

Single crystal neutron diffraction study on rattling in skutterudite compounds

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$\text{PrOs}_4\text{Sb}_{12}$ is the first Pr-based heavy fermion superconductor with $T_{\text{sc}} = 1.85$ K.[1] The non-magnetic singlet ground state and the existence of the field-induced antiferroquadrupolar order suggest the importance of quadrupolar interaction in forming the Cooper pairs. Besides, a recent ultrasound study suggests the important role of ‘rattling’ for the electronic properties.[2] Our initial neutron powder diffraction study has clarified that Pr has a large thermal displacement which shows strong temperature dependence.[3] In order to clarify more details, single crystal neutron diffraction experiments were carried out.

Single crystal neutron diffraction experiments have been carried out on the four-circle diffractometer FONDER, installed at the T2-2 beam port in the guide hall of the research reactor JRR-3. A least-square fitting of the structure analysis for the room temperature gives the good reliable factors of $R=2.71\%$ and $wR=2.72\%$. The enormously large isotropic thermal mean square displacement of Pr was deduced to be $U_{\text{Pr}} \sim 0.04 \text{ \AA}^2$, corresponding to mean thermal displacement of $0.2 \text{ \AA}$. The maximum entropy method (MEM) by using a software PRIMA[4] results in better reliable factors: $R=2.25\%$, $wR=1.60\%$. Figure 1 shows nuclear density images for $\text{PrOs}_4\text{Sb}_{12}$ at the room temperature. This result unveils a widely spread Pr distribution in the Sb cage. It is noticeable that the distribution of Pr has a strong anisotropy towards the $\langle 111 \rangle$ direction. This distribution is almost flat in the density reflecting a shallow potential and has off-center potential minima at (xxx) with $x \sim 0.1 \text{ \AA}$. The nuclear density distribution of Pr is broad even at 8 K. However, the distribution becomes almost isotropic and no off-center potential minima is found within an experimental accuracy. We plan to expand our approach to other skutterudites in order to reveal the relation between rattling and electronic properties.

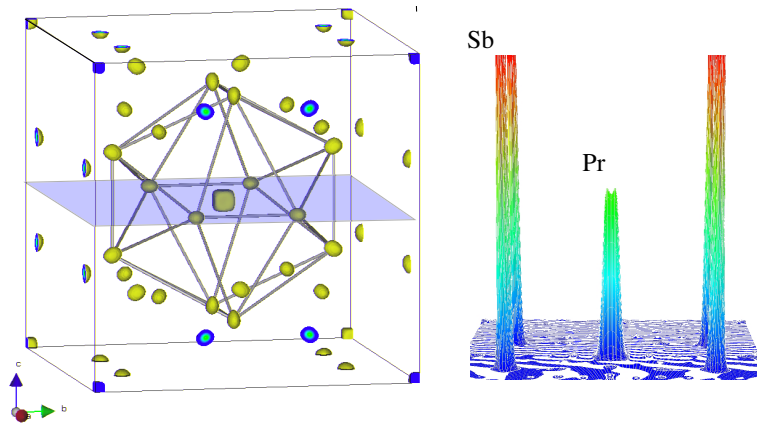


Figure 1: The nuclear density distribution of $\text{PrOs}_4\text{Sb}_{12}$ at the room temperature.

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[2] T. Goto *et al.*: Phys. Rev. B **69** (2004) 180511(R).

[3] K. Kaneko *et al.*: J. Phys. Soc. Jpn. **75** (2006) in press.

[4] F. Izumi and R. A. Dilanian, "Recent Research Developments in Physics," Vol. **3**, Part II.