Experimental report

13/02/2019

Proposal: 5-31-2564 **Council:** 4/2017

Title: Charge and magnetic ordering in Ba3YIr2O9

Research area: Physics

This proposal is a new proposal

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Samples: Ba3YIr2O9
Cu2SO5
Cu2CoSiO5

Instrument	Requested days	Allocated days	From	To
D20	0	2	25/06/2018	27/06/2018
D2B	3	2	25/06/2018	27/06/2018

Abstract:

Iridium compounds are a rather interesting class of materials due to the importance of spin-orbit coupling in these systems which gives rise to the observation of novel phases. Here, we would like to study the perovskite iridate Ba3YIr2O9, which forms a crystal structure with Ir-Ir dimmers along the c-axis and triangular structure in the ab plane. The valence state of Ir ions is 4.5+, and magnetic ordering below ~4 K has been indicated in specific heat, NMR and muSR measurements. But whether there is a charge ordering of Ir4+ and Ir5+ ions, and any information about the magnetic structure are still missing. In order to answer these questions and to study the significance of spin-orbit coupling for the magnetic ordering, we propose to measure the crystal and magnetic structure at the D2B diffractometer.

Charge and magnetic ordering in $Ba_3YIr_2O_9$

Iridates with 5*d* electron systems have attracted considerable interest recently due to the importance of spin-orbit coupling (SOC) in these systems, which may result in novel phases such as SOC-driven Mott-insulators, Weyl semimetals and topological insulators. Apart from SOC, the interplay of lattice, charge and orbital degrees of freedom are important in these transition metal oxide materials. The $Ba_3LnIr_2O_9$ (*Ln* = Y and rare earth elements) systems is such an iridate material with emergent phenomena [1-3]. It crystallizes in the 6H-perovskite type structure with space group $P6_3/mmc$ at room temperature. The crystal structure is composed of face-sharing Ir2O9 octahedra. The two nearest Ir ions exhibit dimerization (along the *c*-axis). These dimers are arranged in a triangular manner within the *ab* plane. Moreover, the valence of Ir ions can be tuned by the use of different *Ln* ions [1]. In this point of view, $Ba_3YIr_2O_9$ is of particular interest among this series of compound because the Ir ions have a mixed valence state of 4.5+. In addition, this compound is magnetically ordered below ~4 K [2], but the magnetic ground state, i.e., the magnetic structure at low temperature is still unknown. In order to investigate whether there is a charge order and the magnetic structure of this interesting compound, we have performed neutron diffraction measurements both on the D2B and D20 diffractometer.

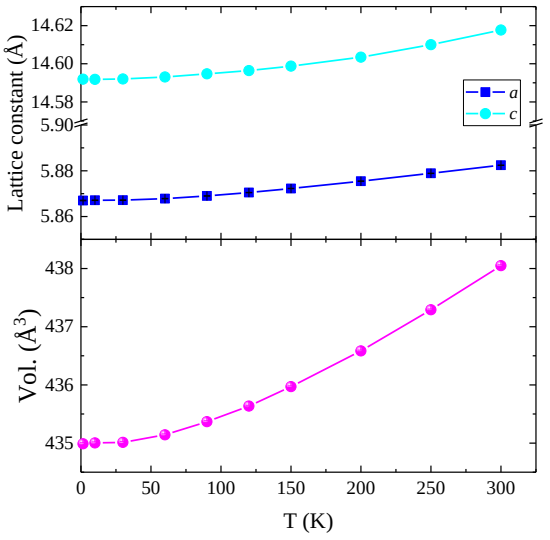

Fig. 1 Temperature dependence of (upper panel) the lattice constants and (lower panel) the volume of the unit cell.

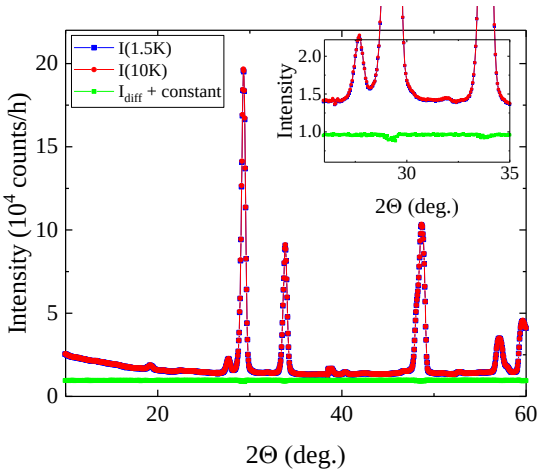

Fig. 2 Neutron diffraction pattern measured on the D20 diffractometer at 1.5 and 10 K. The bottom line shows the neutron intensity difference between 1.5 and 10 K. The inset shows an enlargement of diference intensities in the low angle regime.

The crystal structure was measured on the D2B diffractometer using a neutron wavelength of 1.594 Å at various temperatures. However, the Rietveld refinements of the crystal structure indicate that no observable change of the crystal structure can be detected between 1.5 K and 300 K. Fig. 1 shows the temperature dependence of the lattice constants and volume of the unit cell. No anomaly can be observed in the whole temperature range.

In order to unveil the magnetic structure below 4 K, we have also performed neutron diffraction on the high flux diffractometer D20 with a neutron wavelength of

2.41 Å. No significant change of the neutron pattern can be observed above and below the transition temperature even when the patterns have been measured at each temperature for 10 hours, suggesting that the Ir moments are extremely small in this compound.

References:

[1] Y. Doi and Y. Hinatsu, J. Phys.: Condens. Matter 16, 2849 (2004)
[2] T. Dey, R. Kumar, A. V. Mahajan, S. D. Kaushik, and V. Siruguri, Phys. Rev. B. 89, 205101 (2014)
[3] S. K. Panda, S. Bhowal, Ying Li, S. Ganguly, R. Valentí, L. Nordström, and I. Dasgupta, Phys. Rev. B 92, 180403(R) (2015)