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EXAFS study of filled skutterudites $PrOs_4Sb_{12}$ and $LaOs_4Sb_{12}$

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Introduction

The filled-skutterudite $PrOs_4Sb_{12}$ 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_4Sb_{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 $PrOs_4Sb_{12}$ and further La L_{III}- and Os L_{III}-edge for $LaOs_4Sb_{12}$ to comparethe 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 $PrOs_4Sb_{12}$ and $LaOs_4Sb_{12}$ 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

Figure1 (a) shows temperature dependence of 2nd order cumulant or Debye-Waller factor C_2 for $PrOs_4Sb_{12}$ and $LaOs_4Sb_{12}$. 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].

Figure1 (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 theinteratomic 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.

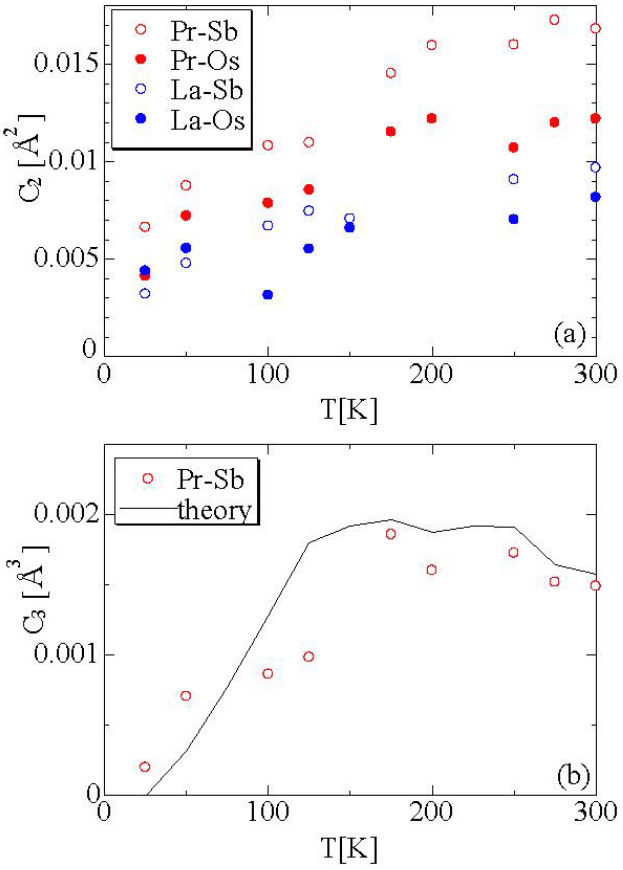

Figure1. (a) Temperature dependence of C_2 for $PrOs_4Sb_{12}$ and LaOs4Sb_{12} and (b) temperature dependence of experimental and theoretically calculated C_3 for Pr-Sb atomic pair.

References

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