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ESRF	**Experiment title:** Charge dynamics in an antiferromagnetic lattice: High resolution RIXS in Nd_2CuO_4 and La_2CuO_4	**Experiment number**: HE2018
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Report:

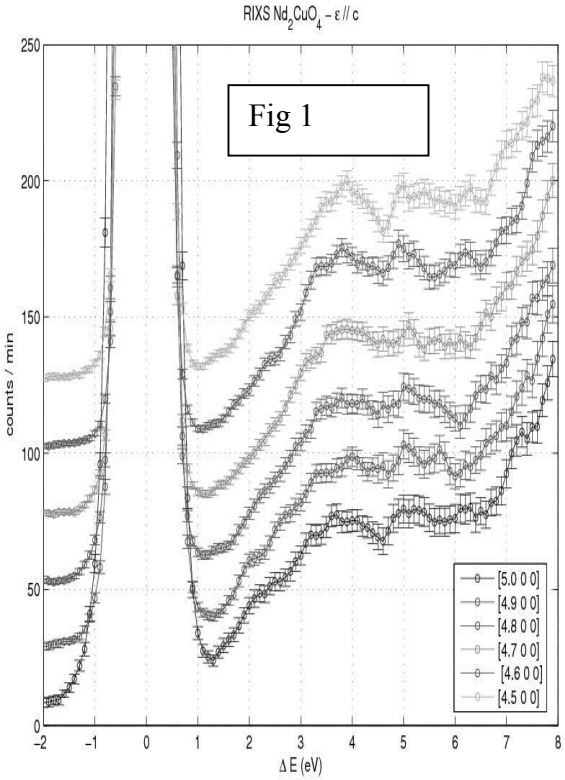
The aim of the experiment was the measurement of resonant inelastic X-Ray scattering at high resolution in two different cuprates, Nd_2CuO_4 and La_2CuO_4 . Given the count-rate of inelastic features available and the relative paucity of data in Nd_2CuO_4 compared to La_2CuO_4 a decision was made to concentrate on Nd_2CuO_4. We used a Si 533 analyser fabricated by us. The monochromator used was a Si 440 channel-cut in addition to the Si 111 pre-monochromator. The total resolution achieved was 400 meV, dominated by the monochromator and a contribution from the source size due to a 10° miscut on the measured face. We measured the absorption curves for polarization both perpendicular and parallel to the *a/b*, CuO_2 plane, the aim being to measure in exactly the same conditions as our earlier measurements in La_2CuO_4, at Spring8 so as to have a one to one comparison between the two systems. This comparison is important since we seek to identify differences between the hole doped La based system and the electron doped Nd based system.

The resonance chosen for this experiment was the main absorption peak, the $1s\text{-}np_\pi 3d^{10}\underline{L}$ transition in the cuprate generated by an incident photon of energy 8992 keV. This resonance is excited whenever the polarization has a significant component parallel to the c-axis and is chosen so as to amplify transitions related to the charge transfer process. We thus ensure that we can detect bound-state formation if there is any. Due to the horizontal scattering geometry of the spectrometer used, we could not access dispersion in the *a/b* plane while keeping the polarization strictly parallel to the c-axis. However, as in our earlier La_2CuO_4 experiment, we could ensure, by using a large scattering angle that the polarization always had a dominant component parallel to the *c*-axis and that while measuring a given dispersion the variation

was small. We also performed some measurements with the polarization in the *a/b* plane. For these, since the absorption curve changes, the incident energy for the measured 1s-$np_\pi 3d^{10}\underline{L}$ transition is different. Here the count-rate was further reduced due to an unfavorable sample configuration leading to a small exit angle for the scattered beam with respect to the sample surface and hence increased absorption.

The angle between the polarization and the *c*-axis for all following measurements varied approximately from 25° for measurements at the BZ center to 35° at the BZ edge and the scattering angle correspondingly varied between approximately 130° at the BZ center to 110° at the BZ edge. We measured dispersion of the RIXS signal in the [100] direction, and the measured Brillouin zone was between [4.5 0 0] and [5 0 0]. This choice was dictated by the need to keep the polarization as close to the *c* axis as possible.

In Figure 1 we show the measured RIXS for six different momentum transfers which span the Brillouin zone from center to edge, for the configuration where the polarisation is almost parallel to the *c* axis. From bottom to top the momentum transfer moves from zone center to zone edge. This is to be compared to our earlier data Figure 2 on La_2CuO_4 (here the momentum transfer moves from zone edge to center from bottom to top, contrary to Figure1).



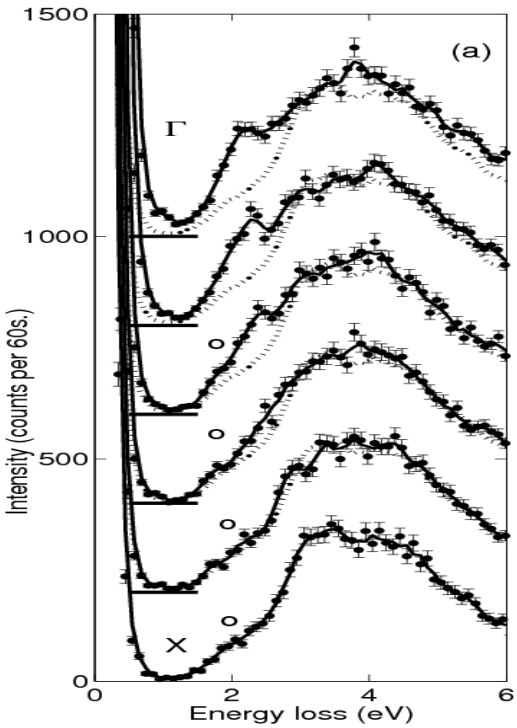


Fig 2

The following remarks can be made:

- As in La_2CuO_4 the gap in intensity between 0 and 2 eV reflects the charge transfer gap.
- The peak at roughly 2 eV, clearly visible in La_2CuO_4 near zone center is seen only as a faint shoulder in Nd_2CuO_4 and that too only in the first two curves near the zone center.

Thus Nd_2CuO_4 seems to exhibit behaviour similar to La_2CuO_4 with important differences.
The optical gap in Nd_2CuO_4 being smaller, the measured gap is less marked in RIXS.
Further, for the same reason, an excitonic state is less probable explaining the very weak excitonic signal.