{\partial t}+\frac{\partial(\rho^\alpha F^\alpha)}{\partial z}+3\frac{e}{m^*}\rho^\alpha\mathcal{E}_z W^\alpha=\rho^\alpha\sum_{\alpha'}C_S^{\alpha\alpha'}$$

in the unknowns (called moments) ρ^α (1-D density), V^α (mean velocity), W^α (mean energy) and S^α (mean energy-flux), and

$$F^\alpha=\frac{2}{(2\pi)}\frac{1}{\rho^\alpha}\int f_\alpha v_z^2\varepsilon_z dk_z$$
$$C_\rho^{\alpha\alpha'}=\frac{2}{(2\pi)}\frac{1}{\rho^\alpha}\sum_\eta\int\mathcal{C}_\eta[f_\alpha,f_{\alpha'}]dk_z$$
$$C_V^{\alpha\alpha'}=\frac{2}{(2\pi)}\frac{1}{\rho^\alpha}\sum_\eta\int\mathcal{C}_\eta[f_\alpha,f_{\alpha'}]v_z dk_z$$
$$C_W^{\alpha\alpha'}=\frac{2}{(2\pi)}\frac{1}{\rho^\alpha}\sum_\eta\int\mathcal{C}_\eta[f_\alpha,f_{\alpha'}]\varepsilon_z dk_z$$
$$C_S^{\alpha\alpha'}=\frac{2}{(2\pi)}\frac{1}{\rho^\alpha}\sum_\eta\int\mathcal{C}_\eta[f_\alpha,f_{\alpha'}]\varepsilon_z v_z dk_z \quad .$$

This system of PDEs is of hyperbolic type.

III. Closure Relations

The above moment system is not closed: there are more unknowns than equations. The maximum entropy principle (MEP) leads to a systematic way for obtaining constitutive relations on the basis of the information theory, as already proved successfully in the bulk case [11]-[16], and for quantum well structures [17], [18]. We define the entropy of the electronic system as

$$S_e = \sum_\alpha|\chi_\alpha(x,y,t)|^2S_e^\alpha \tag{2}$$
$$S_e^\alpha = -\frac{2}{(2\pi)}k_B\int_{\mathbb{R}}(f_\alpha\log f_\alpha-f_\alpha)dk_z \quad , \tag{3}$$

and, according to MEP, we estimate the f_α's as the distributions that maximize S_e under the constraints that the basic moments, which we have previously considered, are assigned. In a neighborhood of local thermal equilibrium, the distribution function writes [19]

$$\hat{f}_\alpha=\exp\left(-\frac{\lambda^\alpha}{k_B}-\lambda_W^\alpha\varepsilon_z\right)\left\{1-\tau\left(\hat\lambda_V^\alpha v_z+\hat\lambda_S^\alpha v_z\varepsilon_z\right)\right\} \tag{4}$$

where the quantities $(\lambda^\alpha,\lambda_W^\alpha,\hat\lambda_V^\alpha,\hat\lambda_S^\alpha)$ are known functions of the moments $\{\rho^\alpha,V^\alpha,W^\alpha,S^\alpha\}$. By using the distribution function (4), the higher-order flux term

$$F^\alpha=\frac{6(W^\alpha)^2}{m^*}$$

as well as the production terms $C_\rho^{\alpha\alpha'},C_V^{\alpha\alpha'},C_W^{\alpha\alpha'},C_S^{\alpha\alpha'}$ have been determined. We underline that this extended hydrodynamic model has been closed by using first principles, and it is free of any fitting parameters.

IV. Local Thermal Equilibrium

When the electric field is small, the system formed by the electrons and phonons is in Local Thermal Equilibrium (hereafter LTE). In this case, we assume that the system under study can be split into a series of sub-systems sufficiently large to allow them to be treated as macroscopic thermodynamic subsystems, but sufficiently small that equilibrium is very close to being realized in each sub-system. In our scheme, this regime will be characterized by setting the smallness parameter $\tau=0$ and, in such a case, the eq.(4) reduces to the local maxwellian. In this regime, Gibbs relations hold for each sub-system, i.e.

