ESRF	**Experiment title:** Magnetic excitations in the high temperature superconducting oxychloride Ca2-xNaxCuO2Cl2	**Experiment number:** HC-2702
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Report:

The copper oxychloride cuprate $Ca_2CuO_2Cl_2$ (CCOC) system, with vacancy or Na doping on the Ca site, is unique among the high temperature superconducting cuprates (HTSCs) since it: lacks high Z atoms; has a simple I4/mmm 1-layer structure, typical of 214 (LSCO) cuprates, but which is stable at all doping and temperatures; and has a strong 2D character due to the replacements of apical oxygen with chlorine [1]. It also show a remarkable phase digram, with a superconducting T_C growing to the optimal doping without any minimum around 1/8 doping, despite the observation of stripes (or CDW) by near-field spectro-microscopy [2].

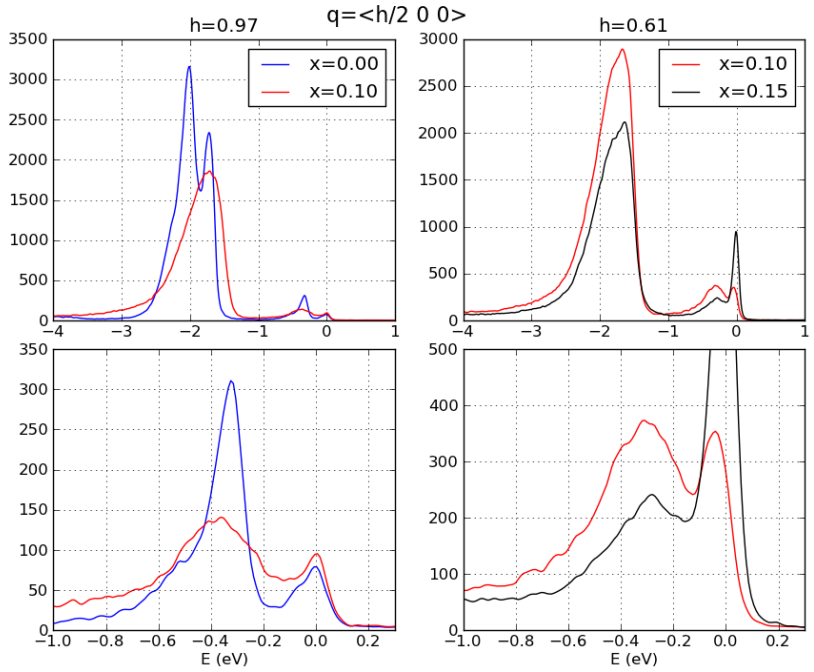

Figure 1: RIXS spectra on $Ca_{2-x}Na_xCuO_2Cl_2$ with x=0.0 (undoped, AF parent compound) and x≈ 0.10, 0.15. Left panels for an exchanged wavevector with *in-plane* projection (0.49,0) comparing x=0.0 with x≈ 0.10. Right panels for an exchanged wavevector with *in-plane* projection (0.3,0) comparing x≈ 0.10 with x≈ 0.15. Top panels shows the energy region including *dd* excitations, while the bottom panels show a zoom on the elastic and (para)magnon energy.

Due to the reduced number of electrons, advanced calculations that incorporate correlation effects, as quantum Monte Carlo [3], are now feasible for the first time in the HTSCs. This makes CCOC a model system to gain insight into the 30-year-old mystery of HTSCs by bridging the gap between theory and experiment. But relatively little is known (for a cuprate) from an experimental point of view.

We are now filling this gap by a comprehensive experimental study covering the whole phase diagram, in particular to the (para)magnon dispersion [4], using recent development in RIXS [5], as well as to the phonon dispersion [6].

In particular, following a first work on the un-doped, antiferromagnetic (AF) parent compound [5], we have performed the present experiment, in order to study the evolution with doping. In Fig. 1 we show three example spectra for x=0.0 and x≈ 0.10, 0.15, at two different wave-vectors, with (polarisation/grazing configuration to add).

The metallization with doping is clear from the broadening of both the *dd* excitation and the magnon. In the AF phase the single magnon is almost resolution limited and can be easily separated from the multi-magnon contribution, while already at x≈ 0.10 the single magnon appear as a maximum in a broad multimagnon feature. Note also that a clear phonon contribution at ≈ 80 meV was apparent, in the parent compound, sometime stronger than the elastic line (not shown).

