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Effective thermal conductivity of rectangular nanowires based on phonon hydrodynamics

M. Calvo-Schwarzwälder [a,b], M.G. Hennessy [a,*], P. Torres [c], T.G. Myers [a,b], F.X. Alvarez [c]

[a] Centre de Recerca Matemàtica, Campus de Bellaterra, Edifici C, 08193 Bellaterra, Barcelona, Spain
[b] Departament de Matemàtiques, Universitat Politècnica de Catalunya, 08028 Barcelona, Spain
[c] Departament de Física, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain

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ABSTRACT

A mathematical model is presented for thermal transport in nanowires with rectangular cross sections. Expressions for the effective thermal conductivity of the nanowire across a range of temperatures and cross-sectional aspect ratios are obtained by solving the Guyer–Krumhansl hydrodynamic equation for the thermal flux with a slip boundary condition. Our results show that square nanowires transport thermal energy more efficiently than rectangular nanowires due to optimal separation between the boundaries. However, circular nanowires are found to be even more efficient than square nanowires due to the lack of corners in the cross section, which locally reduce the thermal flux and inhibit the conduction of heat. By using a temperature-dependent slip coefficient, we show that the model is able to accurately capture experimental data of the effective thermal conductivity obtained from Si nanowires, demonstrating that phonon hydrodynamics is a powerful framework that can be applied to nanosystems even at room temperature.

1. Introduction

Advances in manufacturing processes have brought us to the stage where reliable nanoscale devices are now commonplace. However, in most current and predicted applications of nanostructures, there is a strong concern over the management of heat [1]. One specific issue with heat removal is the dramatic decrease of the thermal conductivity at the nanoscale in comparison to the bulk value [2–5]. This decrease can be rationalised in terms of the manner by which thermal energy is transported across the macroscale and nanoscale. At the macroscale, heat transfer is a diffusive process driven by frequent collisions between thermal energy carriers known as phonons. In contrast, the transport of thermal energy across the nanoscale is a ballistic process driven by infrequent collisions between phonons. As the size of a device approaches that of the phonon mean free path, the phonons become more likely to collide with a boundary than with each other. This results in a conductivity which is more strongly influenced by the scattering dynamics at the boundary than collisions in the bulk. Consequently, thermal energy is transported less efficiently across the nanosystem, yielding a decrease in the thermal conductivity from the bulk value of the material.

Developing mathematical models to aid in the understanding of heat flow has proved problematic due to the breakdown of Fourier's law at small time and length scales [6–8]. With the aim of accurately predicting the effective thermal conductivity (ETC) of nanosystems, a variety of theoretical models of nanoscale heat transport have been proposed, either based on micro- and mesoscopic approaches [9,10] or from a macroscopic point of view [11–18]. A popular approach is the phonon hydrodynamics model [11–17], which is based on the Guyer–Krumhansl (G-K) equation [19,20]. This model was first presented to describe heat transfer in the so-called hydrodynamic regime, where phonon flow behaves as a rarefied gas due to the dominance of normal scattering, i.e., scattering which conserves quasi-momentum, over resistive scattering, which does not conserve phonon quasi-momentum [19–21]. It was originally believed that the hydrodynamic transport regime only occurs at extremely low temperatures. However, recent *ab initio* calculations have demonstrated that phonon hydrodynamics can be valid even at room temperature [22–24]. As with many other macroscopic models such as the thermomass model [18,25] or the equation of phonon radiative transfer [26], the G-K equation can be derived from the Boltzmann transport equation (BTE) [27] or from the extended irreversible thermodynamics (EIT) framework [28]. Thus, the G-K equation provides a

* Corresponding author.
E-mail addresses: mcalvo@crm.cat (M. Calvo-Schwarzwälder), mhennessy@crm.cat (M.G. Hennessy), pol.torres@uab.cat (P. Torres), tmyers@crm.cat (T.G. Myers), xavier.alvarez@uab.cat (F.X. Alvarez).

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link between microscopic (kinetic) and macroscopic (continuum) models. Another attractive feature of the phonon hydrodynamics model is that the governing equations are analogous to those seen in viscous fluid mechanics, which provides an intuitive conceptual framework for model development and interpretation. The analogy between the phonon hydrodynamics and fluid dynamics models has prompted researchers to apply the well-known slip boundary condition to thermal transport [11–14]. In fact, it has been shown that this form of boundary condition naturally arises from the discrete BTE [29] and from the EIT framework [21]. With the correct choice of slip length, this approach was shown to provide excellent agreement with experimental measurements of the ETC of silicon nanowires [11].

Aside from circular nanowires, studies employing the slip boundary condition are mainly confined to two-dimensional thin-film geometries [12–14]. Although the reduced dimensionality of this geometry enables a simple, closed-form expression for the ETC to be obtained, it can only be applied to nanowires with extremely small cross-sectional aspect ratios. However, rectangular nanowires with aspect ratios as high as 0.64 have been reported in the literature [2]. Unlike the thin-film geometry, the cross section of a rectangular nanowire will have two additional boundaries, as well as four corners, that will be detrimental to thermal transport. Therefore, the geometry of the rectangular cross section will play a key role in determining the ETC of the nanowire and have practical consequences in terms of thermal regulation in nanodevices.

The purpose of the present study is to use the phonon hydrodynamic model with a slip boundary condition to calculate the ETC in a rectangular nanowire, with the aim of gaining an improved understanding of how finite cross-sectional geometries influence nanoscale heat transport. Of particular interest is determining the nanowire geometry that leads to the most efficient transport of heat. Theoretical predictions of the ETC are compared against experimentally measured values. We show that the model is able to accurately capture the experimental data across a wide range of temperatures.

