Theoretical and Applied Mechanics Letters 6 (2016) 113–121

Contents lists available at ScienceDirect

Theoretical and Applied Mechanics Letters

journal homepage: www.elsevier.com/locate/taml

Review

Heat transport in low-dimensional materials: A review and perspective

Zhiping Xu *

Applied Mechanics Laboratory, Department of Engineering Mechanics and Center for Nano and Micro Mechanics, Tsinghua University, Beijing 100084, China

State Key Laboratory of Mechanics and Control of Mechanical Structures, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, China

HIGHLIGHTS

- Heat transport is a key energetic process in materials and devices.
- The rich spectrum of imperfections in low-dimensional materials introduce fruitful phenomena.
- We focus on the roles of defects, disorder, interfaces, and the quantum-mechanical effect.
- New physics from theory and experiments is reviewed, followed by a perspective on open challenges.

ARTICLE INFO

Article history:
Received 30 March 2016
Received in revised form
26 April 2016
Accepted 28 April 2016
Available online 9 May 2016
*This article belongs to the Solid Mechanics

Keywords:
Nanoscale heat transport
Low-dimensional materials
Defects
Disorder
Interfaces
Quantum mechanical effects

ABSTRACT

Heat transport is a key energetic process in materials and devices. The reduced sample size, low dimension of the problem and the rich spectrum of material imperfections introduce fruitful phenomena at nanoscale. In this review, we summarize recent progresses in the understanding of heat transport process in low-dimensional materials, with focus on the roles of defects, disorder, interfaces, and the quantum-mechanical effect. New physics uncovered from computational simulations, experimental studies, and predictable models will be reviewed, followed by a perspective on open challenges.

Contents

1. Introduction to thermal energy transport

Nanoscale heat transport is a key energetics process for the functioning and stability of integrated nanosystems and nanostructured materials, which hold great promises in a variety of applications ranging from energy management, conversion [1], phononics based computation [2], and thermotherapy for cells and tissues [3]. The nature of thermal energy transport is the

* Correspondence to: Applied Mechanics Laboratory, Department of Engineering Mechanics and Center for Nano and Micro Mechanics, Tsinghua University, Beijing 100084, China.
E-mail address: xuzp@tsinghua.edu.cn.

http://dx.doi.org/10.1016/j.taml.2016.04.002

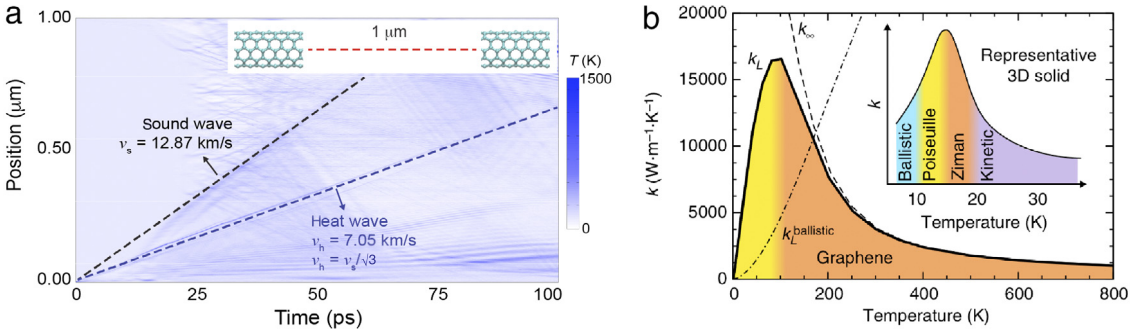

Fig. 1. (a) Temperature evolution as a heat pulse propagates along a 1 μm-long single-walled (5, 5) carbon nanotube (CNT), obtained from classical molecular dynamics simulations. The dash line indicates fronts of the ballistic longitudinal wave and collective heat wave, respectively. The velocities are v_s and $v_h = v_s/\sqrt{3}$. (b) Temperature dependence of thermal conductivity for 3D and 2D solids [4].

redistribution of kinetic energies in materials, toward thermal equilibrium or steady state under temperature gradient. This process demonstrates a ballistic behavior at short length scales, where energy propagation proceeds in forms of coherent waves (Fig. 1(a)). At another limit where the lattice vibration waves are strongly perturbed by scattering sources, diffusive behaviors are expected.