$$T_e^\alpha dS_e^\alpha=d(\rho^\alpha W^\alpha)-\bar\nu^\alpha d\rho^\alpha \quad , \quad T_L dS_L=dW_L \tag{5}$$

where T_e^α is the electron temperature, $\bar\nu^\alpha$ is the chemical potential for the electrons with respect to the energy of the α-th subband [20] , T_L, S_L, W_L the temperature, the entropy, the energy of the lattice respectively. The key point is that, from the Gibbs relations, one can define the entropy-fluxes for the electrons and the lattice

$$J_{Se}^{\alpha i}=\frac{1}{T_e^\alpha}(J_W^\alpha-\bar\nu^\alpha J^\alpha)z^i \quad , \quad J_{S_L}^i=\frac{1}{T_L}J_{W_L}^i \tag{6}$$

where $J^\alpha=\rho^\alpha V^\alpha$, $J_W^\alpha=\rho^\alpha S^\alpha$, and the quantity

$$J_h^{i\alpha}=T_e^\alpha J_{Se}^{i\alpha} \tag{7}$$

is known as electron heat flux density. By defining $S_{tot}=S_e+S_L$ and $J_{Stot}^i=J_{Se}^{\alpha i}+J_{S_L}^i$ then, from the moment system, one can write down the total entropy balance equation [21]

$$\frac{\partial S_{tot}}{\partial t}+\frac{\partial J_{Stot}^i}{\partial x^i}=\sigma \tag{8}$$

$$\sigma=\sum_\alpha J^\alpha z^i\frac{1}{T_L}\frac{\partial\hat\phi^\alpha}{\partial x^i}+\sum_\alpha(J_W^\alpha-\bar\nu^\alpha J^\alpha)z^i\frac{\partial}{\partial x^i}\left(\frac{1}{T_L}\right)-\frac{1}{T_L}\sum_{\alpha\alpha'}\rho^\alpha\bar\nu^\alpha C_\rho^{\alpha\alpha'}. \tag{9}$$

where $\hat{\phi}^\alpha = -\bar{\nu}^\alpha + e\phi^\alpha$ is the electrochemical potential, and we have assumed that the electrons and the lattice are in local thermal equilibrium at the same temperature, i.e. $T_e^\alpha = T_L$. From the previous equation we can identify the thermodynamic forces X_μ and the corresponding generalized fluxes J_ν, i.e.

$$X_\mu = \left\{ \frac{1}{T_L}\frac{\partial \hat{\phi}^\alpha}{\partial x^i}, \frac{\partial}{\partial x^i}\left(\frac{1}{T_L}\right), -\frac{\bar{\nu}^\alpha}{T_L} \right\} \qquad (10)$$

$$J_\nu = \left\{ J^\alpha z^i, \sum_\alpha (J_W^\alpha - \bar{\nu}^\alpha J^\alpha) z^i, \rho^\alpha \sum_{\alpha'} C_\rho^{\alpha\alpha'} \right\} \qquad (11)$$

According to Linear Irreversible Thermodynamics (LIT) [22], linear relations must hold between fluxes and forces, i.e.

$$J_\nu = L_{\nu\mu} X_\mu \quad . \qquad (12)$$

One of the basic principle of LIT is the Onsager Reciprocity Principle (ORP), which is a manifestation of microscopic reversibility for any statistical system near thermal equilibrium and therefore, any properly formulated statistical physical model should satisfy it. The Onsager principle states the symmetry of the constitutive matrix, i.e.

$$L_{\nu\mu} = L_{\mu\nu} \quad . \qquad (13)$$

Close to local thermal equilibrium, we shall suppose the electron kinetic energy can be neglected respect to the thermal one, i.e.

$$W^\alpha \simeq \frac{1}{2} k_B T_e^\alpha = \frac{1}{2} k_B T_L \quad .$$

In this case, in the stationary regime, we can obtain from our hydrodynamic model

$$J^\alpha = b_{11}(\rho^\alpha, W^\alpha)\frac{\partial \hat{\phi}^\alpha}{\partial z} + b_{12}(\rho^\alpha, W^\alpha)\frac{\partial}{\partial z}(k_B T_L) \qquad (14)$$

$$J_W^\alpha = b_{21}(\rho^\alpha, W^\alpha)\frac{\partial \hat{\phi}^\alpha}{\partial z} + b_{22}(\rho^\alpha, W^\alpha)\frac{\partial}{\partial z}(k_B T_L) \qquad (15)$$

where the coefficients b_{ij} are known quantities [19]. Now from the definitions (10),(11) and the eqs.(14), (15) we can identify

$$L_{11} = T_L b_{11} \quad , \quad L_{12} = -k_B (T_L)^2 b_{12}$$

$$L_{21} = T_L (b_{21} - \bar{\nu} b_{11}) \quad , \quad L_{22} = -k_B (T_L)^2 (b_{22} - \bar{\nu} b_{12})$$

and the ORP (13) implies

$$-k_B T_L b_{12} = b_{21} - \bar{\nu} b_{11} \quad . \qquad (16)$$

The validity of the previous equation has been verified numerically up to the machine zero precision.

