EXAFS study of filled skutterudites $\text{PrOs}_4\text{Sb}_{12}$ and $\text{LaOs}_4\text{Sb}_{12}$

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Introduction

The filled-skutterudite $\text{PrOs}_4\text{Sb}_{12}$ is well known to be the first Pr compound that shows the heavy fermion superconductivity. The superconductivity of this material is not belong to $s$-wave type and expected to be new anisotropic type superconductivity. This interesting phenomenon is known to come from rattling motion of Pr ion in the Os$_4$Sb$_{12}$ cage, which suggested by the ultrasonic measurement [1]. Cao et al. have presented the XAFS result for this compound [2]. They reported Debye-Waller factor for Pr-Sb atomic pair is larger than that for Os-Sb atomic pair in the cage. We measured Pr $L_{III}$- and Os $L_{III}$-edge XAFS for PrOs$_4$Sb$_{12}$ and further La $L_{III}$- and Os $L_{III}$- edge for LaOs$_4$Sb$_{12}$ to compare the motion of the center atom in the cage.

Experimental

Pr $L_{III}$- (5.96keV), La $L_{III}$- (5.48keV) and Os $L_{III}$- (10.9keV) edge X-ray absorption spectra were obtained for PrOs$_4$Sb$_{12}$ and LaOs$_4$Sb$_{12}$ powders at beam line BL-9C and BL-12C. The measurements were performed in transmission mode at temperature ranging from 25K to 300K.

Results and Discussion

Figure 1 (a) shows temperature dependence of 2nd order cumulant or Debye-Waller factor $C_2$ for PrOs$_4$Sb$_{12}$ and LaOs$_4$Sb$_{12}$. Cao et al. have presented the XAFS result for this compound: They reported Debye-Waller factor for Pr-Sb atomic pair is larger than that for Os-Sb atomic pair in the cage. We confirmed that the atomic pairs contained center atom in the cage had larger $C_2$ values than that of Os-Sb (cage) atomic pair. And Fig.1 (a) shows that Pr atomic pairs have larger $C_2$ values than that of La atomic pairs. It is interesting that the temperature dependence of $C_2$ cannot be fitted by Einstein curve, but the behavior should be considered as the atomic pair has a double-well potential discussed in the theoretical calculation [3].

Figure 1 (b) shows temperature dependence of experimental and theoretically calculated 3rd order cumulant $C_3$ for Pr-Sb atomic pair. It is characteristic behavior that $C_3$ has maximum point around 150K for this atomic pair. From the theoretical study, a diatomic system which has a double-well interatomic potential is expected to show such a behavior. In the case that atomic potential is asymmetry, the maximum temperature of $C_3$ is almost the same as the temperature height of potential barrier in the interatomic double-well potential. By fitting theoretical calculation to experimental data, we obtained the barrier and width between two wells of Pr-Sb interatomic potential to be 0.025eV and 0.32Å, respectively.

Figure 1. (a) Temperature dependence of $C_2$ for PrOs$_4$Sb$_{12}$ and LaOs$_4$Sb$_{12}$ and (b) temperature dependence of experimental and theoretically calculated $C_3$ for Pr-Sb atomic pair.

References


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