Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Investigation of phonon mass-difference scattering model by molecular dynamics TAKUMA SHIGA, TAKUMA HORI, SHIGEO MARUYAMA, JUNICHIRO SHIOMI, Department of Mechanical Engineering, The University of Tokyo — While nanostructuring has been shown to be a promising approach to effectively reduce lattice thermal conductivity and enhance efficiency of thermoelectrics, alloying still remains to be a key process that determines the base material performance. Therefore, understanding lattice thermal conductivity of alloyed crystals, particularly from the viewpoint of mode-dependent phonon transport, holds importance. In this work, we have investigated phonon scattering rates in alloy crystals by focusing on the mass-difference scattering. The phonon mass-difference scattering rates were obtained through spectral analysis of phase-space molecular trajectories computed by molecular dynamics simulations. Obtained results for simple Lennard-Jones crystals show that the mass-difference scattering rates of long-wavelength phonons follow the frequency dependence of Rayleigh scattering regardless of isotope mass and concentration. Meanwhile we obtained the large deviation from scattering models based on the mass perturbation theory. We will report and discuss details of frequency-dependence of mass-difference scattering rates to clarify validity and limit of the models. Furthermore, the analysis will be extended to thermoelectric materials, such as lead telluride. This work is supported by Global COE Program, Global Center of Excellence for Mechanical System Innovation.

Takuma Shiga
Department of Mechanical Engineering, The University of Tokyo

Date submitted: 11 Nov 2011 Electronic form version 1.4