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A slip-based model for the size-dependent effective thermal conductivity of nanowires

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ABSTRACT

The heat flux across a nanowire is computed based on the Guyer-Krumhansl equation. Slip conditions with a slip length depending on both temperature and nanowire radius are introduced at the outer boundary. An explicit expression for the effective thermal conductivity is derived and compared to existing models across a given temperature range, providing excellent agreement with experimental data for Si nanowires.

1. Introduction

Nanotechnology is currently the focus of extensive research due to its wide range of applications in fields such as industry and medicine [1–7]. Nanowires, in particular, are being used in technologies relating to solar cells [4], flexible screens [5], detection of cancerous cells [7], and energy storage [6]. A key issue facing the practical use of nanodevices is thermal management [8]. Inefficient regulation of heat can lead to large temperatures and melting, possibly resulting in device failure. Understanding and predicting heat flow on the nanoscale is therefore crucial for the manufacturing and operation of nanotechnologies.

It is widely known that many thermophysical material properties become size-dependent at the nanoscale [9–16]. Buffat and Borel [9] showed a dramatic decrease of the melting temperature of gold nanoparticles of almost 50% from the bulk value. For aluminium nanoparticles, a decrease in latent heat by a factor of four has been reported [10]. Experimental observations also demonstrate that the thermal conductivity in silicon nanowires is much lower than the theoretical value predicted by kinetic theory [14]. For instance, it is reported that, at room temperature, the thermal conductivity of Si nanowires with a diameter of 37 nm decreases by approximately 87% with respect to the bulk value. When the characteristic size of the system is much smaller than the phonon mean free path, the thermal conductivity shows an approximately linear dependence on size [17–20].

The size dependence of the thermal conductivity of nanosystems is attributed to the fact that, on the nanoscale, the transport of thermal energy is a ballistic process driven by infrequent collisions between thermal energy carriers known as phonons. This is in contrast to macroscopic heat transfer, which is a diffusive processes driven by frequent phonon collisions. As the size of a device becomes commensurate with the phonon mean free path, bulk phonons are more likely to collide with a boundary than with each other. The ability of a nanodevice to conduct thermal energy, therefore, becomes strongly influenced by the scattering dynamics at the boundary as well as the geometrical structure (e.g., size and shape) of this boundary.

Due to the fundamentally different manner in which heat is transported across nanometer length scales in comparison to heat flow at the macroscale, Fourier's law is unable to provide an accurate description of heat conduction in this regime [21]. Different approaches to modelling nanoscale heat flow have been developed in order to capture the ballistic nature of energy transport and size dependence of the effective thermal conductivity (ETC). These approaches can be classified into three main categories: microscopic, mesoscopic and macroscopic models. Microscopic approaches, such as molecular dynamics or Monte-Carlo methods [22], focus on the evolution of every single phonon while mesoscopic models group them together depending on their wavelength and wavevector. Micro and mesoscopic models are mainly based on the Boltzmann transport equation (BTE) and its solution under

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different approximations. A popular example is the equation of phonon radiative transfer (EPRT) [23], where an expression for the ETC similar to the classical expression from kinetic theory is derived, although here an effective mean free path is now considered. However this model is based on the gray approximation and thus considers a single phonon group velocity and lifetime. A more general model where these quantities are mode-dependent was presented by McGaughey et al. [24]. Starting again from the BTE, Alvarez et al. [18,25] extract a continued-fraction expression to describe the ETC in thin films. Other models, such as those of Callaway [26] and Holland [27], also consider phonon distributions rather than single phonons, but Mingo et al. [28] showed that they fail when predicting the ETC for Si or Ge nanowires.

Macroscopic models aim to describe global variables of the system, such as the temperature and the heat flux. A recent approach at the macroscopic scale is the thermomass model, where heat carriers are assumed to have a finite mass determined by Einstein's mass-energy relation [19,29,30]. Other approaches are based on the Guyer-Krumhansl (G-K) equation [31,32], which is derived from a linearized BTE in dielectric crystals. This equation has become popular since it is analogous to the extensively studied Navier-Stokes (N-S) equations and it is one of the simplest extensions to Fourier's law that includes memory and non-local effects. Models based on the G-K equation are included in the framework of phonon hydrodynamics [33]. For instance, Alvarez et al. [20] use the analogy between the G-K equation and the N-S equations to derive an expression for the ETC in circular nanowires, splitting the heat flux into two separate contributions. This work has been extended to elliptical and rectangular nanowires [34]. However, since the size of the phonon mean free path depends on temperature, the assumptions on which they base their reductions are only valid for low temperatures or very small sizes. Dong et al. [35] find an expression for the ETC by solving the full G-K equations at steady state, although their no-slip boundary condition leads to a quadratic dependence of the ETC on the characteristic size of the device for large Knudsen numbers instead of the known linear behaviour. This does not happen with the expression derived by Ma [17], where a fixed flux is imposed on the outer boundary. However, Ma's solution for the nanowire shows a very poor match to data (their paper contains an error in that they plot the thin film solution in their figure for the nanowire which actually shows reasonable agreement with the data). Further, most of the existing models are only validated at room temperature and therefore a deeper assessment of their accuracy is required.

