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Prediction of Phonon Thermal Conductivity of F.C.C. Al by Molecular Dynamics Simulation

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Abstract : In this work, the phonon thermal conductivity of f.c.c. Al is investigated in detail in the temperature range 100 – 900 K within the framework of equilibrium molecular dynamics simulations making use of the Green-Kubo formalism and one of the most reliable embedded-atom method potentials. It is found that the heat current auto-correlation function of the f.c.c. Al model demonstrates a two-stage temporal decay similar to the previously observed for f.c.c Cu model. After the first stage of decay, the heat current auto-correlation function of the f.c.c. Al model demonstrates a peak in the temperature range 100-800 K. The intensity of the peak decreases as the temperature increases. At 900 K, it transforms to a shoulder. To describe the observed two-stage decay of the heat current auto-correlation function of the f.c.c. Al model, we employ decomposition model recently developed for phonon-mediated thermal transport in a monoatomic lattice. We found that the electronic contribution to the total thermal conductivity of f.c.c. Al dominates over the whole studied temperature range. However, the phonon contribution to the total thermal conductivity of f.c.c. Al increases as temperature decreases. It is about 1.05% at 900 K and about 12.5% at 100 K.

Keywords : aluminum, gGreen-Kubo formalism, molecular dynamics, phonon thermal conductivity
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