ESRF	Experiment title: **ExploRIXS: exploring the scientific opportunities of resonant inelastic soft x-ray scattering measured with the ERIXS instrument at the new ID32**	**Experiment number**: HC886
Beamline: ID32	**Date of experiment**: from: 1/7/2015 to: 10/7/2015	**Date of report**: 9/9/2015
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Report:

First RIXS at ID32 and flash-commissioning

This is a short, preliminary report on the first run of this LTP. Our experiment in July 2015 has been the very first RIXS experiment at the new ID32, coming after only few weeks of commissioning realized in April and May by the beam line staff and the Milano group of this LTP. The very first RIXS spectrum has been obtained on 25/4/2015. In the following days the optical performances (monochromator resolution, refocusing on the sample, spectrometer resolution) have been quickly optimized thanks to the excellent work done by the ESRF staff during the beam line pre-commissioning and in the installation and pre-alignment of the ERIXS spectrometer. Therefore the target energy resolution at Cu L_3 (930 eV) and intensity (with the 3 undulators phased together) have been reached already in the second day of this run in July. This is an exceptional achievement for such a complicated instrument. Even more remarkable if one considers that the liquid He sample cold finger had been tested only 3 days earlier and the new 2.5 m long undulator had been installed at the beginning of June. Finally a decisive contribution has come from the implementation of a single photon counting mode in the Princeton CCD detector (property of the Milano group), an algorithm developed and tested in the preceding year in Milano. In this way the 55 meV combined resolution at Cu L_3, reached with the low resolution gratings of both spectrometer and mono, has immediately set a new standard in the field of high resolution RIXS, being more than 2 times better than the ADRESS instrumentation at the SLS. And this energy resolution is obtained with comparable count rate!

During the April-May commissioning we measured some spectra at room T, as the sample cooling was not available. Therefore we chose very robust samples like the Gd-Ga garnet (Fig. 1), NiO (Fig 2) and MnO. The intensity was still not optimized, also because the new 2.5 m undulator was not in place yet.

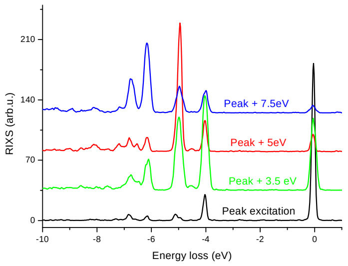

Figure 1. $Gd_3Ga_5O_{12}$ garnet, Gd M_5 RIXS showing sharp *ff* excitations.

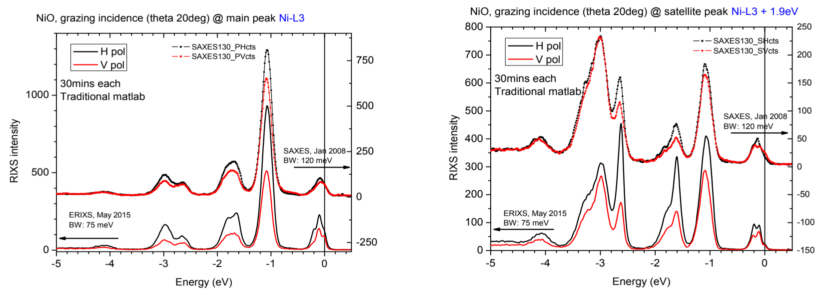

Figure 2. NiO, Ni L_3 RIXS showing rich *dd* excitations and a double magnetic peak. ID32 spectra of may 2015 are compared to those of ADRESS.

Magnetic excitations in AF cuprates

As declared in the proposal, the first milestone was the advanced commissioning of ERIXS to make it reaching the target performances in the “low” resolution - high throughput configuration. We have fully accomplished this task at Cu L_3, whereas in the preceding commissioning significant test measurements had been made at other edges as explained above: Ni L_3, Mn L_3, Ti L_3, Ce M_5, Eu M_5, Gd M_5.

