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Phonon transmission and thermal transport in GaAs-AlAs superlattices from first-principles KEIVAN ESFARJANI, ZHITING TIAN, MARIA LUCKYANOVA, TENGFEI LUO, GANG CHEN, MIT, NANO-ENGINEERING TEAM — Using the Green's function method and Landauer's formula, we formulate phonon transport in a 3D superlattice. The theory is harmonic and describes coherent (elastic) transport of heat through a periodic structure which may also have disorder present at its interfaces. We compute the force constants from first-principles density functional calculations and use them to compute the transmission, and the thermal conductance of a GaAs-AlAs superlattice versus length and temperature. We also investigate the effect of mass disorder at the interface and anharmonicity, to locate the transition from coherent to incoherent transport. Results are finally compared with experimental measurements.

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