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Monte Carlo Simulations of Mode Dependent Phonon Transport in Nanostructured Thermoelectric Materials[1] TAKUMA HORI, The University of Tokyo, JUNICHIRO SHIOMI, The University of Tokyo, PRESTO Japan Science and Technology Agency — Nanostructuring are efficient process to lower the lattice thermal conductivity and thus enhance thermoelectric performance of semiconducting materials. Here, detailed knowledge of phonon transport properties in the nanostructures is needed for prediction of performance and/or optimization of structures. The approach to solve the linearized phonon Boltzmann transport equations stochastically by Monte Carlo method has been demonstrated to be useful to obtain phonon transport properties in mesoscale and complex structures. In this study, we have performed the Monte Carlo simulations to investigate phonon transport properties in nanostructured thermoelectric materials. With the mode-dependent bulk phonon transport properties obtained by first-principles-based calculations, the Monte Carlo simulations are performed to investigate the influence of nanostructure length-scales on the mode-dependent lattice thermal conductivity and its sensitivity to interfacial phonon transmission.

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