The total instrumental band width of 55 meV at 931 eV (resolving power = 17000) has been obtained with 15 micron exit and entrance slit on the monochromator, 4 micron spot size on the sample, the 800 mm^{-1} grating of the mono, the 1400 mm^{-1} grating of the spectrometer, and the single photon detection mode in the Princeton 2048x2048 13.5 micron pixel detector cooled at-110°C by liquid nitrogen. The samples were cooled at ~35 K, and were mounted on the 6 axis in-vacuum Huber diffractometer/manipulator. The instrumental BW was measured as FWHM of the non-resonant diffuse scattering from a piece of polycrystalline graphite tape.

We started from antiferromagnetic layered cuprates, whose RIXS spectra are characterized by sharp *dd* excitations and resolution limited spin-wave excitations whose dispersion in momentum space ranges from zero to 350 meV. The $NdBa_2Cu_3O_6$ (NBCO) is the parent compound of an YBCO-like high Tc superconductor. The superior quality of the spectra is immediately visible in the example of Fig 3: the magnon at 0.3 eV is sharper and next to the elastic peak the phonon peak becomes immediately visible around 60 meV. The resolution has allowed the first observation by RIXS of the magnon optical branch near Γ of this bilayer compound, where a non-negligible interlayer magnetic coupling is present. The fitting of the data according to the model used in PRB 54 6905 (1996) leads to an estimate of the in-plane $J_{//}$ = 136 meV and interlayer $J_{\perp}$ = 6 meV superexchange constants. Similar measurements have been carried on the infinite layer $CaCuO_2$, where a fully 3D AF order develops, as demonstrated by the fact that we could measure a dispersion of the magnetic excitations not only in the CuO_2 planes, but also

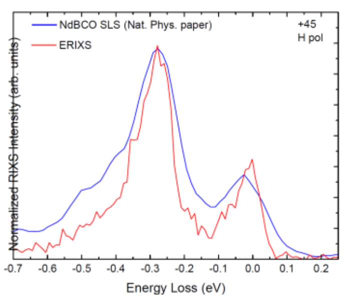

Figure 3. Antiferromagnetic NBCO Cu L_3 RIXS. The red spectrum measured at ID32 shows a sharp magnon peak and the phonon as a shoulder of the elastic.

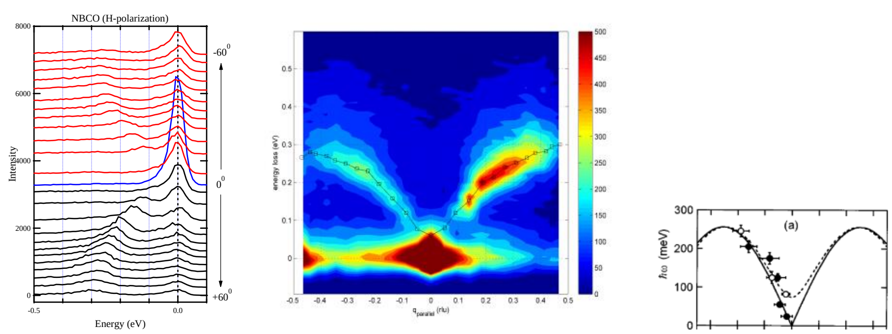

Figure 4. Antiferromagnetic NBCO Cu L_3 RIXS. The dispersing peak is dominated by the single magnon excitation. At Γ point the gapped (“optical”) branch has finite energy ~ 60 meV. By fitting the data according to PRB 54 6905 (1996) we obtain an estimate of the interlayer magnetic coupling $J_{\perp}$ = 6 meV in this bilayer compound. The panel on the right reports the results from INS.

perpendicularly to them. The latter measurements were made possible for the first time, as they exploited the possibility of changing in a continuous way the scattering angle. We could also measure, for the first time, the dispersion of the magnon excitations along diagonal direction and the AF Brillouin zone boundary simultaneously, as shown in Fig. 5, thanks to the azimuthal rotation available on the manipulator.