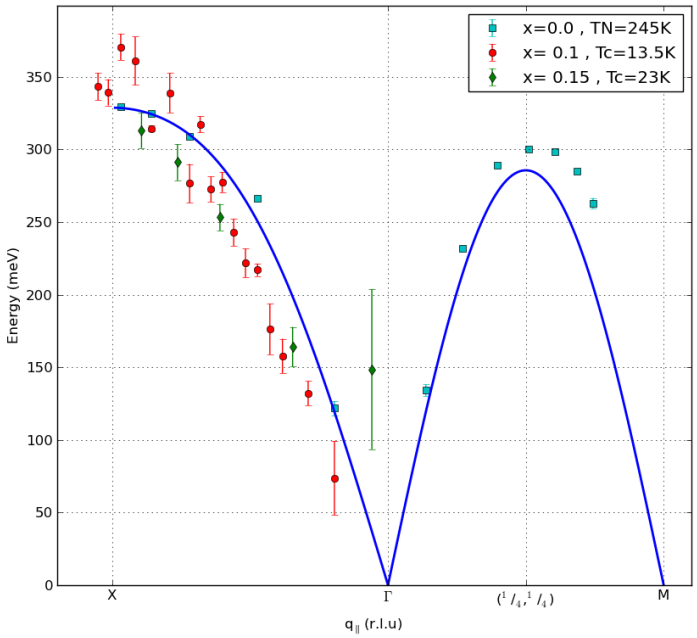

Figure 2: Paramagnon dispersion for x=0.0 and x≈ 0.10, 0.15 (inset shows AF order and superconducting transition temperature for each), along the *in-plane* projection of the Brillouin Zone high symmetry direction Γ-X (h,0) and Γ-M (h, h). Blue line is a spin-wave theory with dispersion for the AF phase including next-nearest-neighborhood exchange parameters.

Fitting all the obtained spectra for each sample and at each measured wave-vector, we can reconstruct the dispersion along the *in-plane* projection of the Brillouin Zone high symmetry direction Γ-X (h,0). For the undoped sample we also measured the Γ-M (h, h) direction, but it was not possible to complete this measurement for the doped samples due to limitation of allocated beam-time. This would be a very interesting completion of the experiment, as along that direction one observe the largest softening with doping in isostructural $La_{2-x}Sr_xCuO_4$. Here we were mainly interested in the spectral weigh evolution along Γ-X. For this, the analysis is under way, but more complex, because of the larger width of the single magnon contribution, that appear strongly mixed with the multi-magnon ones. For this, as complementary measurements with all the grazing/polarization configuration would also be helpful, but was not possible during the present experiment, again for limitation of allocated beam-time.

The x≈ 0.10 sample is particularly interesting, being very close to the magical 1/8 doping for which charge modulation are observed by diffraction in most cuprates, while in oxychlorides only by near-field

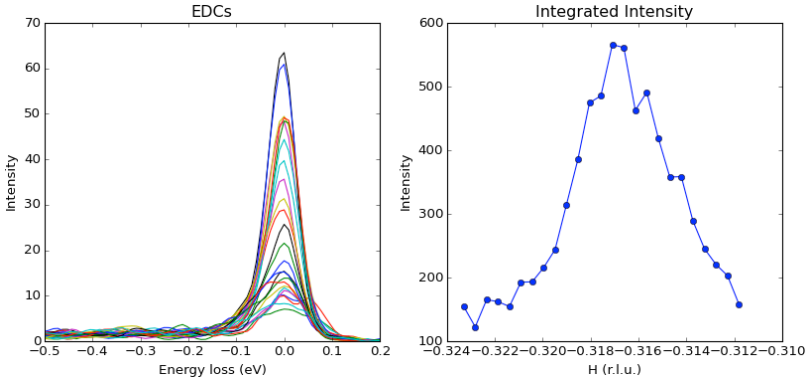

Figure 3: RIXS spectra and integrated intensity along H direction. (Grazing incident with vertical polarization)

spectro-microscopy [2]. We therefore searched in the elastic signal a maxima around the expected charge-modulation propagation vector, and found a signal, as shown in Fig. 3. This is very promising, suggesting that indeed a stripe (or CDW) phase is present in NaCCOC, but we need further data to complete the measurement, with a temperature follow up and out-of-resonance comparison, and demonstrate it is coming really from charge modulations. We are looking forward for additional beamtime in order to complete this part of the experiment. We note also that, due of technical problem and limited allocated beam-time, we were no able to measure the maximal doping x≈ 0.20.

References: [1] Z. Hiroi, N. Kobayashi, M. Takano, Nature 371, 139 (1994); Y. Kohsaka et al. JACS 124, 12275 (2002); [2] T. Hanaguri et al. Nature 430, 1001 (2004); K. Fujita et al. PNAS 111, E3026-E3032 (2014); [3] K. Foyevtsova et al., Phys. Rev. X 4, 031003 (2014); L. K. Wagner, Phys. Rev. B 92, 161116(R) (2015); [4] B. Lebert et al., arXiv:1610.08383 / hal-01388544; [5] M. P. M. Dean, Journal of Magnetism and Magnetic Materials 15, 3 (2015); [6] M. d'Astuto et al. PRB 88, 014522 (2013); B. Lebert et al., article in preparation (2017).