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Rayleigh surface waves, phonon mode conversion, and thermal transport in nanostructures LEON MAURER, IRENA KNEZEVIC, University of Wisconsin-Madison — We study the effects of phonon mode conversion and Rayleigh (surface) waves on thermal transport in nanostructures. We present a technique to calculate thermal conductivity in the elastic-solid approximation: a finite-difference time-domain (FDTD) solution of the elastic or scalar wave equations combined with the Green-Kubo formula. The technique is similar to an equilibrium molecular dynamics simulation, captures phonon wave behavior, and scales well to nanostructures that are too large to simulate with many other techniques. By imposing fixed or free boundary conditions, we can selectively turn off mode conversion and Rayleigh waves to study their effects. In the example case of graphenelike nanoribbons with rough edges, we find that mode conversion among bulk modes has little effect on thermal transport, but that conversion between bulk and Rayleigh waves can significantly reduce thermal conductivity. With increasing surface disorder, Rayleigh waves readily become trapped by the disorder and draw energy away from the propagating bulk modes, which lowers thermal conductivity. We discuss the implications on the accuracy of popular phonon-surface scattering models that stem from scalar wave equations and cannot capture mode conversion to Rayleigh waves.

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