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Thermal conductivity in higher-order generalized hydrodynamics: Characterization of nanowires of silicon and gallium nitride



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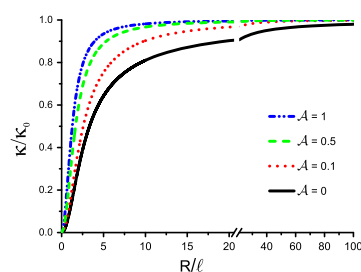
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HIGHLIGHTS

- It is specified a cylindrical geometry in samples of Si and GaN in the macro to nano-scales.
- The study of the thermal conductivity and its influence on the figure-of-merit in thermoelectric devices.
- The thermal conductivity is strongly dependent on the cylinder radius.

GRAPHICAL ABSTRACT

The thermal conductivity is strongly dependent on the ratio of the cylinder radius R to a characteristic length ℓ , the latter given approximately by the velocity of sound times a kind of relaxation time (energy Maxwell time) which has values in the order of hundreds of nanometers.



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ABSTRACT

An analysis of the influence of geometry and size on the thermal conductivity in semiconductors, particularized to the study in Si and GaN, is presented. This is done in the framework of a higher-order generalized hydrodynamics (HOGH) of phonons in semiconductors, driven away from equilibrium by external sources. This HOGH is derived by the method of moments from a generalized Peierls–Boltzmann kinetic equation built in the framework of a Non-Equilibrium Statistical Ensemble Formalism. We consider the case of wires (cylindrical geometry) exploring the effect of size (radius), particularly in the nanometric scale when comparison with experiment is done. Maxwell times, which are quite relevant to define the hydrodynamic movement, are evidenced and characterized.

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1. Introduction

It has been noticed [1] that the ceaseless innovation in semiconductor design creates a demand for a better understanding of the physical processes involved in materials with constrained geometries and functioning in far-from-equilibrium conditions. A particular question is the one of thermal transport in small semiconductor

devices [2] and data centers [3], used in refrigeration processes in microprocessors [4,5]. The heat generated by silicon chips in integrated circuits must be efficiently removed once the performance of modern electronic devices degrades as the temperature increases. One approach for providing active cooling in chips consists in the use of thermo-electric materials, which effectively transport heat via charge-current flow [6].

These questions belong to the area of nonequilibrium phonon dynamics [7] or, more precisely, to the subject of phonon hydrothermodynamics (that is, hydrodynamics associated to nonequilibrium “irreversible” thermodynamics) [8–10]. The hydro-thermodynamics of phonons, driven away from equilibrium by external sources, is built resorting to a theory, the one used in the present work, which, for the

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sake of completeness is summarized in the next section. It is based a nonlinear quantum kinetic theory [11–13] built on the basis of a Non-Equilibrium Statistical Ensemble Formalism (NESEF for short) [14–17]. It follows from the solution via the moments method of a generalized NESEF-based Peierls–Boltzmann kinetic equation for the single-phonon distribution function, to obtain such higher-order phonon hydro-thermodynamics. In a contracted description, meaning using the one of order 1, the solution of the evolution equations of the hydrodynamic motion is obtained; this is described in Section 3. In Section 4 we consider a particular constrained geometry and the thermal conductivity in nanowires is analyzed and compared with experiments. Maxwell times, which are quite relevant to the definition of the hydrodynamic motion, are evidenced and characterized.

2. Summary of a phonon mesoscopic hydro-thermodynamics

We consider a system of longitudinal acoustic $_{LA}$ phonons in a semiconductor in anharmonic interaction with the accompanying transverse acoustic $_{TA}$ phonons. The sample is in contact with a thermostat at temperature T_0 . An external pumping source drives the $_{LA}$ phonon system out of equilibrium. The system is characterized at the microscopic level by the Hamiltonian

$$\hat{H} = \hat{H}_{OS} + \hat{H}_{OB} + \hat{H}_{SB} + \hat{H}_{SP}, \quad (1)$$

which consists of the Hamiltonian of the free $_{LA}$ phonons

$$\hat{H}_{OS} = \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} (a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} + 1/2), \quad (2)$$

where $\omega_{\mathbf{q}}$ is the frequency dispersion relation and the sum on \mathbf{q} run over the Brillouin zone, and the one of the $_{TA}$ phonons, which we call the thermal bath in which the $_{LA}$ phonons are embedded, given by

$$\hat{H}_{OB} = \sum_{\mathbf{q}} \hbar \Omega_{\mathbf{q}} (b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + 1/2), \quad (3)$$

where $\Omega_{\mathbf{q}}$ is the frequency dispersion relation; $a_{\mathbf{q}}^{\dagger}(a_{\mathbf{q}})$ and $b_{\mathbf{q}}^{\dagger}(b_{\mathbf{q}})$ are the corresponding creation (annihilation) operators in mode \mathbf{q} .

Moreover, the interaction of the $_{LA}$ phonons with the thermal bath is given by

$$\hat{H}_{SB} = \sum_{\mathbf{k}, \mathbf{q}} M_{\mathbf{k}, \mathbf{q}} a_{\mathbf{q}} b_{\mathbf{k}+\mathbf{q}}^{\dagger} b_{-\mathbf{k}}^{\dagger} + \text{h.c.}, \quad (4)$$

where we have retained the only process that contributes to the kinetic equations ($_{LA} \rightleftharpoons _{TA} + _{TA}$) and we have neglected nonlinear contributions; $M_{\mathbf{k}, \mathbf{q}}$ accounts for the coupling strengths. Finally \hat{H}_{SP} is the interaction energy operator for the phonons and an external pumping source, to be specified in each case.

