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Phonon Heat Conduction In Nanostructures: Ballistic, Coherent, Localized, Hydrodynamic, and Divergent Modes[1]

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In this talk, we will discuss different modes of heat conduction in nanostructures. Ballistic transport happens when phonon mean free path is longer than the characteristic size of the structure. We will discuss how we compute phonon mean free path distributions based on first-principles and measure the distributions with optical pump-probe techniques by exploring ballistic phonon transport processes. In superlattice structures, ballistic phonon transport across the whole thickness of the superlattices implies phase coherence. We observed this coherent transport in GaAs/AlAs superlattices with fixed periodic thickness and varying number of periods. Simulations show that although high frequency phonons are scattering by roughness, remaining long wavelength phonons maintain their phase and traverse the superlattices ballistically. Accessing the coherent heat conduction regime opens a new venue for phonon engineering. We show further that phonon heat conduction localization happens in GaAs/AlAs superlattice by placing ErAs nanodots at interfaces. This heat-conduction localization phenomenon is confirmed by nonequilibrium atomic Green's function simulation. These ballistic and localization effects can be exploited to improve thermoelectric energy conversion materials via reducing their thermal conductivity. In another opposite, we will discuss phonon hydrodynamic transport mode in graphene via first-principle simulations. In this mode, phonons drift with an average velocity under a temperature gradient, similar to fluid flow in a pipe. Conditions for observing such phonon hydrodynamic modes will be discussed. Finally, we will talk about the one-dimensional nature of heat conduction in polymer chains. Such 1D nature can lead to divergent thermal conductivity. Inspired by simulation, we have experimentally demonstrated high thermal conductivity in ultra-drawn polyethylene nanofibers and sheets.

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