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Phonon backscatter, trapping, and misalignment effects on microscale thermal conductance below the Casimir limit

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ABSTRACT

At nanometer to micron length scales, there exists a strong competition between intrinsic and extrinsic scattering mechanisms that can curtail the free flight of phonons and ultimately affect the thermal transport. Despite significant progress in showing the ability to reach behaviors significantly below the Casimir limit, little appears to be understood about the competition between these scattering sources. In this investigation, we propose a simple one-parameter geometry that simultaneously modulates backscattering and trapping effects to enable directed study of these different means of controlling phonons. The geometry is a simple sequence of chambers offset from one another by a defined distance. We use the geometry to study the effects of phonon backscatter, trapping, and corner-turning on the thermal conductance in Si nanowires (NWs). We employ a full Brillouin zone Boltzmann Transport Equation (BTE) method to determine spatially-varying phonon densities in the geometry. Significantly greater impact is seen due to backscatter than any other means of arresting phonon flow. By creating a geometry that maximizes backscatter, a roughly 8-fold reduction in thermal conductance below the Casimir limit can be achieved at room temperature which is a factor of four smaller than the nearest reported value in the literature. The geometry is also useful for systematic investigation of other means of controlling phonons and affecting thermal transport; particularly, we investigate diffuse versus specular boundary scattering and the induced misalignment between the phonon flow and thermal flux due to the shape of the geometry. These effects combine to offer new insights into fundamental phonon behaviors and possible routes to phonon control.

1. Introduction

As the trend towards smaller, more powerful, and more efficient microelectronic and MEMs devices continues, high fidelity control over thermal energy transport continues to grow in importance for maximizing the performance of these devices. Advances in silicon-on-insulator technologies have made devices with nanoscale features smaller than 100 nm commonplace [1]. Furthermore, while early nanostructures were primarily simple nanowires or thin films, it is now possible to engineer nanostructures with novel geometries that deviate significantly from those earlier designs. However, at the submicrometer length scale, classical boundary Brillouin zone-averaged scattering expressions, such as those derived in [2,3], neglect discrete effects such as the propagation direction of individual phonon modes, an important mechanism in heat transport in nanostructures [4]. Therefore, in order to utilize novel device geometries to engineer desirable thermal transport characteristics, a more complete understanding is required of how nanodevice geometries affect phonon transport, resist heat flow, and alter the carriers' ability to conduct heat at the level of individual phonon modes. Many types of devices stand to benefit from the improved ability to engineer heat transport behavior including transistors, photodiodes, and thermoelectrics.

The quest to manipulate heat transport at small scales has brought considerable attention to phononic crystals, i.e. crystalline systems with an artifical secondary periodicity. Such crystals can be developed to have desirable heat transport properties such as a high degree of anisotropy, phononic band gaps, or reduced thermal conductivity. Three types of phononic crystal concepts are found in the present literature. One uses nanopillars [5] or nanodots [6] periodically arranged on structures. The additional features create nonpropagating vibrational modes which can trap thermal energy and reduce thermal conductivity. Another concept uses membranes patterned with periodically-arranged circular [7], square [8], hexagonal [9], and triangular [10] pores. The pores can obstruct phonon flow and thereby reduces thermal conductivity, enhances anisotropy of the heat flow, and in the coherent limit

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creates phononic band gaps. A third concept uses NWs with periodically modulated thickness [11] or irregular surface geometries such as sawtooth [12], corrugated [13], or fishbone [14] features that backscatter phonons or also create nonpropagating modes thereby leading to increased thermal resistance and reduced conductivity. All of these concepts are motivated by the potential to exert control over phonon behaviors using mechanisms that manipulate the way scattering occurs in the conductor. Efforts to combine concepts, such as pores and nanowires [15] and films and nanowires [16], have also shown some degree of effectiveness.

A fourth class of approach operates in a different MFP regime than is of current interest. Whereas our interest is for long MFP phonons, approaches that modulate transport through control over small MFP phonons using defects such as impurities [17], voids/vacancies [18], and dislocations [19], or superlattice constructions [20] have been pursued.

Tangential to these studies has been the surge of interest in reducing thermal conductivity in materials for thermoelectric applications [7,13,14,21–23]. Silicon nanowires (NWs) have gained increasing use as components of thermoelectric systems over the past 10 years due to their desirable thermal conductivity of 25 $\mathrm{W\,m^{-1}\,K^{-1}}$ [24] which is nearly an order of magnitude smaller than its bulk value (156 $\mathrm{W\,m^{-1}\,K^{-1}}$ at 300 K [25]). Findings that roughened sidewalls of NWs can further reduce the conductivity to as low as 1.6 $\mathrm{W\,m^{-1}\,K^{-1}}$ for a 52 nm cross-sectional dimension at room temperature [22] are among efforts that motivate, and are motivated by, the phononics literature.

