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

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The superconductivity of $PrOs_4Sb_{12}$ is known to come from rattling and tunneling motion of Pr ion in the Os_4Sb_{12} cage [1]. On the other hands, extended X-ray absorption fine structure (EXAFS) is effective technique to study local atomic structure around excited atom and one can obtain the useful information about atomic vibration.

Pr L_{III}-, La L_{III}- and Os L_{III}- edge X-ray absorption spectra were obtained at BL9C(Si(111) monochrometer) and BL12C(Si(111) monochrometer) at Photon Factory (KEK) in transmission mode with the detector of the ionization chamber. In order to obtain the structural parameters, non-linear-least-square-fitting was applied to experimental data. Figure 1 (a) shows the temperature dependence of second order cumulant or Debye-Waller factor (C_2). C_2 shows the static and thermal atomic fluctuation. It is clear that C_2 for Pr-Sb atomic pair is larger than that for La-Sb atomic pair in all temperature region and Pr-Sb atomic pair has more static fluctuation and its thermal oscillation is larger than La-Sb pair because the value of C_2 near 0K and dC_2/dT is larger for Pr-Sb pair. Figure 1 (b) shows the temperature dependence of third order cumulant (C_3). C_3 shows the degree of asymmetry of the interatomic potential. From the theoretical consideration [2], for asymmetric double-well potential, C_3 has a maximum point (T_m) in that temperature dependence, which corresponds to the activation energy (or potential barrier) of the double-well potential. Comparison between experimental and theoretically calculation (path-integral effective potential method), we obtained the shape of the double-well interatomic potential of Pr-Sb atomic pair.

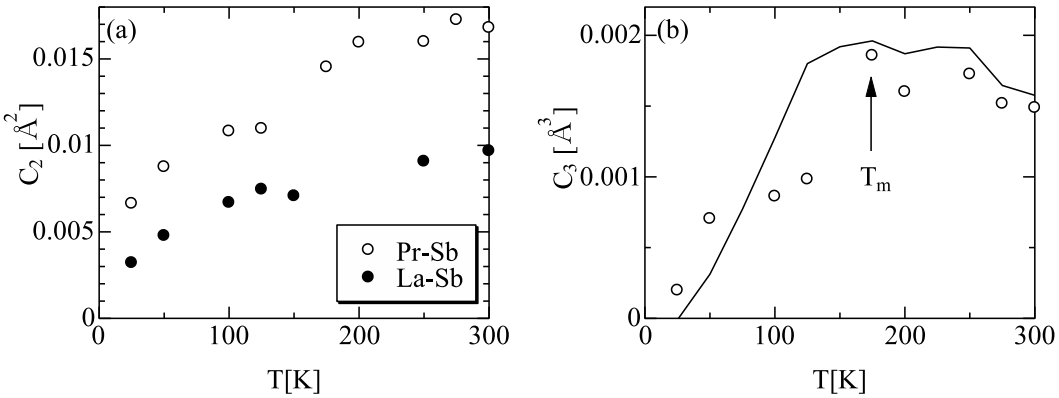

Figure 1: (a) Temperature dependence of C_2 (Debye-Waller factor) for atomic pairs of Pr-Sb, Pr-Os, La-Sb and La-Os. (b) C_3 obtained by experimental and theoretical calculation for Pr-Sb atomic pair.

[1] T. Goto, *et al.*: Phys. Rev. B **69** (2004) 180511
[2] K. Nitta, *et al.*: J. Phys. Soc. Jpn. **75** (2006) 054603