Dynamics of Long-Wavelength Phonons Near Boundaries and Interfaces in Nanomaterials

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ABSTRACT

Long-wavelength phonons undergo infrequent phonon-phonon scattering and propagate ballistically over long distances in single-crystalline, high-quality bulk materials, thereby making a major contribution to thermal conductivity in these systems. The dynamics of long-wavelength phonons and their interaction with boundaries and interfaces can be accurately modeled within the elastic-continuum limit. We present our modeling of thermal transport in the long-wavelength limit in the presence of boundary and interface disorder that relies on the finite-difference time-domain (FDTD) solution to the elastic wave equation and is strongly informed by experiment. We show the emergence of phenomena such as the incoherent-to-coherent transition in thermal transport in III-V superlattices and the changes in the power-law dependence of phonon lifetime on frequency for rough nanowires and membranes with varying correlation types. The work illustrates the complexity of phonon interaction with disorder, and the utility and flexibility of numerical techniques such as the finite-difference time-domain (FDTD) method for elucidating the dynamics of phonons in nanomaterials.

ELASTIC-WAVE MODELING OF LONG-WAVELENGTH PHONON DYNAMICS

We present thermal transport in a) III-V alloy superlattices, such as those used in quantum cascade lasers, and in b) rough silicon nanowires. Our simulation work is corroborated with experimental data. We solve the elastic wave equation using the finite-difference time-domain (FDTD) technique in the velocity-stress formulation, starting from the code base we developed earlier [1]. Interface and boundary roughness are generated according to a correlation type with a given rms roughness and correlation length [1].

To simulate thermal transport in InGaAs/InAlAs alloy superlattices, we performed FDTD calculations with several rms roughness values and correlation lengths, and all of which are close to experimental observations [2]. We then used these FDTD calculations as training data for a neural-network-based machine-learning algorithm in order to identify the optimal values of rms roughness and correlation lengths that give the best agreement between measurements and calculations. Both experiment and simulation show a cross-over between incoherent and coherent phonon transport in alloy superlattices as the interface density increases (Fig. 1).

As for transport in nanowires, a Gaussian longitudinal wave packet is launched at the center of a Si nanowire (Fig. 2) toward the rough interface formed between Si and Al (right boundary of the domain). The Gaussian pulse is centered around a certain frequency, typically one that coincides with a resonant mode. The Fourier transform of this signal is peaked around the launch frequency and its harmonics, and there is a notable broadening to it that depends on roughness properties. Each prominent peak is fitted with a Lorentzian to extract the line width, which corresponds to the scattering rate (inverse of scattering lifetime). Lifetime versus frequency power-law dependence carries valuable information about the interplay between wire dimensions and roughness features.

This work was funded by the AFOSR (award FA9550-22-1-0407), NSF (award 2212011), and the Splinter Professorship.

REFERENCES

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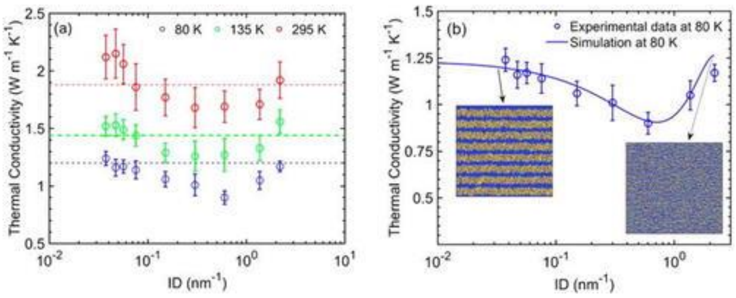

Fig. 1: (a) Experimental values of the cross-plane thermal conductivity at 80 K (blue), 135 K (green), and 295 K (red) vs interface density ranging from 0.0374 to 2.19 nm^{-1}. The dashed horizontal lines represent the reference values for the bulk quaternary alloys of the same stoichiometry as the SLs. (b) Experimental (open symbols) and modeling values (solid curve) for the cross-plane thermal conductivity as a function of interface at 80 K. Symbols are experimental averages, and error bars are the standard deviation of four measurements. Insets to panel (b) depict simulated structures with low and high interface densities. Reprinted with permission from AIP Publishing from Appl. Phys. Lett. 121, 232201 (2022).

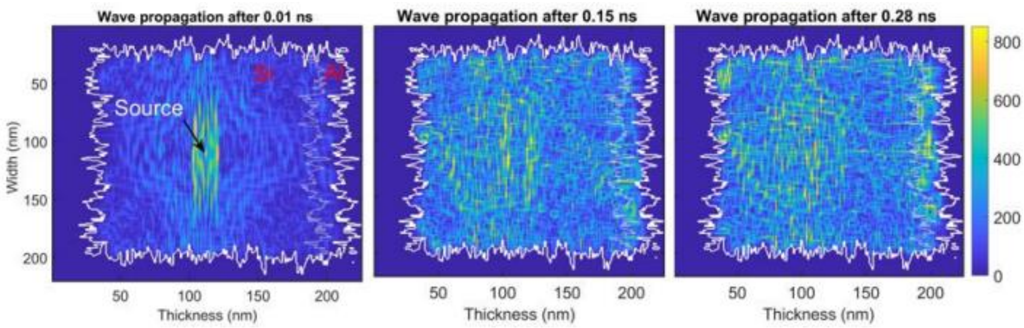

Fig. 2: (Preliminary work) A Gaussian wave packet launched from the center of a Si nanowire (170 nm width; 200 nm thickness) capped with Al (layer on the right). Snapshots taken 0.01 ns (left), 0.15 ns (center), and 0.28 ns (right) after launch. The rough surface is exponentially correlated with a correlation length of 1.7 nm (0.01 of the width) and rms roughness of 5 nm.

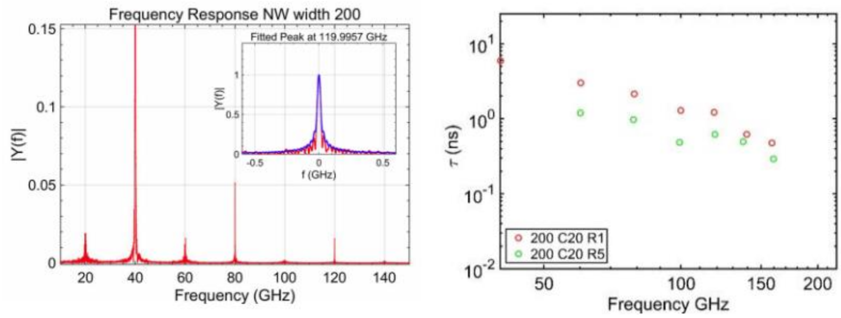

Fig. 3: (Left) Fourier transform of the time-resolved, spatially averaged velocity magnitude (divided by velocity magnitude of the launched Gaussian wave). Each prominent peak is fitted with a Lorentzian (see inset) whose width corresponds to the scattering rate, the inverse of lifetime due to roughness as averaged over the whole surface. (Right) Sample data presenting lifetime versus elastic-wave frequency for two different rms roughness (1 and 5 nm), but the same wire dimensions (200 nm x 200 nm) and correlation length (20 nm). The dependence of the lifetime on frequency carries important information about the interplay between aspect ratio of the wire cross section, the rms roughness, and the roughness correlation length and type.