At the macroscopic level (the nonequilibrium thermodynamic state) NESEF requires first to specify the basic variables that are to be used to characterize the nonequilibrium ensemble [14–17]. A priori, when the system is initially driven away from equilibrium, it is necessary to include all the observables of the system what is attained introducing many-particle dynamical operators [18,19]; in the present case it suffices to take only the single-phonon dynamical operators $\hat{\nu}_{\mathbf{q}, \mathbf{Q}} = a_{\mathbf{q}+\mathbf{Q}/2}^{\dagger} a_{\mathbf{q}-\mathbf{Q}/2}$ in the second-quantization representation in reciprocal space. The two-phonon dynamical operator and higher-order ones can be ignored because of Bogoliubov's principle of correlation weakening [19]. Moreover, for bosons it would be necessary to also include the amplitudes $a_{\mathbf{q}}^{\dagger}$ and $a_{\mathbf{q}}$ because their eigenstates are the coherent states [20], and the boson pairs [21], both are disregarded because they are of no practical relevance for the problem considered here. In Appendix A we describe the corresponding nonequilibrium statistical operator. Another basic microdynamical variable that needs to be incorporated

is the energy of the bath, and then the basic set is composed of

$$\{\hat{\nu}_{\mathbf{q}}, \hat{\nu}_{\mathbf{q}, \mathbf{Q}}, \hat{H}_{OB}\}, \quad (5)$$

with $\mathbf{Q} \neq 0$, where we have separated out the so-called populations, $\hat{\nu}_{\mathbf{q}} = a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}}$, from those with $\mathbf{Q} \neq 0$ which are related to the change in space of the populations (they are also called coherences [22]).

The average values of the microdynamical variables in set (5) over the nonequilibrium ensemble provide the variables that characterized the nonequilibrium macroscopic state of the system, which we indicate by

$$\{\nu_{\mathbf{q}}(t), \nu_{\mathbf{q}, \mathbf{Q}}(t), E_B\}, \quad (6)$$

and are also introduced, see Appendix A, the nonequilibrium thermodynamic variables conjugated to those above, which we designate as

$$\{F_{\mathbf{q}}(t), F_{\mathbf{q}, \mathbf{Q}}(t), \beta_0\}, \quad (7)$$

with $\beta_0^{-1} = k_B T_0$.

Going over to direct space (anti-transforming Fourier in variable \mathbf{Q}) we obtain the space and crystalline momentum-dependent distribution function $\nu_{\mathbf{q}}(\mathbf{r}, t)$, in terms of which is built the phonon Higher-Order Hydro-Thermodynamics which consists of two families of hydrodynamical variables, namely, the one associated to the quasi-particles (the phonons) motion (we call it the n -family)

$$\{n(\mathbf{r}, t), \mathbf{I}_n(\mathbf{r}, t), \{I_n^{[\ell]}(\mathbf{r}, t)\}\}, \quad (8)$$

where $\ell = 2, 3, \dots$, $n(\mathbf{r}, t)$ stands for the number of phonons at time t in position \mathbf{r} , namely

$$n(\mathbf{r}, t) = \sum_{\mathbf{q}} \nu_{\mathbf{q}}(\mathbf{r}, t), \quad (9)$$

the first flux of this quantity is

$$\mathbf{I}_n(\mathbf{r}, t) = \sum_{\mathbf{q}} [\nabla_{\mathbf{q}} \omega_{\mathbf{q}}] \nu_{\mathbf{q}}(\mathbf{r}, t), \quad (10)$$

and the higher-order fluxes are

$$I_n^{[\ell]}(\mathbf{r}, t) = \sum_{\mathbf{q}} u^{[\ell]}(\mathbf{q}) \nu_{\mathbf{q}}(\mathbf{r}, t), \quad (11)$$

with $\ell = 2, 3, \dots$, defining the ℓ -order flux (ℓ -rank tensor) and where

$$u^{[\ell]}(\mathbf{q}) = [\nabla_{\mathbf{q}} \omega_{\mathbf{q}} : \dots \ell \text{-times} \dots : \nabla_{\mathbf{q}} \omega_{\mathbf{q}}], \quad (12)$$

is a ℓ -rank tensor consisting of the tensorial inner product of ℓ -times the group velocity of the \mathbf{q} -mode phonon, $\nabla_{\mathbf{q}} \omega_{\mathbf{q}}$.

On the other hand we do have the family associated to the energy motion (heat transport, and we call it the h -family)

$$\{h(\mathbf{r}, t), \mathbf{I}_h(\mathbf{r}, t), \{I_h^{[\ell]}(\mathbf{r}, t)\}\}, \quad (13)$$

where

$$h(\mathbf{r}, t) = \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} \nu_{\mathbf{q}}(\mathbf{r}, t), \quad (14)$$

$$\mathbf{I}_h(\mathbf{r}, t) = \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} [\nabla_{\mathbf{q}} \omega_{\mathbf{q}}] \nu_{\mathbf{q}}(\mathbf{r}, t), \quad (15)$$

$$I_h^{[\ell]}(\mathbf{r}, t) = \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} u^{[\ell]}(\mathbf{q}) \nu_{\mathbf{q}}(\mathbf{r}, t), \quad (16)$$

which are, respectively, the energy density, its first (vectorial) flux, and the higher-order ($\ell = 2, 3, \dots$) tensorial fluxes at time t in position \mathbf{r} .

Consequently, the hydrodynamic equations of motion (evolution equations for the quantities above) are

$$\frac{\partial}{\partial t} I_p^{[\ell]}(\mathbf{r}, t) = \sum_{\mathbf{q}} K_p^{[\ell]}(\mathbf{q}) \frac{\partial}{\partial t} \nu_{\mathbf{q}}(\mathbf{r}, t), \quad (17)$$

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