Neutron scattering study of phonon dynamics on La3Pd20Ge6

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Large vibration of an atom in an oversized atomic cage, so called rattling, has attracted a great interest since it can be the origin of some exotic physical properties. For example, the rattling can be responsible for an extremely low thermal conductivity. Electronic properties could also be affected via electron-phonon coupling. In beta-pyrochlore compound KOs2O6, it has been proposed that rattling may assist the appearance of superconductivity [1]. Clarifying the nature of the rattling motion is now a very important issue.

La3Pd20Ge6 is one of compounds that has large Ge and Pd atomic cages filled with La guest atoms. Ultrasonic measurements show that the elastic constant C44 of La3Pd20Ge6 exibits a Debye-type dispersion of around T=20K [2]. It is proposed that the phenomenon is originated from rattling motion of La atoms. However the relationship between the rattling and Debye-type dispersion is still controversial. In the present work, we study phonon dynamics of La3Pd20Ge6 and try to understand the reason of the Debye-type dispersion as well as the nature of the rattling.

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

Figure 1 shows typical phonon spectra of La3Pd20Ge6 at Q=(8.4,0,0). Peaks at E = 3 and 6 meV correspond to an optical mode where La guest atoms on 4c sites vibrate largely and an acoustic mode. Comparable intensity is due to mixture of both phonon modes. Phonon peaks above E = 8 meV correspond to optical modes where lattice cages vibrate mainly. As other cage compounds, clear anti-crossing behaviour is also observed in La3Pd20Ge6. Analysis in details is now in progress.

[1] S. Yonezawa et al., J. Phys.: Condens. Matter 16 (2004) L9
[2] T. Goto et al., Phys. Rev. B 70 (2004) 184126

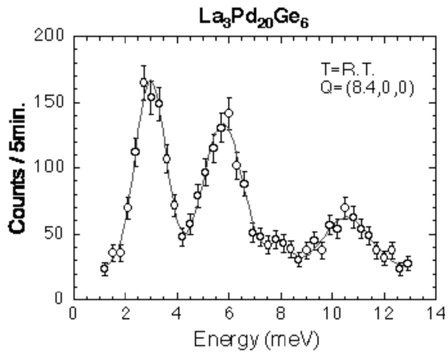

Fig. 1. Energy spectra of longitudinal acoustic and optical phonon peaks with propagation vector [100] in La3Pd20Ge6. The solid lines are the results of Gaussian fits.