Molecular Dynamics Study of One Dimensional Heat Conductivity

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Abstract

The behavior of individual atoms and their interaction with one another in condensed matter is not easily observed using conventional instruments in the laboratory. This leads to difficulty testing proposed theories about how such a system behaves. Molecular dynamics takes advantage of computer simulations that can test these theories by "measuring" fundamental quantities at discrete time intervals and observing how they change.

In this work, a computer program written in the Fortran 90 language was developed to observe heat conduction in a one dimensional crystal lattice. One dimensional crystal samples were created with random displacements in atomic positions. Forces between atoms were governed by a Lennard-Jones nearest neighbor potential. A temperature gradient was constructed by driving the ends of the sample with Langevin equations incorporating damping and Gaussian white noise driving terms. The simulations were carried out using a modified Verlet time step algorithm.

We obtain results for the effective thermal conductivity for varying chain lengths up to fifteen thousand atoms and select temperature gradients and damping factors that exemplify the anharmonicity of the Lennard-Jones potential. Work has begun on the extension of the program to two dimensions and comparing results with those obtained by phonon gas and perturbation theory.

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