Hydrodynamic transport in Silicon Nano Wire devices

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INTRODUCTION

Transport phenomena in Silicon nanowire (SiNW) devices can be described using a semiclassical formulation based on the 1-D multisubband Boltzmann Transport Equation (MBTE), supposing the channel length is larger than some nanometers. Solving the MBTE numerically is not an easy task, because it forms an integro-differential system in two dimensions in phase-space and one in time, with a complicate collisional operator. The collisional operator can be approximated using the so called Relaxation Time Approximation, where the microscopic relaxation time is considered an adjustable parameter which is determined by fitting the solution to some experimental or simulated data when available [1]. The full solution of the MBTE can be obtained or by using the Monte Carlo (MC) method [2] or by using deterministic numerical solvers [3], 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). One way to tackle these problems is by means of the Maximum Entropy Principle (hereafter MEP) of Extended Thermodynamics [4], where the distribution function is assumed to be that which maximizes the entropy under the constraints of the given set of moments. In this way one obtains a representation of the distribution function valid up to the first order from Local Thermal Equilibrium (LTE). Recently, a consistent hydrodynamic model for SiNWs using the MEP has been developed [5] where, without any fitting procedure, the higher-order moments and the production terms have been analitycally determined.

THE HYDRODYNAMIC MODEL

We shall assume the parabolic band approximation, and scattering with (bulk) optical and acoustic phonons. By taking the moments of the MBTE, one obtains the following system [5]

$$\frac{\partial \rho^\alpha}{\partial t} + \frac{\partial (\rho^\alpha V^\alpha)}{\partial z} = \rho^\alpha \sum_{\alpha'} C_\rho^{\alpha\alpha'}$$

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

$$\frac{\partial (\rho^\alpha W^\alpha)}{\partial t} + \frac{\partial (\rho^\alpha S^\alpha)}{\partial z} + \rho^\alpha e \mathcal{E}_z V^\alpha = \rho^\alpha \sum_{\alpha'} C_W^{\alpha\alpha'}$$

$$\frac{\partial (\rho^\alpha S^\alpha)}{\partial t} + \frac{6}{m^*}\frac{\partial (\rho^\alpha (W^\alpha)^2)}{\partial z} + 3\frac{e}{m^*}\rho^\alpha \mathcal{E}_z W^\alpha = \rho^\alpha \sum_{\alpha'} C_S^{\alpha\alpha'}$$

where ρ^α is the α-subband electron density in the z-direction of the wire, V^α the electron velocity, W^α the electron energy, S^α the electron energy flux, and the right-hand-side are the production terms which are known functions. The above system must be coupled to the Poisson equation and the Schrödinger equation in the effective mass approximation. In this preliminary study, for the sake of simplicity, we shall assume that the oxide gives rise to an infinitely deep potential barrier. This justifies the use of analytical expressions as bottom energies and envelope functions [6]. The above system of PDEs is of hyperbolic type, and can be numerically solved by using high-order WENO finite-difference

schemes together with explicit RungeKutta time discretizations.

THERMOELECTRIC PROPERTIES

Our model can be also useful used to investigate thermoelectric phenomena in SiNWs. Under the hypothesis of small electric field, the system formed by the electrons and phonon is in LTE, i.e. the local and instantaneous relations between the thermal and mechanical properties of the physical system are the same as for a uniform system at equilibrium. From our model, which is valid in a larger neighborhood of LTE, by taking the appropriate limit we can obtain the following constitutive equations, linking the fluxes to the thermodynamic forces (i.e. the gradients) [5]

$$J^\alpha = b_{11}\frac{\partial \hat{\phi}^\alpha}{\partial z} + b_{12}\frac{\partial}{\partial z}\left(k_B T_e^\alpha\right) \qquad (1)$$

$$J_W^\alpha = b_{21}\frac{\partial \hat{\phi}^\alpha}{\partial z} + b_{22}\frac{\partial}{\partial z}\left(k_B T_e^\alpha\right) \qquad (2)$$

where $\hat{\phi}^\alpha$ is the electrochemical potential, T_e^α the electron temperature, where the coefficients b_{ij} are known functions. From the eq.(1), under the hypothesis of open circuit (i.e. $J^\alpha = 0$), we can define the Thermopower (or Seebeck coefficient)

$$\mathcal{S}_d = \frac{\sum_\alpha \rho^\alpha \mathcal{S}_d^\alpha}{\sum_\alpha \rho^\alpha} \quad , \mathcal{S}_d^\alpha = \left.\frac{\Delta \hat{\phi}^\alpha}{\Delta T_L}\right|_{J=0} \qquad (3)$$

In the figure 1 we have plotted $\mathcal{S}_d$ versus the lattice temperature, where we have considered a SiNW with square cross section of 15 $\times$ 15 nm^2, and doped to 5 $\times 10^{17}$ cm^{-3}. The Thermopower shows a straight-line behaviour in the temperature interval [200, 300], in qualitative agreement with the available experimental data [7].

CONCLUSION

A hydrodynamic model for SiNWs is formulated by means of the Maximum Entropy Principle of Extended Thermodynamics, whose main advantage is the complete determination of the transport coef ficients without any fitting procedure. Under suitable approximations, the model is able to describe the Seebeck effect, obtaining a good qualitative agreement with the results available in the literature.

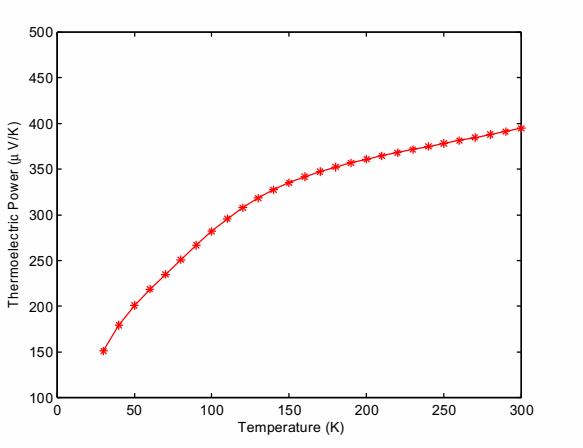

Fig. 1. The Thermopower $\mathcal{S}_d$ versus the lattice temperature, evaluated by means of eq.(3).

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