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Lattice thermal conductivity with first-principles anharmonic lattice model TERUMASA TADANO, YOSHIHIRO GOHDA, SHINJI TSUNEYUKI, Department of Physics, The University of Tokyo — First-principles calculation of lattice thermal conductivity is important to design new devices such as high-efficiency thermoelectric materials. For lattice thermal conductivity calculations of complex materials and nanostructures, non-equilibrium molecular dynamics (NEMD) is more suitable than widely used Boltzmann transport theory. However, a combination of NEMD and FPMD is almost impossible because of its high computational cost, so that NEMD has been performed only with classical model potentials for specific materials. In order to overcome this limitation in materials, we have developed a new methodology for calculating lattice thermal conductivity without relying on any experimental values. In this method, the potential energy of a system is expressed as a many-body anharmonic model, that is, a Taylor expansion of the total energy with respect to displacements of atoms up to 4th order. Parameters of the anharmonic lattice model are determined with Hellmann-Feynman force of FPMD by least-square fitting. We performed thermal conductivity calculations with the anharmonic lattice model combined with NEMD and obtained reasonable agreements with experimental values.

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