Engineering Phonon Transport at Multiple Scales: Phonon Coherence and Localization

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The last decade has seen a rising notion of the wave nature of phonons. For instance, ballistic transport of coherent phonon in superlattices was observed in both experiments and atomistic simulations. These coherent phonons allegedly arise from the interference of backscattered phonon waves at the densely packed interfaces, which should otherwise greatly hinder the transport of particle-like phonons. In this invited talk, we will discuss our recent explorations of the exotic behaviors of coherent phonons and their relations with conventional incoherent phonons, of which the transport and scattering processes were commonly treated in a particle-like manner. First, we will demonstrate that randomizing the layer thicknesses of a superlattice, which leads to localization of phonons, can reduce its thermal conductivity to even below the amorphous material limit, which can hardly be achieved by merely scattering phonons. Notably, machine learning can be very helpful to guarantee sufficient structural optimization to fulfill this purpose. Second, we will discuss how the coexistence of coherent phonons and incoherent phonons, which can scatter and convert into each other, in the same material can lead to complex temperature dependence or length dependence of thermal conductivity of superlattices. In particular, we will rigorously explain these behaviors by decomposing thermal transport into coherent phonon and incoherent phonon contributions via the Landauer-Datta-Lundstrom approach. Detailed spectral phonon analysis will further reveal the interplay between coherent and incoherent phonons, as well as their respective effect on thermal transport. Finally, we will discuss the feasibility of engineering coherent and incoherent phonons in a decoupled manner. This provides the opportunity to continuously reduce the lattice thermal conductivity of the superlattice structure towards improved thermoelectric or thermal barrier applications.