Thus, the net effects of phononic features on thermal conductivity can be significant. Blanc et al. experimentally studied corrugated Si NWs at low temperatures (0.3–5 K) and found that corrugation resulted in thermal conductance of roughly half the Casimir limit at 1 K [13]. Poborchii et al. studied corrugated Si nanowires at temperatures ranging from 300 to 400 K observing a 60–70% reduction in κ for strongly corrugated wires at 300 K [26]. Monte Carlo simulations indicated that the observed reduction in thermal conductance may be due to phonon trapping or backscattering within the corrugations. Several groups have studied NWs with periodically modulated thickness [11,14,27–31].

Based on the emerging findings, there is now strong evidence that backscattering or trapping plays some role in reducing thermal conductance from intrinsic bulk. Yet, a careful study does not appear to be available presently. In this article we develop a parametric model for altering a Si NW geometry systematically in order to study the phonon transport properties near the limit of vanishing transport. The goal is to study the effect on below-Casimir-transport due to variations in the device dimensions and determine if thermal conductivity can be substantially reduced in simply connected domains by using the interplay and competition between boundary and intrinsic scattering mechanisms. Namely, we examine the interactions of backscatter and constriction and attempt to isolate these from the effects of intrinsic scattering. For the sake of future experimental fabrication ease and potential three dimensional device designs, we eschew interior scattering features such as in [7–10] and instead favor nearly-simply connected domains that contain jogs or offsets. The offsets cause periodically-spaced regions where increased backscattering occurs. Phonons must flow around obstructions, creating regions of misalignment between the phonon flux and the macroscopic temperature gradient. Furthermore, the offset produces constriction effects that lead to a greater degree of "phonon trapping", or when a phonon undergoes multiple backscattering events before exiting. In contrast to previous studies showing reductions in thermal conductivity of 35–70% compared to the uniform NW of same cross-section area [12,14,26,32,33], we find that backscattering and trapping, and not intrinsic scattering due to increased constriction, are the dominant mechanisms for reducing transport and can alone achieve reductions over 90%. The increased backscatter shifts the modewise thermal conductance and serves as a filter for modes of a certain mean free path. Wires with rough sidewalls allow phonons to more easily realign with the macroscopic temperature gradient and flow around offsets. Approaches that do not maximize backscattering produce a less optimal reduction in conductance.

The outline of this article is as follows. The chamber-offset NW and its geometrical parameters are defined in Section 2.1. Section 2.2 describes the methodologies used for ray-tracing and three dimensional full Brillouin Boltzmann transport models. Section 3 presents the modeling results for NW thermal conductance as well as the analyses of the fundamental mechanisms leading to the reduction in phonon transport. Finally, in Section 4 we provide our concluding remarks.

2. Methodology

2.1. Model Geometry

We use Si NW models in this paper. These are composed of cubical chambers with an offset between adjacent chambers. A section of the geometry is shown in Fig. 1 with $\hat{\boldsymbol{x}}$ as the transport direction. The chamber-offset is composed of a periodically repeating segment (indicated by the dash line box), with period $\boldsymbol{T} = W\hat{\boldsymbol{x}} + H\hat{\boldsymbol{y}}$ where W is 50 nm and H is the free parameter varied from 0 nm to 40 nm. NWs of both infinite and finite (450 nm) length are studied. These dimensions are in contrast to previous experimental studies which considered NWs with cross sectional areas ranging from 20 nm $\times$ 20 nm to 196 nm $\times$ 550 nm and lengths ranging from 1.7 μm to 18.8 μm [34–36]. When $H = 0$ the geometry reduces to straight uniform wire with square cross-section. This case provides the reference transport properties. A vertical surface is introduced for any value of $H \neq 0$, which promotes phonon backscattering leading to a reduction in thermal conductance. The backscattering increases thermal resistance even when reflections at the sidewalls are purely specular. The inlet is the face on the left, normal to the x axis, and the outlet is the opposite face on the right. Despite this nomenclature, phonons can leave through either the inlet or the outlet. Phonon backscattering is defined as any scattering event in which the component of the phonon group velocity aligned with the macroscopic temperature gradient changes sign. Thus while the phrase is suggestive of a resistive scattering event, backscattering may, on occasion, lead to an increase in thermal conductivity i.e. when phonons are "forward" scattered toward the outlet.

The phonon scattering mechanisms that are presently considered include boundary scattering and intrinsic Umklapp scattering.

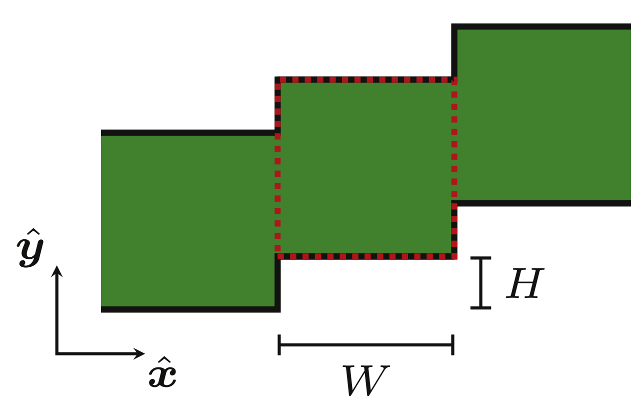

Fig. 1. Finite section of chamber-offset NW geometry. The red dotted area denotes a single *chamber*. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)