# Rattling vibration of cage compounds

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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. For example, rattling can be responsible for the extremely low thermal conductivity in cage compounds. Electronic properties could be also affected by rattling via electron-phonon coupling. To clarify the effect of rattling motion on these exotic physical properties, it is very important to understand the nature of rattling.

Type-I clathrate X8Ga16Ge30 (X=Ba, Sr or Eu) is one of compounds that has large Ga and Ge atomic cages filled with X guest atoms. According to crystal structure analysis, the positions of Sr and Eu atoms split into four sites. Phonon dynamics of cage compounds with off-centered guest atoms are a controversial issue. Therefoire, we studied the phonon dynamics of Sr8Ga16Ge30 by inelastic neutron scattering [1,2].

Neutron scattering measurements were carried out using a triple-axis spectrometer, TOPAN, at the JRR-3 reactor of JAEA at Tokai. The final neutron energy was fixed at Ef=14.8 meV using a pyrolytic graphite (PG) monochromator and analyzer. The sequences of horizontal collimators were 40′-30′-S-30′-30′ where S denotes the sample position. A single crystal of Sr8Ga16Ge30 was grown by a self-flux method using excess Ga. The volume of the single crystal used for the measurements was about 2 cc. All measurements were conducted at room temperature.

Figure 1 shows the phonon dispersion of Sr8Ga16Ge30 with propagation vector of [100]. The optical phonon mode observed at E = 4 meV corresponds to a guest mode, in which Sr atoms vibrate largely. The guest mode shows anti-crossing behavior with the acoustic phonon mode, though the gap energy is relatively small comparing with that of Ba8Ga16Ge30. Analysis based on a Born-von Karman force model has clarified that the Sr atoms are bound very weakly to surrounding atoms, with a force constant of 0.007 ~ 0.009 mdyn/A. The results suggest that hybridization between the guest atoms and host lattice vibration is weak in Sr8Ga16Ge30 compounds.

[1] C. H. Lee et al., J. Phys. Soc. Jpn. 77 (2008) 260, Suppl. A.
[2] C. H. Lee et al., J. Phys.: Conf. Ser. 92 (2007) 12169.

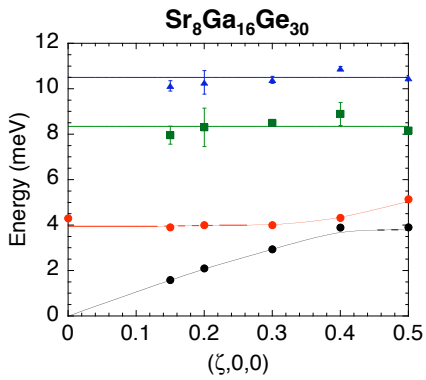


Fig. 1. Phonon dispersion curves of transverse acoustic and optical phonon modes with propagation vector [100] in Sr8Ga16Ge30.