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**Simulation of Nanostructure and Thermal Conductivity in Binary Alloys** YUSUKE KONISHI, NRI-AIST, TETSUYA FUKUSHIMA, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University, YOSHIHIRO ASAI, NRI-AIST — Thermoelectric materials attract much attention because of concerns about energy conservation. Recently, Sugihara et al. made nanostructures using phase separation of Ni-Cu binary alloy [1]. This structure is about 10nm and has the large Seebeck coefficient. However, the way to make better thermoelectric material is under discussion. For this purpose, we need a large Seebeck coefficient, large electric conductivity, and small phonon thermal conductivity. The goal of this study is finding the condition of making good thermoelectric materials. In our simulation, we made structures in various conditions and evaluated phonon thermal conductivity. First, we simulated quenching binary alloy at high temperature by using Monte Carlo method. The potential between atoms are determined by KKR-CPA method [2]. In this simulation, nanostructures have the size distribution between 1 nm and 50 nm. Next, we simulated phonon conduction by molecular dynamics. Heat baths were placed at both ends and the thermal gradient was made. By calculating energy flux, we determined the value of phonon thermal conductivity. [1] A Sugihara et al., Appl. Phys. Exp. 3, 065204 (2010). [2] H. Akai, J. Phys.: Condens. Matter 1, 211 (1989).

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