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Calculation of Phonon Conductivity and Seebeck Coefficient in Cu-Ni Alloy YUSUKE KONISHI, YOSHIHIRO ASAI, NRI-AIST — In recent years, thermoelectric materials have been attracting a lot of attention because they are expected to be applied for utilization of waste heat. Many kinds of materials are studied for this purpose; semiconductors, alloys, organic materials, etc. 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. Although this material is a great candidate for a thermoelectric material, we need to find the condition for a large thermoelectric coefficient that requires a large Seebeck coefficient, large electric conductivity, and small phonon conductivity. We calculated phonon conductivity in Cu-Ni alloy by using nonequilibrium molecular dynamics simulation and calculated Seebeck coefficients via ab-initio methods. [1] A. Sugihara et al., Appl. Phys. Exp. 3, 065204 (2010).

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