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Neutron scattering study of phonon dynamics in a filled skutterudite CeRu₄Sb₁₂

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Filled skutterudite compounds RM_4X_{12} (R = rare-earth; M = Fe, Ru or Os; X = P, As or Sb) have attracted great attention due to their potential as thermoelectric devices. Their low lattice thermal conductivity is advantageous to achieve high thermoelectric performance. For further improvement in their performance, the origin of their low lattice thermal conductivity needs to be investigated. Previous studies suggest that the suppression of thermal conductivity is a consequence of free vibration of rare-earth atoms in a large lattice cage, which is so called rattling effect. To confirm the hypothesis, phonon behavior should be studied.

In this work, we have studied phonon dynamics of $\text{CeRu}_4\text{Sb}_{12}$ by neutron scattering using single crystal samples. The measurements were conducted using the 3-axis spectrometers, TAS-1 and TOPAN, at JRR-3M reactor of Japan Atomic Energy Research Institute in Tokai. The incident (final) neutron energy was fixed at E_i (E_f) = 14.7 meV or 13.7 meV using the (002) reflection of a pyrolytic graphite monochromator and an analyzer. In order to increase the sample volume, five single crystals were assembled and mounted in an Al container filled with He thermal exchange gas. Total volume of the samples is about 0.2 cc. Note that all previous neutron scattering studies of phonons were restricted to powder samples and this is the first report on a phonon study using single crystals. Fig. 1 shows energy dispersion of transverse acoustic phonon at T = 300 K. As shown, the energy dispersion deviates from linear relationship above k = 0.4. Details will be discussed in the conference.

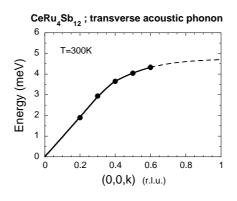


Figure 1: Energy dispersion of transverse acoustic phonon at T = 300 K for CeRu₄Sb₁₂.