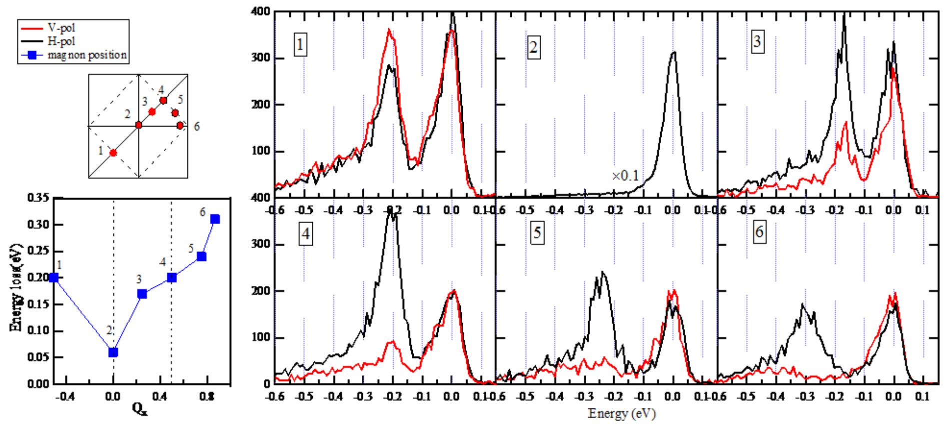

Figure 5. Dispersion of magnon excitations along diagonal direction and the AF Brillouin zone boundary of antiferromagnetic NBCO.

Preliminary measurements on superconducting cuprates

We used part of the beam time to take partial sets of data on underdoped and optimally doped YBCO and single layer Bi2201. These results provide information on the counting time, spectral quality and reproducibility that will serve for future runs of this LTP and other standard proposals on specific scientific cases on doped cuprates. That type of experiments requires systematic measurements, where parameters such as temperature and doping are varied in order to gain valuable information on the physics of high Tc superconductors. In fact the magnetic excitation features of doped cuprates are **not** resolution limited and only phonons sharpen up visibly when improving energy resolution. Therefore the superiority of ERIXS over the competing instruments in this field has to be found more in the precise sample manipulation and in the variable scattering angle rather than in the energy resolution only. In figure 6 and 7 we show some false-color maps of $YBCO_{6.6}$ (cleaved in air) and Bi2201 (cleaved in vacuum), measured with π polarization at 35 K. The goniometer guarantees that the beam does not move on the sample surface when the angle of incidence is scanned to change the in-plane momentum transfer: the resulting dispersion maps are of higher quality and the charge density wave peaks can be detected very directly around 0.26 rlu in underdoped Bi2201.

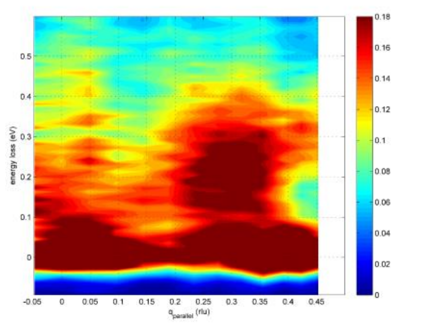

Figure 6. Underdoped YBCO Cu L_3 RIXS. Dispersion of the magnetic excitations for positive q// values.

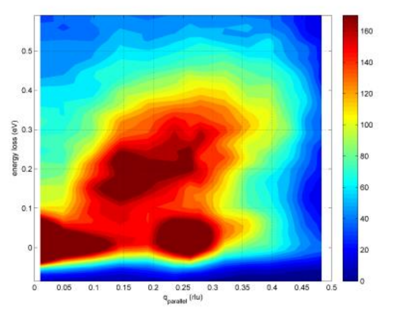

Figure 7. Underdoped Bi2201 Cu L_3 RIXS. Dispersion of the magnetic excitations for positive q// values, and strong CDW peak at zero energy loss and q//=0.26 rlu