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Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** Is Sr_2IrO_4 a realisation of a J_{eff}=1/2 spin-orbit insulator?	**Experiment number**: 28-01 932
Beamline: BM28	**Date of experiment**: from: 20/07/2011 to: 26/07/2011	**Date of report**: 03/10/2011
Shifts: 18	**Local contact(s)**: Didier Wermeille	*Received at ESRF:*

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Report:

We carried out X-ray Resonant Scattering (RXS) experiments on a $Sr_3Ir_2O_7$ sample at the Ir L_2 and L_3 edges and Ir M_2 and M_3 edges. After Kim *et al*. found that for a sample of Sr_2IrO_4 the X-ray resonant magnetic scattering was strong at the Ir L_3edge and very weak at the Ir L_2 edge they interpreted this strong difference with a J_{eff}=1/2 model for the spin-orbit Mott insulator [1]. The purpose of our experiments was to confirm the branching ratio found by Kim at the L edges and in addition we intended to study in detail the magnetic structure of the $Sr_3Ir_2O_7$ crystal and to study the temperature dependence of different magnetic reflections. Furthermore we studied the RXS at the M edges.

The sample, a $Sr_3Ir_2O_7$single crystal, is a double-layered perovskite (Space group I4/mmm) where, compared to the sample of Ref. [1] , is present a double layer of IrO_6 instead of a single layer . The sample was mounted on a 4K displex cryostat. A monochromatic X-ray beam was used tuned at the Ir $L_{2,3}$ (12.831 keV , 11.217 keV) and Ir $M_{2,3}$ edges (2.92 keV, 2.55 keV). The scattering geometry was always kept vertical with a *sigma* polarized incoming beam. The polarization analyzer used was an Au(333) crystal for the L_3 edge , Al (600) for the L_2 edge and Ge (111) for the M edges
The crystal presents a reasonable quality with a mosaicity calculated as the FWHM of the (0.5 0.5 24) reflection of about 0.044 degrees

$L_{2,3}$ edges

Whit the incident energy tuned at the Ir L_3 edge we found several reflections at hkl=(0.5 0.5 L). In Fig.1 (top left) we presented the energy scan for the (0.5 0.5 24), (0.5 0.5 23) and (0.5 0.5 22) reflections both in sigma-pi channel. The complete suppression of the sigma-sigma channel could be reasonably a fingerprint of dipole-dipole resonant magnetic scattering. Based on this fact and on the shape and the position of this resonance (see Fig.1 (top left)) very similar to that presented by Kim *et al.* [1] in Sr_2IrO_4, we can conclude that the origin of these reflections is magnetism and consider a magnetic propagation vector $\boldsymbol{\tau}$=(0.5 0.5 0). Since all the magnetic reflections are quite narrow in reciprocal space we can conclude that the magnetic ordering is long ranged.

