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Neutron scattering study of phonon dynamics on cage compounds C.H. LEE, AIST Jpn, H. YOSHIZAWA, ISSP, I. HASE, AIST, H. SUGAWARA, Tokushima Univ., M.A. AVILA, T. TAKABATAKE, Hiroshima Univ., H. SATO, Tokyo Metropolitan Univ. — Filled skutterudite compounds have attracted great attention due to their potential as thermoelectric devices. In particular, their low lattice thermal conductivity is advantageous to achieve high thermoelectric performance. To improve the performance further, it is important to clarify the origin of their low lattice thermal conductivity. Previous studies suggest that the low thermal conductivity is a consequence of free vibration of rare-earth atoms in large lattice cages, which is so called rattling effect. To confirm the hypothesis, we have studied phonon dynamics of $CeRu_4Sb_{12}$ by neutron scattering using single crystal samples at JRR-3M reactor of JAERI in Tokai. As results, we have found optical phonons associated with large vibration of Ce atoms at relatively low energy of E=6 meV, which show an anticrossing with acoustic phonons. According to the analysis based on a Born-von K'arm'an force model, the longitudinal force constants of the nearest Ce-Sb and Ce-Ru are both estimated to be 0.025 mdyn/A, while that of the nearest Ru-Sb shows a large value of 1.4 mdyn/A, indicating that the Ce atoms are bound very weakly with surrounding rigid RuSb₆-octahedron cages. We will discuss that the origin of the low lattice thermal conductivity can be intensive Umklapp scattering originating from low-lying optical phonons.

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