The paper is organised as follows. The model and boundary conditions are presented in Section 2 and expressions for the ETC are given in Section 3. In Section 4, the modelling results are discussed and the theoretical predictions are compared against experimental data. The paper then concludes in Section 5.

2. Mathematical model

We model the transport of thermal energy across a long nanowire with rectangular cross section that is suspended in a vacuum; see Fig. 1. The length of the nanowire L_3^* is assumed to be much greater than both the half-width L_1^* and half-height L_2^* of the cross section. The * notation is used to denote dimensional quantities. Without loss of generality, the cross section can be taken to be wider than it is tall, $L_2^*/L_1^* < 1$. Under these conditions, the cross-sectional aspect ratio $\phi = L_2^*/L_1^*$ and the longitudinal aspect ratio $\epsilon = L_2^*/L_3^*$ satisfy $\epsilon \ll \phi < 1$. The transverse coordinates x^* and y^* denote points within a given cross section whereas the longitudinal coordinate z^* describes distances along the length of the nanowire. The origin of the cross section $(x^*, y^*) = (0, 0)$ is chosen to coincide with the center of the rectangular face. The transport of heat is driven by a longitudinal temperature gradient $\Delta T^* > 0$ that is imposed by fixing the temperature T^* at the ends of the nanowire to be $T^* = T_0^* + \Delta T^*$ at $z^* = 0$ and $T^* = T_0^*$ at $z^* = L_3^*$. The thermal flux is assumed to be symmetric about the $x^* = 0$ and $y^* = 0$ planes.

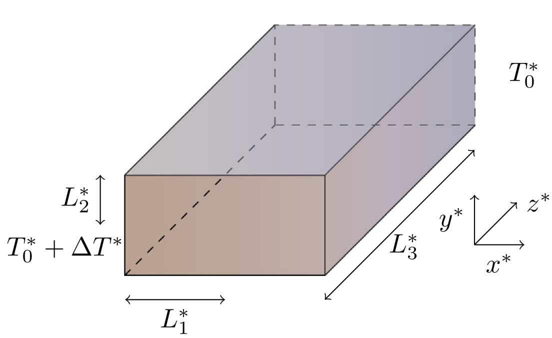

Fig. 1. The experimental setup consists of a rectangular nanowire of length L_3^* and a cross section of dimensions $2L_1^* \times 2L_2^*$. The heat flux $\mathbf{Q}^*$ is induced by a constant temperature difference $\Delta T^* > 0$.

2.1. Governing equations

The mathematical model consists of an equation representing conservation of thermal energy and the G-K (or hydrodynamic) equation describing the evolution of the thermal flux. Under the steady-state assumption, the governing equations are

$$\nabla \cdot \mathbf{Q}^* = 0, \tag{1a}$$

$$\mathbf{Q}^* = -k^* \nabla T^* + \ell^{*2} \nabla^2 \mathbf{Q}^*, \tag{1b}$$

where $\mathbf{Q}^* = u^* \hat{\mathbf{x}}^* + v^* \hat{\mathbf{y}}^* + w^* \hat{\mathbf{z}}^*$ is the thermal flux written in terms of Cartesian components, $k^*(T^*)$ is the bulk thermal conductivity, and $\ell^*(T^*)$ is a non-local length related to the bulk phonon mean free path (MFP), *i.e.*, the mean distance between phonon–phonon collisions. In the original equation derived by Guyer and Krumhansl, the parameter ℓ^* represents the bulk MFP defined as $\ell^{*2} = (v_g^{*2} \tau_N^* \tau_R^*)/5$, where v_g^* is the phonon group velocity and τ_N^* and τ_R^* are the normal and resistive mean free times, i.e., the mean times for normal and resistive scattering. Other researchers have proposed alternative definitions for ℓ^*, such as the geometric mean of the bulk MFP and a local MFP, the latter of which decreases near a boundary [12]. We take ℓ^* to be the non-local length computed from the Kinetic Collective Model (KCM), which is an accurate approach for predicting the thermal conductivity in a number of materials [30]. We refer to Appendix A for a more detailed description of how ℓ^* is obtained from the KCM.

For simplicity, the dependence of the parameters on the temperature will not be explicitly written unless required by the context. The second term on the right-hand side of (1b) accounts for non-local effects, *i.e.*, phonon collisions. The strong increase in the length scale ℓ^* as the temperature decreases can make non-local effects relevant in relatively large systems, including those with dimensions exceeding the nanoscale [28,31].

The size-dependent effective thermal conductivity (ETC) of the nanowire k_{eff}^* is defined in terms of the mean thermal flux through a cross section Q^* and the longitudinal temperature gradient $\partial T^*/\partial z^*$ as

$$k_{\mathrm{eff}}^* = -\frac{Q^*}{\partial T^*/\partial z^*}, \quad Q^* = \frac{1}{4L_1^* L_2^*} \int_{-L_2^*}^{L_2^*} \int_{-L_1^*}^{L_1^*} w^* \, \mathrm{d}x^* \mathrm{d}y^*. \tag{2}$$

By construction, w^* is the only component of the flux that is not tangential to the cross-section. Therefore, to compute the effective thermal conductivity of a rectangular slab, we need to find only the normal component of the heat flux w^*.

2.2. Boundary conditions

The boundary conditions for the temperature at the endpoints of the nanowire are