Molecular Dynamics Simulation of the Effects of Atomic Vacancies on the Thermal Conduction of Solid Argon

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A nonequilibrium molecular dynamics simulation has been performed to investigate the effects of vacancies on the thermal conductivity of solid argon. The thermal conduction of solid argon is dominated by lattice vibration, and the electron effect is negligible. Therefore, the thermal conductivity is affected by the internal stress due to the atomic vacancies. The interatomic potential of solid argon is expressed by a simple Lennard-Jones potential. Analysis was performed on a system that consisted of 2600 argon atoms. The temperature of the upper region of the system was controlled at 8 K and the lower region was controlled at 12 K, using the velocity scaling method. The pressure of the system was varied from –50 to 50 MPa. The thermal conductivities were calculated by measuring the heat flux that passed through the system and, also, the temperature gradient of the system. Four vacancies and eight vacancies were arrayed in the system in various arrangements. Simulation results show that the thermal conductivities decrease inversely with the number of vacancies, and that nonequilibrium molecular dynamics simulation results agree well with the results of the equilibrium molecular dynamics simulation. Furthermore, the depression rate of the thermal conductivity varies with the arrangement of the vacancies, and it is found that the depression rate of the thermal conductivity increases when the vacancies are arrayed perpendicular to the direction of heat flow. These results suggest that the effect of vacancies in solid argon is localized around the vacancies.