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Molecular Dynamics Simulation of the Phonon Conductivity in Cu-Ni Binary Alloy YUSUKE KONISHI, NRI, AIST, TETSUYA FUKUSHIMA, KAZUNORI SATO, Graduate School of Engineering Science, Osaka University, YOSHIHIRO ASAI, NRI, AIST, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — In 2010, a giant Peltier effect was observed in a Cu-Ni/Au junction [1]. It is considered that this giant Peltier effect is caused by nano-scale phase separation formed in the sputtering process. The giant Peltier coefficient in the Cu-Ni/Au junction indicates the great Seebeck coefficient in Cu-Ni alloy. Although this alloy is a prospective thermoelectric material because of its great Seebeck coefficient, the low phonon thermal conductivity is also necessary for a large thermoelectric coefficient ZT. In order to find conditions for the low phonon conductivity, we calculate the thermal conductivity in Cu-Ni Alloy in various shapes with or without nanostructures by using nonequilibrium molecular dynamics simulation. In this simulation, we use a semi-empirical potential [2] and the reverse nonequilibrium molecular dynamics [3] method. [1] A. Sugihara et al., Appl. Phys. Exp. 3, 065204 (2010). [2] J. Cai and Y. Y. Ye Phys. Rev. B 54, 8398 (1996). [3] F. Müller-Plathe J. Chem. Phys. 106, 6082 (1997).

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