

Raman scattering on $\text{La}_3\text{Pd}_{20}\text{X}_6$ ($\text{X}=\text{Si}, \text{Ge}$)

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Recently, a frequency dependence of the elastic constant C_{44} of $\text{La}_3\text{Pd}_{20}\text{Ge}_6$ has been found around 20K by the Niigata group¹. This anomaly is interpreted in terms of a rattling motion of La atoms between off-center positions around the La(1) site. If there is the rattling motion, one or more peaks can be found in Raman spectra in addition to the Raman active modes. In fact, the additional A_{1g} peak has been found in the Raman spectra of $\text{A}_8\text{Ga}_{16}\text{Ge}_{30}$ ($\text{A}=\text{Eu}$ and Sr)², in which the guest atoms locate on the off-center position³. On the other hand, the Niigata group also shows that there is no anomaly in the elastic constants of $\text{La}_3\text{Pd}_{20}\text{Si}_6$. Therefore a comparison between Raman spectra of both compounds can elucidate the rattling motion from a view of optical phonon modes.

We measured Raman spectra of $\text{La}_3\text{Pd}_{20}\text{X}_6$ ($\text{X}=\text{Si}$ and Ge) single crystals from 4K to room temperature. The observed Raman spectra of both crystals at 4K are shown in Fig. 1. If all La atoms locate on the center of the cages, 13 Raman active modes, $3A_{1g}+4E_g+6T_{2g}$, can be observed. In Fig. 1, all of the Raman active modes were found for both crystals and there is no additional mode. Therefore, in the Raman spectra there is no evidence of the off-center positions. In these observed modes, the lowest T_{2g} mode is a vibration of La atoms. The energy of the mode slightly decreases at low temperatures in $\text{La}_3\text{Pd}_{20}\text{Ge}_6$, while the energies of the other modes in $\text{La}_3\text{Pd}_{20}\text{Ge}_6$ and all modes in $\text{La}_3\text{Pd}_{20}\text{Si}_6$ increase with decreasing temperature. This anomalous temperature dependence has been also found for guest modes of $\text{A}_8\text{Ga}_{16}\text{Ge}_{30}$ ($\text{A}=\text{Sr}$, Eu , and Ba) and KOs_2O_6 . Therefore we think that this anomalous behavior is universal for thermal rattling motion of guest atoms.

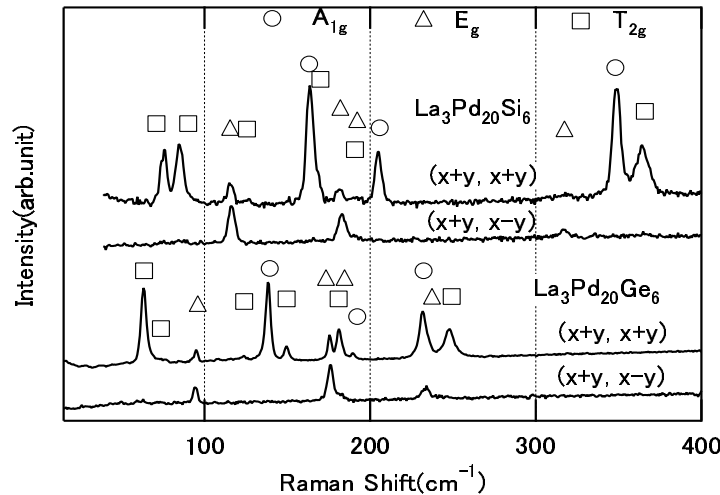


Figure 1: Raman spectra of $\text{La}_3\text{Pd}_{20}\text{X}_6$ ($\text{X}=\text{Si}$ and Ge) at 4K.

¹T. Goto, *et al.*, Phys. Rev. B **70**, 184126(2004)

²Y. Takasu, *et al.* P1-18 in this workshop.

³B. C. Chakoumakos, *et al.*, J. Alloys Comp. **322**, 127(2001)