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Abstract
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Disciplines
Engineering | Materials Science and Engineering

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Dynamical behavior of heat conduction in solid Argon

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Abstract. Equilibrium molecular dynamics is performed to obtain the thermal conductivity of crystalline argon using the Green-Kubo formalism, which permits the study of dynamical details of the transport process. A large system run to longer times is used to derive the heat flux autocorrelation functions from the low temperature solid to the liquid state. The power spectrum of an autocorrelation function reveals the change in the nature of the underlying atomic motions across the temperature range.

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PACS: 02.70.Ns, 66.70.-f

The theory of thermal conduction in electronically insulating crystals is based on the phonon concept in which the individual (rapid) atomic motions are averaged out. Molecular dynamics method enables us to look into both fast and slow atomic motions, at the cost of computational efforts. Crystalline argon is a good benchmark target because the interatomic potential is well described by the Lennard-Jones potential and experimental data are available. The temperature dependence of thermal conductivity has been studied using the equilibrium molecular dynamics method with the Green-Kubo formalism and the results compared with experiment. We have previously performed a simulation [1] for a system of 864 particles with 10^7 time steps, and the resulting thermal conduc-

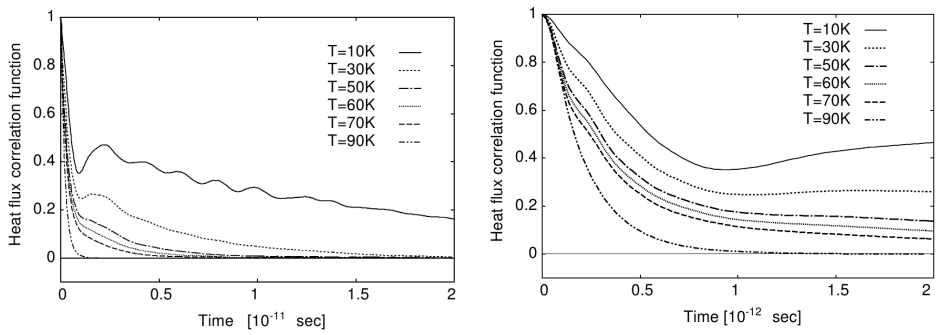

FIGURE 1. Heat flux autocorrelation function for the long (left) and short (right) time range

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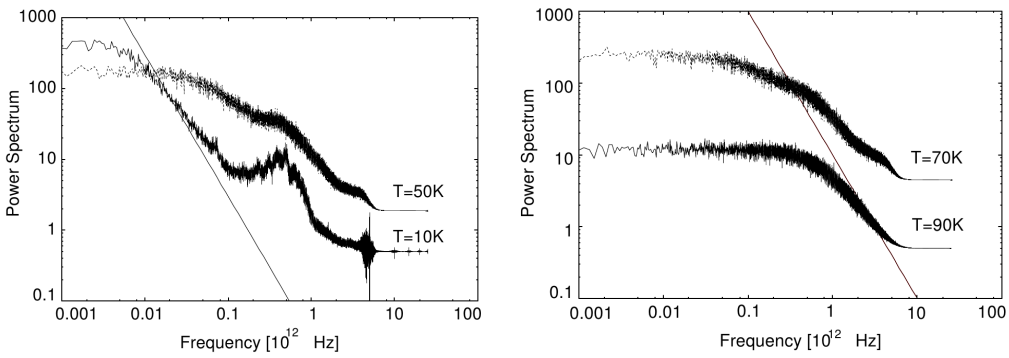

FIGURE 2. Power spectra at $10K, 50K$(left) and $70K, 90K$(right). The data of $50K$ and $70K$ are shifted upward for easy comparison. The linear line in the figure shows a guide to $(frequency)^{-2}$ relation.

tivity was found to be in good agreement with experiment. However, we did not obtain the power spectrum with adequate accuracy due to insufficient sampling. Here, a larger system of 4000 atoms with total time steps of 10^8 is employed to obtain a good power spectrum.

Figure 1 shows the results of the heat flux autocorrelation function at various temperatures. The form of the heat flux autocorrelation function for $N = 4000$ is almost the same with the previous $N = 864$ case, so the values of thermal conductivity are mostly the same. However, a slight reduction of the autocorrelation is observed in the lower temperatures with increasing the system size, suggesting that longer-wavelength phonons, now allowed to exist in the supercell, enhances scattering. A more quantitative analysis should be made on the N-dependence of thermal conductivity. We see clearly in Fig.1 (left) the two-stage relaxation process, except in the liquid case($90K$), where the first (fast) relaxation is ascribed to single-particle like motions and the second relaxation to collective atomic motions (phonons) [1, 2]. Single particle motions, which are observed in the diffusion of atoms in the liquid state, can be expected to become more prominent in the solid state during the continuous transition from high-temperature solid to the liquid. At the lower temperatures, the autocorrelation is oscillatory at the beginning of the second stage[2, 1], corresponding to the resonant peak in the power spectrum(Fig.2 (left)). Also, a slight shoulder, likely a damped shear mode in a solid, is observed in the first stage[1]. A wide range of power spectra has been obtained by taking Fourier-transform of the heat flux correlation functions (see Fig.2) which show from low frequency collective motions to high frequency atomic motions. Oscillatory modes are seen as characterized by the resonant peak at 0.5 THz and the step at 4 THz. These features appear to persist even below the melting point. Because the highest phonon frequency in Ar is 1.9 THz, the step at 4 THz appears to be due to frequency cutoff of second harmonic generation.

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