Abstract Submitted
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Micro to Nano Scale Heat Conduction in Thermoelectric Materials MARTIN MALDOVAN, MIT — Understanding and controlling heat transfer in solids is very important for increasing the efficiency of thermoelectric materials such as skutterudites, clatharates, superlattices, nanowires, and quantum dots. Although the mechanisms governing the thermal conductivity have been understood for years, a comprehensive theoretical method to calculate heat transfer, particularly at small scales, has not been available. This is mainly due to the complexity of anharmonic processes and phonon boundary scattering. We present a comprehensive theoretical model to calculate the thermal conductivity of thermoelectric materials at small length scales. The approach involves an exact calculation of the reduction of the phonon mean free paths due to boundary scattering and removes the need to solve the Boltzmann equation or to use adjustable terms as in the Callaway or Holland models. The analysis is based on the kinetic theory of transport processes and considers general expressions for dispersion relations, phonon mean free paths, and surface specularity parameters. The results show an excellent agreement with experiments for thin films, nanowires, and superlattices over a wide range of temperature and across multiple length scales. The theoretical approach can further be applied to a wide variety of problems involving the conduction of heat in micro/nanostructured thermoelectrics. This research was funded by the MIT Energy Initiative.

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