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Title: Molecular dynamics simulation of phonon transport in the Green-Kubo formalism of thermal conductivity

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Thermal conductivity for electronically insulating crystals is obtained atomistically through the Green-Kubo fluctuation formula using the equilibrium molecular dynamics data. Our previous study revealed that temperature dependence of thermal conductivity for solid argon, derived using the system of 864 particles, is in good agreement with experiment, and that the time correlation function of heat flux decreases in two stages, consisting of fast decaying single-particle like motions and slowly decaying collective atomic (phonon) motions. The system of 864 particles is minimally required to obtain the good thermal conductivity, although how the longer-wavelength phonons affect the relaxation process, in particular, the second stage, is not precisely known. Also, the conventional calculation of thermal conductivity based on the phonon Boltzmann equation is not well founded in this atomistic formalism. We have performed molecular dynamics simulations for the argon crystals with the system size ranging from 864 to 2916 particles at 30K to study the relaxation process. Various ensemble averages are taken from the long time trajectory, up to the 10^{9} steps, of the molecular dynamics simulation to reduce the correlation effects. It is found that the oscillatory motions in the second phonon relaxation process observed in the system of 864 particles tend to be smooth as the system size increases. We also performed the molecular dynamics simulation using the harmonically approximated Lennard-Jones (LJ) potential to observe the relaxation process. The results show that the relaxation in the phonon stage tends to disappear although the fast decaying part is mostly the same with the low temperature LJ case. The power spectra for the harmonic and LJ cases at various temperatures show the relaxation process in the second phonon stage in perspective.