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Research Paper

Ballistic thermal wave propagation along nanowires modeled using phonon Monte Carlo simulations

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HIGHLIGHTS

- Ballistic thermal wave propagation along nanowires is investigated using a phonon-traced Monte Carlo method.
- The effects of boundary scattering on thermal wave propagation differ for ballistic-diffusive and diffusive phonon transport.
- Different phonon transport regimes will be measured using different temporal resolution, and their dependencies on phonon scattering regimes are different.

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ABSTRACT

The propagation of ballistic thermal waves when the phonon transport is in the ballistic-diffusive regime is markedly affected by the boundary. This work simulates ballistic thermal wave propagation in nanowires with a phonon-traced Monte Carlo method to investigate the effects of the nanowire characteristics including the radial Knudsen number and the specularity parameter, and the effects of the temporal resolution of the measurements. The phonon boundary scattering accelerates the evolution of the phonon transport from ballistic to ballistic-diffusive and finally to diffusive transport and increases the thermal conduction resistance by reducing the effective thermal conductivity. High heat pulse frequencies lead to thermal wave propagation in ballistic regime, moderate heat pulse frequencies lead to thermal wave propagation in ballistic-diffusive regime and very low heat pulse frequencies lead to purely diffusive thermal wave propagation, i.e. the Fourier thermal conduction. The ballistic-diffusive thermal wave propagation relies heavily on the specific type of the dominated phonon scattering mechanism while the purely ballistic and diffusive propagations do not. Thus, ballistic-diffusive thermal wave propagation should be modeled by a new constitutive equation with new characteristic parameters.

1. Introduction

Rapid developments of micro-electromechanical systems (MEMS) and nano-electromechanical systems (NEMS) [1–4] are placing higher demands on micro/nano devices with the need for excellent physical properties. Semiconductor nanowires and nanowire arrays are being developed as micro/nano devices due to their novel physical optical [5,6], electrical [7,8] and thermoelectric properties [9–11]. The ultra-short pulse laser technique has become an effective tool in micro device machining due to its high precision [12–17]. The interactions between the ultra-short laser pulse and the materials involve a complex set of optical, electrical and thermal processes [12–17] such as photon-electron interactions, electron-electron interactions and transport, electron-phonon interactions, and phonon-phonon interactions and transport. Since the interactions are very fast, the carriers do not relax diffusively but have non-diffusive characteristics. Another area needed in the development of micro/nano devices is thermophysical properties measurements [18]. The small scales require ultra-high temporal and spatial resolution. Ultra-short pulse lasers offer the necessary resolution for the nanomaterial measurements in a non-contact method called pump-probe optical measurements [19–22] which can be used to measure the properties of thin films [19–23] and nanowire arrays [24]. However, for semiconductor nanostructures like nanowires, the special nature of these nanoscale devices requires more detailed information about the nanowires such as the mean free path (or relaxation time) distributions which require ultrafast carrier dynamics measurements [8,25,26] in addition to their macroscopic thermal physical

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properties to tune and optimize their optical, electrical and thermal properties.

In both ultra-short pulse laser machining and laser measurements, theoretical research on ultrafast heat conduction is needed to guide process analyses. In semiconductor materials, the phonons dominate the thermal conduction as the main carrier [27]. When the characteristic thermal time is on the order of picoseconds, comparable with the phonon relaxation time, the classical Fourier's law fails to predict the phenomena because the heat is transported in the phonon ballistic-diffusive regime [28–33] as thermal waves [34,35]. As a result, more precise modeling and analyses for measurements should start from a more fundamental basis (e.g. the phonon Boltzmann transport equation) instead of the macroscopic models (e.g. Fourier's law). Classical phonon transport theory has two kinds of thermal waves including ballistic thermal waves from the phonon ballistic transport and the second sound from phonon normal scattering dominated transport [34,35]. This research focuses on the ballistic thermal waves occurring in phonon ballistic-diffusive transport. Previous theoretical and numerical analyses have mostly focused on one-dimensional models [36,37] with few studies of three-dimensional effects that include lateral boundaries. However, research on thermal wave propagation in three-dimensional nanostructures is essential as there are more and more measurements of complicated nanostructures such as nanoporous silicon [23] and nanowire arrays [24]. In one-dimensional cases, the thermal wave is mostly affected by the phonon boundary emissions and is dissipated by the intrinsic phonon scattering [34,35], with more phonon boundary scattering involved in three-dimensional cases. Typical boundaries and interfaces include the lateral boundaries in nanowires [38–41], emission and reflection boundaries in nanofilms [34,35] and the interfaces in superlattice nanofilms [42] and polycrystals [43,44]. Unlike steady state heat conduction [38–44], ultrafast heat conduction is a non-equilibrium process with both spatial and temporal variations, making it more complicated and more easily influenced by the properties and spatial distribution of the boundaries in addition to the internal properties of the materials [33].