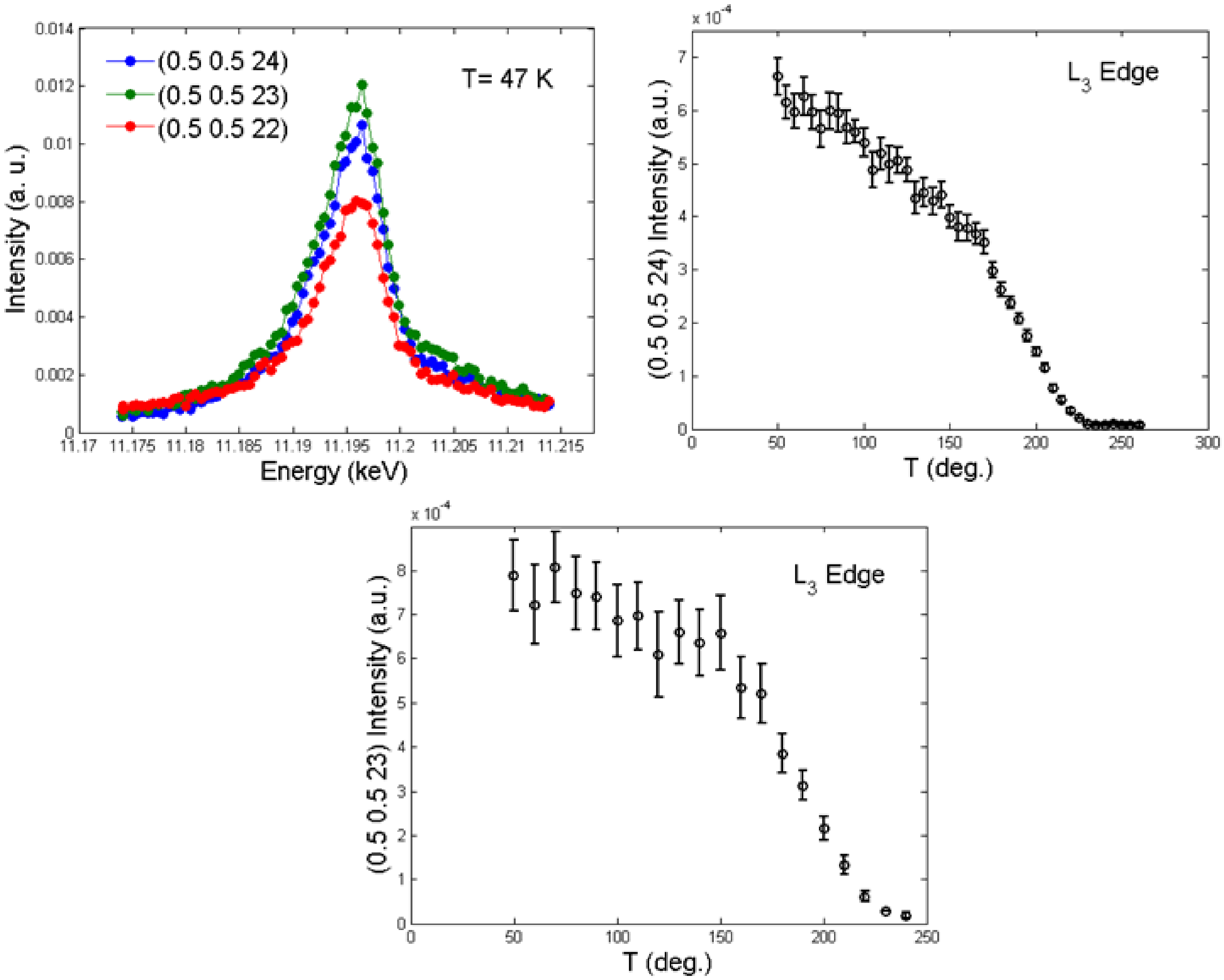

Figure 1: Top left: Energy scan of the (0.5 0.5 24), (0.5 0.5 23) and (0.5 0.5 22) magnetic reflection in the σ-π channel at the L_3 edge. Top right: Temperature dependece of the intensity of the (0.5 0.5 24) magnetic reflection at the L_3 edge. Bottom: Temperature dependece of the intensity of the (0.5 0.5 23) magnetic reflection at the L_3 edge.

From the half-width at half maximum (HWHM) of the l scan, defining the magnetic correlation length as 1/HWHM we obtain that ξ_{MAG} >106 Å, thus magnetic ordering extends substantially also between different Ir planes. Regarding the L_2 edge, almost no resonant enhancement has been found . This results is in perfect agreement with the findings of Kim

[1]. Regarding the temperature dependence of the magnetic ordering, it was measured by theta-2theta scans across the (0.5 0.5 24) and the (0.5 0.5 23) magnetic reflection. The peak was then fit to a Lorentzian function. Fig.1 (top right) shows the temperature dependence of the intensity of the (0.5 0.5 24) magnetic reflection at the L_3 edge, whereas Fig.1 (botton) shows the temperature dependence of the intensity of the (0.5 0.5 23) magnetic reflection at the L_3 edge . The width and the centre of the peak are almost constant as a function of the temperature. The transition to the antiferromagnetic state is T_N~ 240 K for both reflections.

$M_{2,3}$ edges

Whit the incident energy tuned at the Ir M_3 edge we found several reflections at hkl=(0.5 0.5 L). In the same way as the L edges we can see a strong enhancement of the magnetic scattering when the energy of the incoming x-rays is tuned to the Ir absorption edge.Unfortunately, at the time of these measurements, a proper in-vacuum stage for the polarization analyser (PA) was not available, thus polarization analysis of RXS was not possible. In Fig.2 (left) we presented the L-scan across the (0.5 0.5 7) peak. Evaluating the magnetic correlation length as above we obtain ξ_{MAG} >140 Å, thus as for the L edges case we have a long-ranged order magnetism that is not confined to the IrO_6 planes.

