Thermal Transport in Micro-Scale Phononic Crystals: Observation of Coherent Phonon Scattering at Room Temperature and its implications to Thermoelectrics

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Abstract: We report on the experimental observation of coherent phonon boundary scattering in micro-scale phononic crystals (PnCs) at room temperature. We show that the neglecting coherent boundary scattering leads to gross overestimation of the measured thermal conductivities of the PnC samples. We introduce a hybrid model that accounts for partial coherent and partial incoherent phonon boundary scattering. Excellent agreement with the experiment is achieved.

Almost all physical processes produce heat as a byproduct making thermoelectric (TE) systems very attractive for energy scavenging applications. Energy conversion in TE devices is based on the so called Peltier effect. Here the temperature gradient resulting from expelled heat is used to force electronic transport resulting in an electric current. As such, heat transported via phonons represents a leakage mechanism and serves to reduce the efficiency of TE systems. Indeed the inability to suppress or eliminate the relative phonon contribution to thermal transport as compared to the electronic one has hindered the development of efficient TE devices. Recently, it has been proposed that coherent boundary scattering in micro-scale phononic crystals (PnCs) may hold the key to solving this problem by scattering phonons with minimal influence on electrons. PnCs are artificial structures with a periodic variation in mechanical impedance brought about by the introduction of holes or plugs of one material into a homogenous matrix of another. This periodic variation results in rich phonon dispersion with unusual behaviors. In this communication, we focus on micro-scale PnCs formed by the introduction of air holes in a Si matrix with minimum feature sizes ≥100nm. As a phonon population traverses such a lattice, it can undergo two types of scattering processes: simple incoherent scattering as a result of encountering a boundary; and coherent Bragg-like scattering due to the periodic topology of the artificial lattice of air holes. In the first type, it is assumed that the phonons will retain no phase information after each scattering event. This implies that the phonon dispersion remains unaltered due to the introduction of the air-holes. In the second type, on the other hand, it is assumed that the phase is preserved throughout several scattering events thus enabling coherent interference to occur. Consequently, this would imply a modified phonon dispersion that is sensitive to the topology of the PnC air-hole lattice. Practically, this can have profound implications because: while incoherent boundary scattering depends only on the shape, size, and separation of the holes; coherent boundary scattering additionally depends on the symmetry and topology by which these holes are distributed. Thus, the existence of coherent scattering would allow one to further reduce the thermal conductivity of the underlying material without the need for additional boundaries (e.g. more air-holes) by simply altering the PnC topology.

The claim of coherent phonon scattering in micro-scale Si/Air PnCs at room temperature has generated widespread controversy in the literature given the relatively small wavelength characteristic of the phonon population dominating the thermal transport. Experimentally however, the thermal conductivity (κ) of PnC samples have consistently been measured to be significantly lower than that of an unpatterned film. In fact far lower than what would be expected due to the combination of material removal and simple incoherent boundary scattering, thereby suggesting that another κ reduction mechanism, possibly coherent scattering, must be taking place. The
controversy was heightened by the discovery that ~50% of \( \kappa \) in Si is carried by phonons with mean free paths (MFPs) from 100nm up to 1\( \mu \)m\textsuperscript{15}, which was recently verified experimentally\textsuperscript{16}. Since it is logical to assume that a phonon remains coherent over its MFP, we suggest here that the MFP, rather than wavelength, should be used when judging whether or not coherent scattering events can take place. In which case, a large enough fraction of the phonon population could travel sufficient distances to experience the PnC lattice periodicity and thus undergo coherent scattering.

We report on the experimental observation of coherent phonon boundary scattering in micro-scale phononic crystals (PnCs) at room temperature. We investigate the existence of coherent phonon boundary scattering resulting from the periodic topology of the PnCs and its influence on the thermal in silicon. To delaminate incoherent from coherent boundary scattering, PnCs with a fixed minimum feature size, differing only in the unit cell topologies, were fabricated. A suspended island platform was used to measure the thermal conductivity. We show that the neglecting coherent boundary scattering leads to gross overestimation of the measured thermal conductivities of the PnC samples. We introduce a hybrid model that accounts for partial coherent and partial incoherent phonon boundary scattering. Excellent agreement with the experiment is achieved emphasizing the influence of coherent zone folding in PnCs. Our results yield conclusive evidence that significant room temperature coherent phonon boundary scattering does indeed take place.

References
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