

Rattling motion in $\text{PrOs}_4\text{Sb}_{12}$ studied by neutron diffraction

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$\text{PrOs}_4\text{Sb}_{12}$ is the first Pr-based heavy fermion superconductor with $T_c=1.85$ K[1]. The existence of field-induced antiferroquadrupolar ordered state indicates the important role of antiferroquadrupolar interaction in this compound. In addition, previous study reported that weakly bounded rare earth ion in the oversized cage exhibits the strong Einstein oscillation, so-called 'rattling' in the skutterudites[3]. Recent ultrasound experiments reported the rattling motion in $\text{PrOs}_4\text{Sb}_{12}$ due to the existence of off-center Pr site in the Sb cage[4]. They suggested that the mixing of the off-center rattling motion with the quadrupolar fluctuation may be responsible for the heavy fermion superconductivity in $\text{PrOs}_4\text{Sb}_{12}$. In order to study the rattling motion in $\text{PrOs}_4\text{Sb}_{12}$ more directly, we have carried out the neutron powder diffraction.

The powder neutron diffraction pattern was analyzed with the Rietveld method by using the software RIETAN-2000[5]. The observed neutron powder diffraction pattern was well reproduced by $\text{PrOs}_4\text{Sb}_{12}$ and small portion of Os with $R_{\text{wp}}=7.2$, $S=1.6$ and $R_1=3.6$ for 8 K as shown in Fig. 1. We have obtained the large thermal atomic displacement parameter $B_{\text{Pr}}=2.8 \text{ \AA}^2$ for 300 K, corresponding to the mean square displacement $U_{\text{Pr}}=0.036 \text{ \AA}^2$. This result is consistent with the existence of rattling motion in $\text{PrOs}_4\text{Sb}_{12}$. With decreasing temperature, the thermal atomic displacement parameter of Pr shows an gradual decrease but still large even at 8 K, $B_{\text{Pr}}=0.5 \text{ \AA}^2$. In order to clarify the existence of off-center site and anisotropy, neutron diffraction experiments on single crystal are in progress.

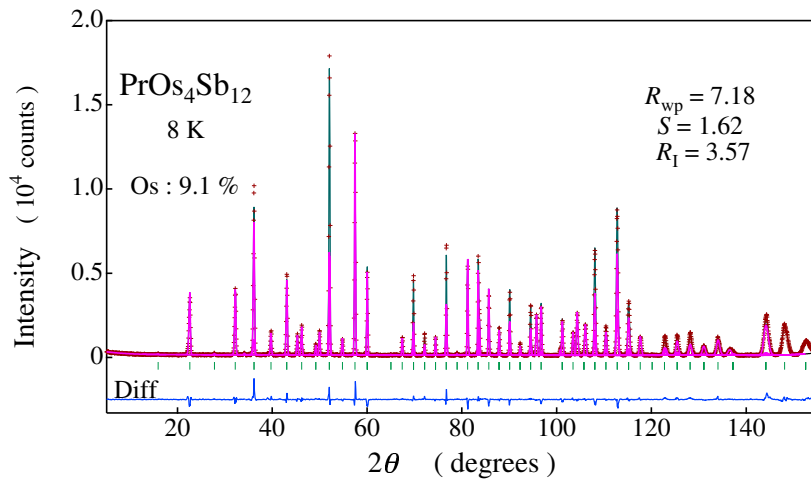


Figure 1: Neutron powder diffraction pattern for $\text{PrOs}_4\text{Sb}_{12}$ at 8 K.

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