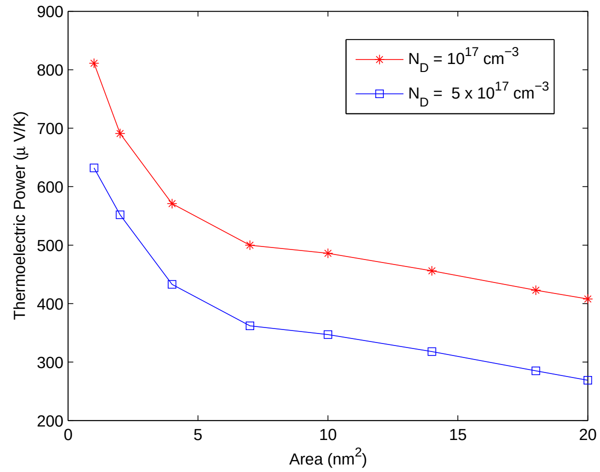

Fig. 1. The Thermopower $\mathcal{S}_d$ (17) versus the cross sectional area of the SiNW, at room temperature.

V. Thermoelectric properties

Our extended hydrodynamic model is able to describe thermoelectric effects in SiNWs. In fact under the hypothesis of small electric field, the system formed by the electrons and phonon is in LTE and we can apply the previous arguments. From the eq.(14), under the hypothesis of open circuit (i.e. $J^\alpha = 0$), we can define the Thermopower (or Seebeck coefficient) as

$$\mathcal{S}_d = \frac{\sum_\alpha \rho^\alpha \mathcal{S}_d^\alpha}{\sum_\alpha \rho^\alpha} \quad , \mathcal{S}_d^\alpha = \left.\frac{\Delta \hat{\phi}^\alpha}{\Delta T_L}\right|_{J=0} = -k_B \frac{b_{12}}{b_{11}} . \qquad (17)$$

This coefficient S_d represents the diffusive contribution which, at room temperature, is two order of magnitude with respect to the phonon-drag contribution [23], [24].

Let us consider the case in which the temperature gradient vanishes. Then eqs. (7),(14),(15) reduce to

$$J^\alpha = b_{11}\frac{\partial \hat{\phi}^\alpha}{\partial z} \quad , \quad J_h^{i\alpha} = \frac{b_{21} - \bar{\nu} b_{11}}{b_{11}} J^\alpha z^i \qquad (18)$$

hence a particle flux J^α produces a heat flux density $J_h^{i\alpha}$, which can be understood as the Peltier effect. Since $J_h^{i\alpha} = (0, 0, J_h^\alpha)$ then the Peltier coefficient is defined as

$$\Pi^\alpha = \left.\frac{\partial J_h^\alpha}{\partial J^\alpha}\right|_{\nabla T_L = 0} \qquad (19)$$

and the eq.(18) gives the Peltier coefficient for the α-th subband

$$\Pi^\alpha = \frac{b_{21}(\rho^\alpha, W^\alpha)}{b_{11}(\rho^\alpha, W^\alpha)} - \bar{\nu}^\alpha \quad . \qquad (20)$$

Moreover we have

$$\Pi = \frac{\sum_\alpha \rho^\alpha \Pi^\alpha}{\sum_\alpha \rho^\alpha} = \frac{\sum_\alpha \rho^\alpha \left[\frac{b_{21}(\alpha)}{b_{11}(\alpha)} - \bar{\nu}^\alpha\right]}{\sum_\alpha \rho^\alpha} \quad . \tag{21}$$

Another well known results of LIT is the Kelvin relation, which states that the Thermopower and the Peltier coefficient are linked by the following relation

$$\Pi = \mathcal{S}_d T_L \quad . \tag{22}$$

If we substitute (17), (20) into the previous equation, we obtain the eq.(16), and the Kelvin relation is a consequence of the ORP. So far we have verified that the extended thermodynamic model, for small electric fields, is compatible with the ORP. In order to obtain quantitative results, we have considered a wire with square cross-section and infinite confining potential. Consequently, the kinetic energies associated to the confinement and the corresponding envelope functions have analytic expressions. Figure 1 shows the cross sectional area effect on $\mathcal{S}_d$, at room temperature. The Thermopower decreases remarkably in accordance to the simulation results obtained in [25], where atomistic calculations for electronic structures and the BTE in the relaxation time approximation have been used.

VI. Conclusion

An extended hydrodynamic model for SiNWs has been formulated with the use of the maximum entropy principle. The transport coefficients are completely determined without any fitting procedure. For small electric fields, we have verified that our model is compatible with the ORP, and the Thermopower and the Peltier coefficient have been obtained.

VII. Acknowledgment

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