In this paper, we introduce a new phenomenological slip boundary condition that, when used with the G-K equations, results in ETC predictions that are in excellent agreement with experimental data for Si nanowires over a range of radii and temperatures. The proposed model is remarkably simple and only requires knowledge of the temperature dependence of the bulk thermal conductivity and phonon mean free path, both of which may be obtained experimentally or computationally, making it well suited for use in practical applications. A detailed comparison of the proposed and existing models is performed, the results of which show that the proposed model consistently yields the most accurate predictions of the ETC compared to existing models. Furthermore, this comparison establishes the validity of each model in terms of temperature and nanowire radius.

2. Mathematical modelling

We consider a circular nanowire (NW) of radius R^* and length L^* that is suspended in a vacuum; see Fig. 1. The radius of the NW is assumed to be much smaller than its length, i.e., $R^*/L^* \equiv \epsilon \ll 1$. A temperature gradient $\Delta T = T_0^* - T_1^* > 0$ is imposed along the axial direction of the NW by fixing the temperature at its left and right ends to be T_0 and T_1, respectively. The thermal flux that is driven by this temperature gradient is assumed to be axisymmetric. Therefore, it is sufficient to consider a two-dimensional model with radial and axial coordinates r^* and x^*, respectively. The mathematical model will consist

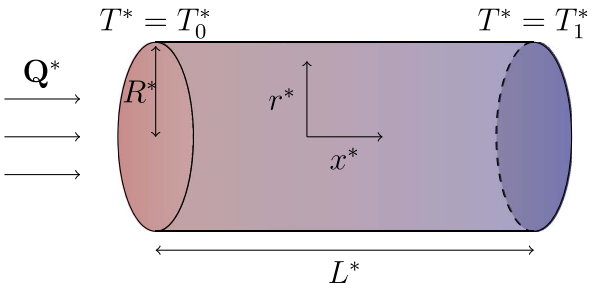

Fig. 1. A circular nanowire with radius R^* and length L^* is held at different temperatures T_0^*, T_1^* at the left and right ends respectively, which induces a heat flux $\mathbf{Q}^*$.

of an equation representing conservation of thermal energy and the G-K equation describing the evolution of the thermal flux.

2.1. Bulk equations

Conservation of energy requires

$$\frac{\partial u^*}{\partial t} = -\nabla\cdot\mathbf{Q}^*, \tag{1}$$

where $u^*(T^*)$ is the internal energy per unit mass and T^* is the temperature. The thermal flux $\mathbf{Q}^* = v^*\hat{\mathbf{r}} + w^*\hat{\mathbf{x}}$ is assumed to satisfy the G-K equation

$$\tau^*\frac{\partial \mathbf{Q}^*}{\partial t} + \mathbf{Q}^* = -k^*\nabla T^* + \ell^{*2}(\nabla^2\mathbf{Q}^* + 2\nabla\nabla\cdot\mathbf{Q}^*), \tag{2}$$

where v^* and w^* are the radial and axial components of the heat flux, $\tau^*(T^*)$ is the total mean free time and $k^*(T^*)$ and $\ell^*(T^*)$ are the bulk thermal conductivity and a non-local length related to the bulk phonon mean free path (MFP), i.e., the mean distance between phonon-phonon collisions. In this model, both k^* and ℓ^* will be based on the Kinetic Collective Model (KCM) framework [36]. Zhu et al. [37] propose that ℓ^* is the geometric mean of the bulk and a local MFP, the latter of which decreases near a boundary. In the following we opt for simplicity and model the decrease in local MFP through an analogy with fluid flow, by introducing a slip boundary condition. For convenience, we will not write the temperature dependence of the parameters explicitly unless it is required due to the context. However, we note that, for the temperature ranges considered here, both the bulk thermal conductivity and non-local length monotonically decrease with temperature. As will be shown in Section 4, the non-local length of silicon decreases from about 5 μm at 50 K to 55 nm at 300 K.

The first term on the left-hand side of Eq. (2) captures memory effects and, in particular, the dependence of heat flux on the history of the temperature gradient. The second term on the right-hand side of Eq. (2) captures non-local effects, such as the interaction of phonons with the boundary of the NW. When the characteristic time and length scales are much larger than the resistive mean free time and non-local length, the G-K Eq. (2) reduces to Fourier's law.

For the remainder of the paper, we restrict our attention to the case of steady-state heat flow. This focus is motivated by the available experimental data. Under the steady-state assumption, $\partial u^*/\partial t = \partial \mathbf{Q}^*/\partial t = 0$. Conservation of energy (1) and the G-K Eq. (2) then reduce to

$$\nabla\cdot\mathbf{Q}^* = 0, \tag{3a}$$

$$\mathbf{Q}^* = -k^*\nabla T^* + \ell^{*2}\nabla^2\mathbf{Q}^*. \tag{3b}$$

This system is clearly analogous to an incompressible, viscous flow with a source term proportional to the velocity. Under this analogy, the parameter $\mu^* = \ell^{*2}/k^*$ may be interpreted as a thermal viscosity. These observations allow us to use well-known techniques from viscous flow to analyse the problem.