Between these two extremes there are mechanistic transitions taking place at specific length and time scales, or a critical concentration of resistive sources in the material. One feasible approach to formalize the intermediate regime is to divide the heat flux into two components in the transport processes, known as the ballistic–diffusive model [5,6]. One originates from the thermal boundaries and represents the ballistic part. The other component is contributed by scattered and excited carriers as diffusive processes. To characterize the transition in between, a mean free path l_{MFP} can be defined for the carriers, below which a wave-like behavior is preserved. For crystalline nanostructures such as carbon and boron-nitride nanotubes, the phonon mean free path could reach hundreds of nanometers, which exceeds the characteristic length of structural ripples and approaches the theoretical limit set by their radius of curvature [7]. The robustness of heat conduction in these nanostructures refines the ultimate limit far beyond the reach of ordinary materials. In the ballistic limit, coherent wave propagation can be outlined by the Landauer formula through a transmission function defined for both elastic or inelastic scattering processes [8]. Beyond the length scale of $\sim l_{MFP}$, a thermal excitation emitted at the heat source loses its memory of both phase and momentum, and this diffusive nature allows a phenomenological description based on the diffusive Fourier's law. However, the parabolic diffusion equation predicts that a pulse of heat at the origin is felt at any distant point instantaneously, admitting an infinite speed of propagation of heat signals, which is in contradiction with the theory of relativity. To recover part of the wave-like nature into the diffusive picture and approach the ballistic limit, a number of updated models have been proposed by adding characteristic time scales in a hyperbolic form of equation, for example. Although being successful in solving some practical problems, works by Cattaneo [9], Vernotte [10], and Chester [11] following this spirit have been criticized for their phenomenological treatment that leads to both conceptual ambiguity in the definition of temperature and unrealistic behaviors in their predictions. Additional parameters have to be included for the time delay between heat flux and the temperature gradient in the fast-transient processes.

For crystalline solids where the notion of phonon is well defined, one can perform lattice dynamics calculations to determine harmonic and anharmonic force constants. These parameters can then be used to construct a semi-classical theory based on the phonon Boltzmann–Peierls transport equation (phBPE), which is able to bridge the ballistic and diffusive models coherently [12]. The thermal conductivity of materials, κ, could be predicted within this framework by including multiple-phonon scattering effects through high-order force constants, which can be calculated from density-functional theory based first-principles calculations. For example, the predicted values of κ for silicon agree well with experimental measurements in a wide range of temperature [13,14]. This approach has also been validated for a wide spectrum of materials including those with complex structures such as the clathrate [15]. Moreover, this first-principles approach using phonon as the propagating quanta also yields detailed information of the heat transport process, such as mode-resolved relaxation time and resistance, and the resistive contribution from phonon–phonon interactions at different orders [14,16,17]. By decomposing the thermal resistance from individual scattering events including normal, resistive (Umklapp, isotopic) and extrinsic processes, classification of thermal transport regimes can be made. The Umklapp and isotopic processes are resistive, while the normal process can result in energy flow between phonon modes. The temperature dependence of thermal conductivity serves commonly as a spectroscopy to extract information of these scattering sources, and the resistive contribution from them can be added up using the Matthiessen's rule by assuming they are independent. Recent studies show that the dimension of materials plays a key role in the selection of regimes [4,18]. In graphene, as an example of two-dimensional (2D) crystals, normal processes dominate over the Umklapp scattering well-above the cryogenic condition, extending to room temperature and even more, which allows the Poiseuille and Ziman hydrodynamic regimes emerging at ordinary conditions, as demonstrated through drift motion of phonons, significance of boundary scattering and second sound (Fig. 1(b)) [4,18]. These facts indicate that the low-dimensional nature grants these nanostructures uncommon significance as model materials for the study of heat transport in the non-diffusive manner.

For material samples measured in thermal transport experiments, imperfections inevitably present at large length and time scales, which not only introduce thermal resistance, but may also alter the mechanism of heat transport. Defects, disorders, and interfaces in materials lead to weak or strong wave scatterings, and even localization of wave propagation. Scaling theory predicts that wave localization is more significant in lower dimensions [19], although compared to quantized waves such as the electrons, the spatial extension of vibrational waves, especially low-frequency waves at the continuum limit, is much larger and this effect is less significant [20]. These fundamental mechanisms of heat conduction considering these factors have not been well understood yet because of the lack of efficient control and characterization tools in exploring microscopic heat transport and dissipation processes in materials. The mean free path of phonons in nanostructures such as CNTs or graphene is expected to be extraordinarily