Experimental Report

Proposal: **5-14-255** **Council:** 4/2014

Title: Rattling oscillation in strong coupling superconductor KOs2O6

This proposal is a new proposal

Researh Area: Physics

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Samples: KOs2O6

Instrument	Req. Days	All. Days	From	To
D9	9	8	28/11/2014	06/12/2014

Abstract:

We would like to investigate rattling motion of a K ion in beta-pyrochlore superconductor KOs2O6, in which rattling is considered to induce strong coupling superconductivity in this compound. By single crystal neutron diffraction, we want to clarify detailed characteristics of K oscillation including anharmonicity and anisotropy, and how it changes on passing through Tc, and additional first order phase transition Tp inside the superconducting phase. This result will provide us indispensable information to deepen our understanding on relationship between rattling and superconductivity in AOs2O6.

Rattling oscillation in strong coupling superconductor KOs_2O_6

A large-amplitude anharmonic oscillation of a guest ion incorporated in an oversized cage, called *rattling*, is considered to play a vital role to induces (or enhance) superconductivities in β-pyrochlore oxides, $A\mathrm{Os_2O_6}$ (A=K, Rb and Cs).[1] In $A\mathrm{Os_2O_6}$, $\mathrm{KOs_2O_6}$ has largest free space for a cation inside $\mathrm{Os_2O_6}$ cage which results in the largest thermal displacement parameters and lowest energy of rattling phonon. Accordingly, superconductivity has highest T_c and its character becomes strong coupling in $\mathrm{KOs_2O_6}$.[2, 3] Furthermore, an additional first-order transition appears inside superconducting state at T_p=7.5 K.[4] While the electric properties undergo substantial change on passing through T_p, no apparent change was observed in the structure. No additional superlattice reflection was detected in single crystal x-ray diffraction, and K NMR cannot observe symmetry breaking as well. In order to elucidate characteristics of rattling motion of K in $\mathrm{KOs_2O_6}$ and its variation at the transitions T_c and tp, we carried out single crystal neutron diffraction experiment.

Single crystal of $\mathrm{KOs_2O_6}$ with the volume of roughly 0.1 mm^3 was used in this measurements. The experiment was performed on the hot neutron four-circle diffractometer D9. Neutrons with a wavelength of $\sim$0.8 Å were provided via a Cu monochromator. The sample was cooled down to 2 K using the standard cryostat.

Due to weak intensity and limited beam time, measurement was focused on 2 temperatures at 15 K ($T > T_\mathrm{c}$, paramagnetic state) and 2 K ($T < T_\mathrm{p} < T_\mathrm{c}$, superconducting ground state). In total 931 and 1214 reflection intensity data were collected for 15 and 2 K, respectively. Tentative least-square analysis for the data at 15 K worked fairly well with the reported crystal structure with the space group $Fd\bar{3}m$, as shown in the figure. On the other hand, the same approach does not go satisfactory for the data at 2 K, whereas no superlattice reflection was detected. Namely, we succeeded to find trace of structural anomaly in $\mathrm{KOs_2O_6}$. Further analysis is in progress.

Unfortunately, we do not have enough time to investigate the intermediate temperature at 8.5 K ($T_\mathrm{p} < T << T_\mathrm{c}$). This hinders to reveal whether this structural anomaly occurs at T_c or T_p. To clarify nature of this structural anomaly, additional experiment is indispensable.

References

[1] Z. Hiroi *et al.*, J. Phys. Soc. Jpn. **81**, 011012 (2012), and reference therein.

[2] S. Yonezawa *et al.*, J. Phys.: Condens. Matter **16**, L9 (2004).

[3] Z. Hiroi *et al.*, Phys. Rev. B **76**, 014523 (2007).

[4] Z. Hiroi *et al.*, J. Phys. Soc. Jpn. **74**, 1682 (2010).

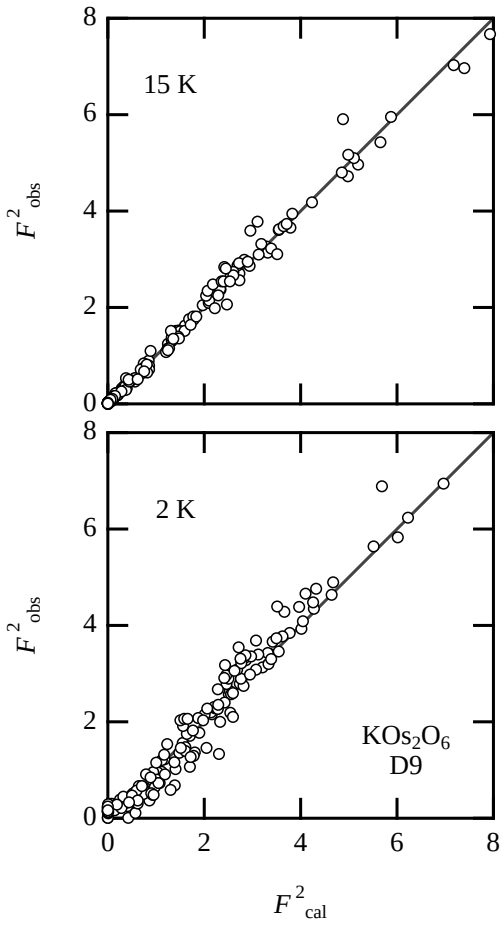

Figure 1: Tentative results of least-square analysis of KOs_2O_6 at 15 and 2 K.