ESRF	**Experiment title:** The evolution of the magnetic and electronic excitations in layered iridate spin-orbit Mott insulatrors under pressure	**Experiment number**: HC-987
Beamline: ID20	**Date of experiment**: from: 19/02/2014 to: 25/02/2014	**Date of report**: 27/02/2015
Shifts: 18	**Local contact(s)**: M. Moretti	*Received at ESRF:*

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Report:

The aim of the experiment was to probe the electronic and magnetic excitations of Sr3Ir2O7 under the external stimulus of pressure. Indeed, among the Ir-based 5d transition-metal oxides, the bilayer Sr3Ir2O7, is attracting a lot of attention because proximal to a metal-insulator transition boundary. Owing to the bilayered structure of Sr3Ir2O7, a larger number of Ir nearest-neighbours translates into a broader bandwidth compared to Sr2IrO4, thus mitigating the effect of electron-electron correlation. Applying pressure to the system causes in fact two major effects: an increase in the bandwidth, and a significant variation of the tetragonal crystal field (CF) and the local symmetry in general. Both these effects should modify the balance between different energies at play in a way that the Jeff =1/2 ground state is perturbed in favor of a less insulating state. The question how the magentic excitation spectrum changes as the system undergoes this transition is extremely interesting.

The beamline was set-up with a Si(844) post-monochromator and Si(844) diced crystal analysers with a curvature radius of 2 m. The target energy-resolution of 25 meV was reached with a mask size of 60 mm.

The sample, a 50x50x20 μm^3 single crystal of $Sr_3Ir_2O_7$, was gas (He) loaded in a panoramic diamond anvil cell of 500 μm cult-size. Be was chosen as the gasket material and the experimental geometry was such that both the incident and scattered beam were passing through the gasket. The DAC was then inserted in a liquid nitrogen cryostat in order to cool the sample below the magnetic ordering temperature.

Unfortunately, we encountered a number of problems which made the experiment extremely difficult and, to a large extent, unsuccessful. In particular,

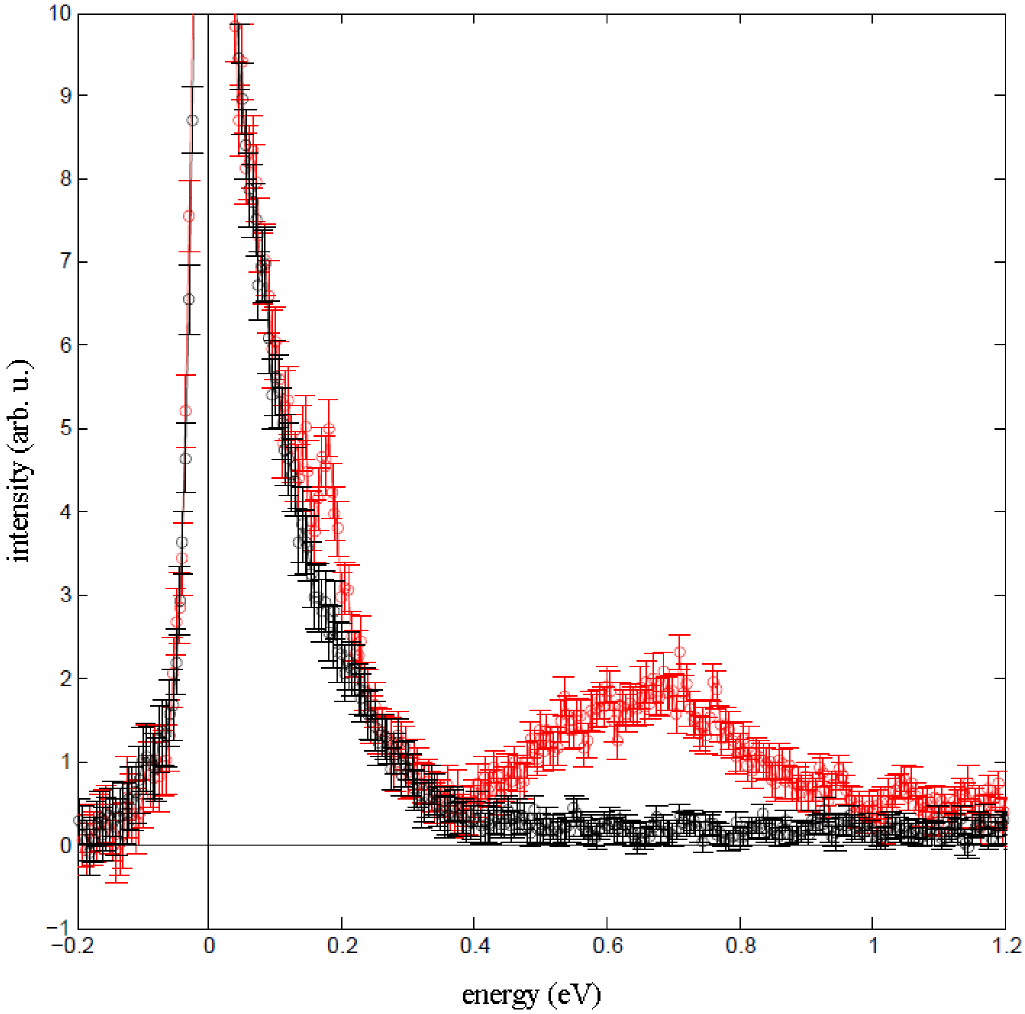
1) The gasket material, Be, turned out not to be perfectly amorphous. This complicated enormously the alignment of the sample as Be contains grains of sufficient size to produce unwanted Bragg peaks which are easily confused with those from the sample.

A solution to this problem would be to pre-align the sample in the beam before gas loading, i.e. with the sample sitting on the bottom diamond and without the Be gasket.

2) Be grains also produced spurious elastic scattering, which appears at an energy loss in the spectrum because the source is geometrically offset with respect to the center of the rotation of the goniometry. In addition, we did not manage to suppress the contribution coming from the phonon/multi-phonon of Be (off-resonance scattering). In principle, this can be zeroed by working at scattering angle 2θ=90 but some intensity leaked through because of the finite collecting solid angle of the spectrometer and eventually this was comparable or larger than the signal expected for magnetic excitations in $Sr_3Ir_2O_7$.

In the figure below we report two spectra taken at 3 GPa. The red spectrum corresponds to the scattering from the sample, while the black one was obtained by shifting the sample stage so to intercept only the Be gasket with the beam. As it can be seen, the low energy region (< 0.4 eV, the one where magnetic excitations are expected to occur) is fully dominated by the Be contribution. The tiny feature at 0.2 eV, apparently related to the sample, looks unphysical in its energy position and we believe is related to scattering from Be grains that are missed when moving to the black spectrum.

By simple geometric considerations, we believe it should be possible to partially cut the contribution from Be by adding motorized slits as close as possible to the sample. Also, the analyser horizontal acceptance could be reduced to minimize the off-resonant scattering from Be and the vertical acceptance increased to keep the collecting solid angle unchanged.



The energy feature at 0.65 eV is, instead, real and corresponds to intra-t_{2g} excitations within the 5d shell.