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Molecular Detection and Phonon Filtering in Heat-Transfer Spectroscopy[1] KAMIL WALCZAK, KIRK YERKES, Air Force Rsch Lab - WPAFB — We examine heat transport carried by acoustic phonons in the systems composed of nanoscale chains of masses coupled to two thermal baths of different temperatures. Thermal conductance is obtained by using linearized Landauer formula for heat flux with phonon transmission probability calculated within atomistic Green's functions (AGF) method. AGF formalism is extended onto dissipative chains of masses with harmonic coupling beyond nearest-neighbor approximation, while atomistic description of heat reservoirs is also included into computational scheme. The resonant structure of phonon transmission spectrum is analyzed with respect to reservoir-dimensionality effects, molecular damping, and mass-to-mass harmonic coupling. Analysis of transmission zeros (antiresonances) and their accompanied Fano-shape resonances are discussed as a result of interference effects between different vibrational modes. Specifically, we show that the heat-transfer-based characterization method may be used to identify individual molecules or filter out specific phonon modes from the whole frequency spectrum.

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