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Phonon anomaly of $PrRu_4Sb_{12}$

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Recent subjects in the study of rare-earth filled skutterudite are atomic vibration with large amplitude of the filled rare-earth atoms in a cage composed of pnictogens and its effect on electronic states. Ultrasonic measurement suggested that Pr ions in $PrOs_4Sb_{12}$ exhibit off-center motion within the Sb cage icosahedron (T. Goto *et al.*: PRB **69** (2004) 180511). Recent inelastic x-ray scattering experiment on Sm-based compounds (S. Tsutsui *et al.*: Physica B in press) and inelastic neutron scattering experiment on $CeRu_4Sb_{12}$ (C. H. Lee *et al.*) also revealed lower-frequency flat phonon mode which can cross the normal acoustic mode. We have also reported anomalous phonon modes softening with decrease of temperature in $PrOs_4Sb_{12}$ (K. Iwasa *et al.*: Physica B in press).

In the present study, we focused on the phonon in $PrRu_4Sb_{12}$ and their temperature dependence, in order to investigate the expected low-frequency modes and anharmonic atomic potential for Pr ion sites. Inelastic neutron scattering experiments for the single crystalline samples synthesized by the Sb self flux method has been performed at the triple axis thermal neutron spectrometer TOPAN installed at the 6G beam line in JRR-3M reactor, JAEA, Tokai.

Figure 1 (a) shows inelastic spectra measured at the reciprocal lattice points $\mathbf{Q} = (\xi, 3, 3)$. A distinct peak was observed at 4.7 meV near $\xi = 0$ corresponding to the zone center. It is less dispersive and the intensity decreases with varying ξ of $\mathbf{Q} = (\xi, 3, 3)$, which can be attributed to the low-frequency optical mode with the atomic displacement vector along the [0, 1, 1] axis. It is notable that this mode shows distinct softening behavior with decreasing temperature. We measured phonon spectra also at $\mathbf{Q} = (6, \zeta, \zeta)$, as show in Fig. 1 (b). The data measured at $\zeta = -0.4$ shows two peaks, and the ζ dependence of the spectra can be interpreted as the anti-crossing between the transverse acoustic phonon and the low-frequency optical mode. However, the spectrum at $\zeta = 0$ is an unexpectedly overdamped with its center located at $E = 0$. The tail of spectrum extending up to 4 meV is suppressed with decrease of temperature, while the Bragg reflection intensity at $\mathbf{Q} = (6, 0, 0)$ is enhanced. This phenomenon can be interpreted as that the low-frequency mode with the propagation vector $\mathbf{q} = 0$ with the atomic displacement along the $[1, 0, 0]$ axis has finite life time like the atomic diffusion. These experimental facts indicate the Pr ion in an anharmonic and anisotropic potential.

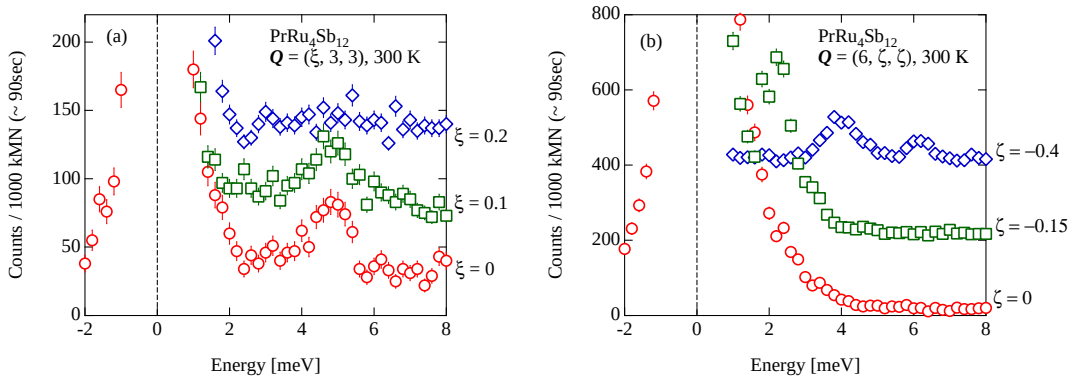

Figure 1: Inelastic neutron scattering spectra at $\mathbf{Q} = (\xi, 3, 3)$ (a) and at $\mathbf{Q} = (6, \zeta, \zeta)$ (b) of $PrRu_4Sb_{12}$. Both spectra were measured at 300 K.