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A first principles approach for thermal transport in nanostructures with defects DEREK STEWART, Cornell Nanoscale Facility, Cornell University, IVANA SAVIC, CEA-Grenoble, NATALIO MINGO, CEA-Grenoble and UC Santa Cruz — Efficient heat transport is essential for developing viable nanoscale devices. On these small scales, defects, impurities, and even isotopic composition can dramatically affect thermal transport in heat conduits such as nanowires and nanotubes. We present a first principles approach that combines a non-equilibrium Green's function formalism for thermal transport with interatomic force constants derived from density functional calculations. We apply this approach to examine the thermal conductance in several potential heat conduits such as carbon nanotubes, boron nitride nanotubes, and silicon based nanowires. These nanostructures are treated in terms of a central region linked to two semi-infinite leads and interatomic force constants are calculated for the three separate regions. The role of defects on thermal conductance is examined for the different devices and the results are compared to empirical potential calculations and commonly used analytical models.

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