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Nanoscale Interface Scattering of Phonons in Multilayered Nanostructures KARTIK KOTHARI, MARTIN MALDOVAN, Georgia Inst of Tech — Nanostructures can be employed to control thermal and electrical properties and increase thermoelectric energy conversion efficiency. An insight into surface and interface scattering in nanostructures is essential in manipulating these properties, which in turn affect the thermoelectric figure of merit ZT. An understanding of the surface conditions is imperative for predicting the amount of specular reflection and transmission of phonons. A crucial challenge is to incorporate this along with different physical properties of constituents across an interface. We employ an extension of the electromagnetic wave scattering theory for rough surfaces developed by P. Beckmann and A. Spizzichino to account for thermal phonon interface scattering. This is supplemented with the Fuchs-Sondheimer theory to formulate thermal transport in layered nanostructures. A rigorous analysis incorporating complete layer coupling, reflection and refraction conditions, and surface shadowing effects is presented. Thermal conductivities of superlattices, bi-layers and sandwich-layered structures made of different constituent materials including Si-Ge, AlAs-GaAs and Si-$\mathrm{Si_xGe_{1-x}}$ are calculated. An evaluation of the amount of heat flow confined within a constituent, and extended over multiple layers is performed. A detailed analysis of the heat spectrum is also presented which allows to predict the amount of heat carried by phonons of different frequencies and mean free paths. The proposed accurate description of phonon surface scattering and prediction of heat spectra would allow for the design of nano-engineered materials and devices with improved thermoelectric properties.

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