With the same procedure as above, we measured the temperature dependence of the (0.5 0.5 7) peak at the M_3 edge.The results shown in Fig.2 (right) are the integrated area after the fitting to a lorentzian function. The last points near T_N, where the intensity of the peak is not very high compared to the background, have been fit keeping the width and the background of the lorentzian function fixed. From the curve we can obtain a value of T_N of about 210 K. This value is slightly less that what we have found for the L_3 edge and the reason of this behavior is not clear.

As far as we are aware, these are the first XRS measurements done at the M edges for 5d elements.

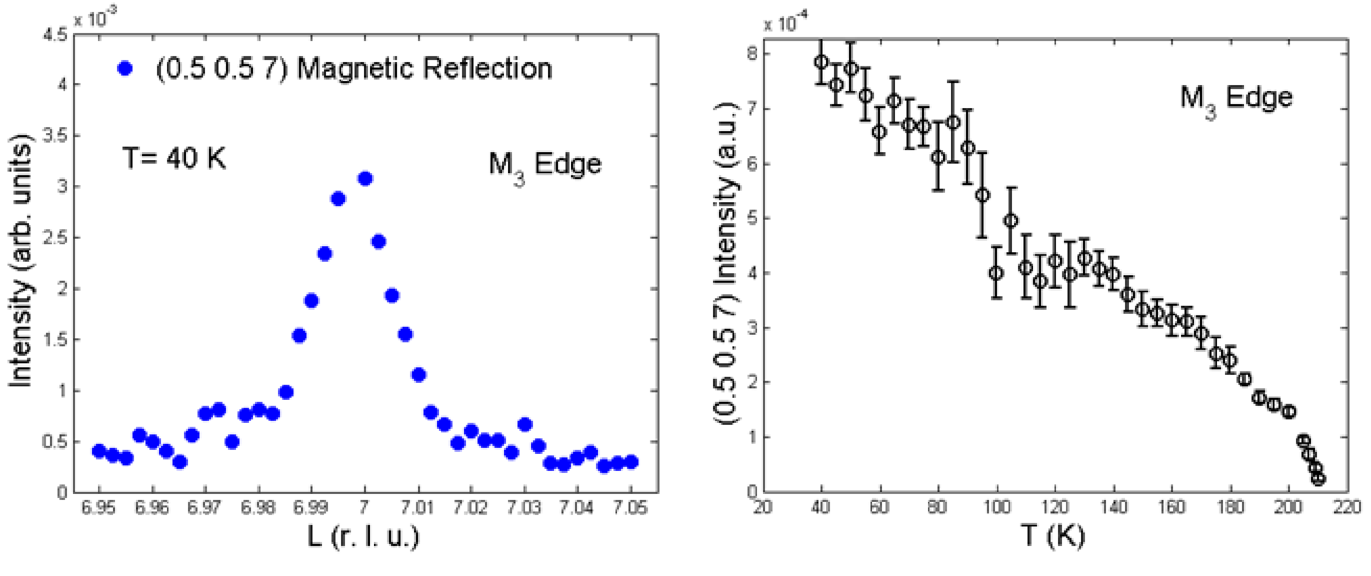

Figure 2: Left:L-scan across the (0.5 0.5 7) magnetic reflection at the M_3 edge. Right: Temperature dependece of the intensity of the (0.5 0.5 7) magnetic reflection at the M_3 edge.

Conclusions and Future work

In our first experiment we were able to observe X-ray resonant scattering from a $Sr_3Ir_2O_7$ crystal at the L edges and M edges. Our findings confirm the branching ratio between L_3 and L_2 edges observed by Kim *et al.* [1]. Furthermore we found that the transition temperature to the antiferromagnetic state is about 240 K. Several magnetic peaks has been measured confirming an antiferromagnetic long range order with the magnetic moments probably align in the ab plane of the crystal. Future experiments at XMaS will be carried out with the purpose of determine precisely the orientation of the magnetic moments by means of the RXS dependence on the azimuthal angle and the XRS at the M edges will be performed including polarization analysis (a proper in vacuum stage for the PA in now available). Furthermore, in order to understand better what is the driving mechanism of the $J_{eff}=1/2$ model measurement of non-resonant magnetic scattering will be performed in order to separated the orbital from the spin contribution.

References

[1] B. J. Kim *et al.*, Science **323**, 1329 (2009)