Although many studies have carried out to develop the macroscopic constitutive heat conduction equation using the phonon Boltzmann transport equation [29,37], especially for cross-plane ultrafast heat conduction, modeling on the boundaries both in microscopic and macroscopic levels which dominate for large Knudsen number conditions are few. Analyses of thermal transport problems that are heavily affected by the boundaries need a comprehensive understanding of the effect of the boundaries to develop a practical constitutive heat conduction equation and make reasonable extensions. Finally, since the effective thermal physical properties of nanomaterials are closely related to the measurement characteristics including the measurement parameters [45] and methods [46], development of a new constitutive equation must carefully considers experimental and engineering practices. Consequently, the characteristic parameters in thermal applications and measurements should be taken into consideration in establishing a new macroscopic constitutive equation with new characteristic parameters to describe the thermal processes and guide the data analyses in experiments.

This work investigates ballistic thermal wave propagation in nanowires using a phonon-traced Monte Carlo (MC) method. Cases with different radial Knudsen numbers, Kn_r and specularity parameters, p, are simulated to study the effects of the general characteristics of the nanowires in both phonon ballistic-diffusive transport and diffusive transport. Heat pulses with various periods are simulated to investigate the effects of the temporal resolution of the measurements. The results give a comprehensive understanding of ballistic thermal wave propagation in nanowires to guide further experimental analyses.

2. Phonon Monte Carlo methods

A phonon-traced Monte Carlo simulation method is used to model the ballistic-diffusive phonon transport [32,47] to simulate the ballistic thermal wave propagation in nanowires by directly solving the phonon Boltzmann transport equation in the nanowires,

$$\frac{\partial f}{\partial t} + v_g \cdot \nabla f = -\frac{(f - f_0)}{\tau_R}, \tag{1}$$

in which f and f_0 are the phonon distribution function and the phonon equilibrium distribution function, τ_R is the relaxation time for phonon resistive scattering, t is the time and v_g is the phonon group velocity. The heat pulse trace and the nanowire model with a circular cross section are shown in Fig. 1. The heat pulse is input from the left end ($x = 0$) of the nanowire and propagates in the x direction, i.e. the axial direction. The radial direction is described by the radius r and the circumferential direction by the angle φ. The initial temperature of the nanowire is set to be 300 K, room temperature. Phonons are emitted according to the Lambert cosine law at the emission boundary. As Eq. (1) shows, phonon intrinsic scattering is treated with the relaxation time approximation. Phonons interact with the lateral boundary and are scattered back into the nanowire. The phonon boundary scattering is modeled using a specularity parameter, p, according to the formula proposed by Ziman [27],

$$p = \exp(-16\pi^3\delta^2/\lambda^2), \tag{2}$$

in which δ is the root mean square surface roughness and λ is the phonon wavelength. Generally, when the lateral boundaries of the nanowires and nanofilms are flat and the surface roughness is smaller than the phonon wavelength, this classical formula, i.e. Eq. (2), is applicable. In this work, we study the phonon boundary scattering effect using the classical framework in which the boundary roughness is described by the specularity parameter, p. The boundary condition for the lateral boundary in the nanowire is [27]

$$g(\vec{k}, r_B)_{v_n} = pg(\vec{k}', r_B)_{-v_n}, \tag{3}$$

in which g is the deviation distribution function $(f - f_0)$, $\vec{k}'$ and $\vec{k}$ are the wave vectors for the incident and reflected phonons at the boundary, and r_B is the phonon boundary scattering location. Eq. (3) means that $p \times 100\%$ of the phonons colliding with the boundary are scattered specularly with the rest scattered diffusively. The specular scattering conserves the phonon momentum and the non-equilibrium part of the distribution function while the diffuse scattering does not. For a nanowire, the radius of the circular cross section is R and the thickness of the nanowire is described by the radial Knudsen number, Kn_r, defined as $Kn_r = l/R$ where l (56 nm) is the mean free path of the phonon intrinsic scattering [29]. Here, the phonon group velocity, v_g, is 5000 m/s [29]. The heat pulse period, t_p, is 0.2, 2, or 20 ps for the investigations. The gray model is used for the phonon frequency spectrum and the Debye approximation is used for the dispersion [30].

3. Results and discussion

3.1. General discussion

There are several key factors that affect the propagation of the ballistic thermal wave in nanostructures including the phonon emissions at the boundary, the characteristics of the heat pulse (especially the period, t_p), the time, t, of the thermal wave propagation, the relaxation time, τ, for the phonon intrinsic scattering (including τ_N for normal scattering, τ_R for resistive scattering and τ_i for isotopic scattering), the specularity parameter, p, the radial