Neutron scattering study of phonon dynamics on La3Pd20Ge6

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A large vibration of an atom in an oversized atomic cage, so called rattling, has attracted great interest since it can be the origin of exotic physical properties. La3Pd20Ge6 is one of those compounds that have large atomic cages filled with La guest atoms. Ultrasonic measurements show that the elastic constant C44 of La3Pd20Ge6 exhibits a Debye-type dispersion around T = 20K [1]. It is proposed that the phenomenon is originated from the rattling motion of La atoms, but there is still no direct evidence. Rather, the feature of a rattling motion is still controversial. In the present work, thus, we study phonon dynamics of La3Pd20Ge6 by inelastic neutron scattering and try to understand the reason of the Debye-type dispersion as well as the nature of rattling.

Neutron scattering measurements were carried out using the triple-axis spectrometer, TOPAN, GPTAS and HER, at the JRR-3 reactor of JAEA at Tokai. The final neutron energy was fixed at Ef = 14.8 meV or 5.4 meV using a pyrolytic graphite monochromator and an analyzer. The sequences of the horizontal collimators were 40′-40′-S-40′-40′, 40′-60′-S-60′-60′, open-S-80′-80′ or open-S-40′-40′, where S denotes the sample position. Total sample vomule of La3Pd20Ge6 single crystals used for the measurements was about 1.3cc.

Fig. 1 shows the phonon dispersion curve of La3Pd20Ge6 with propagation vector of [100]. The optical phonon mode observed at E = 1 meV around zone center corresponds to a guest mode, in which La atoms vibrate largely. Around q=(0.08,0,0), the guest mode shows anti-crossing behavior with acoustic phonon mode as other cage compounds[2-4]. Characteristically, the guest mode is quite dispersive, different with other cage compounds where guest modes are almost dispersionless. This suggests that an interaction between La-La atoms exists. Temperature dependence of the guest phonon energy exhibits hardening below T = 50 K, indicating strong anharmonicity. The relationship between the hardening and the Debye-type dispersion observed by ultrasound measurements is now under consideration.

[1] T. Goto et al., Phys. Rev. B 70 (2004) 184126
[2] C. H. Lee et al., J. Phys. Soc. Jpn. 75, (2006) 123602
[3] C. H. Lee et al., J. Phys.: Conf. Ser. 92, (2007) 12169
[4] C. H. Lee et al., J. Phys. Soc. Jpn. Suppl. (2008) in press

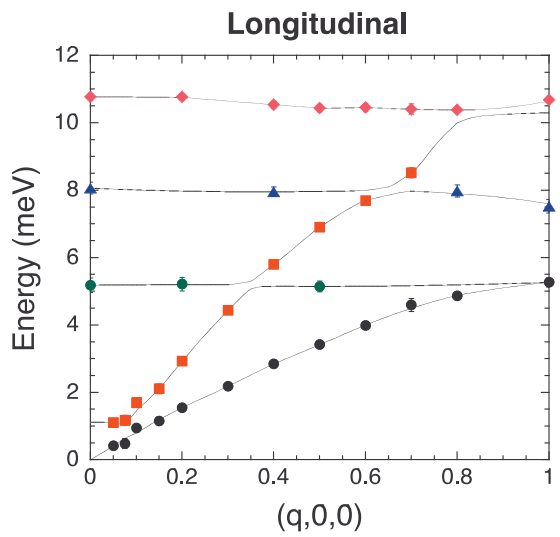

Fig. 1. Phonon dispersion curves of longitudinal phonon modes with propagation vector [100] in La3Pd20Ge6.