$KCuF_3$ under uniaxial strain: a resonant X-Ray Scattering investigation of $KCuF_3$.

C. Mazzoli[1], L. Paolasini[1], F. de Bergevin[1] and P. Ghigna[2]
[1] European Synchrotron Radiation Facility, Grenoble, France
[2] Dipartimento di Fisica Chimica di Pavia, Italy

March 1, 2005

New samples of the low dimensional magnetic pseudo-cubic perovskite $KCuF_3$ have been recently available for Resonant X-Ray Scattering (RXS) measurements. The new batch of sample has been grown by Bridgman method (B); previous experiments [1,2] on this orbitally ordered strongly correlated system were performed on crystals grown by aqueous solution precipitation (A).

We have carefully characterized the B samples by susceptometry and specific heat measurements as well as by local bulk probe techniques. Samples of the two batches give consistent results from a magnetic point of view; the B ones seems to be less disordered, as seen by Nuclear Magnetic Resonance (NMR), with a magnetic transition temperature higher of $\sim$1 K and a typical transition width of $\frac{\Delta T_B}{T_B} \simeq \frac{1}{2}\frac{\Delta T_A}{T_A}$.

In this system an intense Templeton scattering is expected due to orbital order of Cu^{2+} ion wave functions ($3d^9$ configuration with $3d_{x^2-z^2}$ and $3d_{y^2-z^2}$ alternatively occupied in adjacent sites, below $T_{OO} \approx$800 K); strong resonances at the energy of the dipolar transition between 1s core state and the 4p empty states of Cu^{2+} have already been detected in the $\sigma - \pi$ scattering [1,2].

A recent theoretical work [3] has shown how it is possible to deduce important characteristics of the orbital order parameter, and its relation with the magnetism, from features of the resonant orbital spectrum.

In fig.1 a typical spectrum of an orbital peak ([331], 12K) is shown at correspondent azimuth in two samples of the different batches (filled and empty symbols for A and B samples, respectively). Detector counts (π channel configuration) have been divided by monitor ones and corrected for absorption, as deduced by fluorescence measurements (identical within experimental errors in the two samples). Intensities are normalized to the respective maxima.

The A sample shows a complex spectrum made of at least three features, peaked at 8.986, 8.993, 9 keV [1,2]. Conversely, in the B sample the lower energy feature only has been detected. In both the spectra broad features at 9.02 keV are due to residual fluorescence.

Magnetic peaks form the three dimensional AF-magnetic structure ($T_N \simeq$39 K) have been investigated, also.

Fig.2 shows the typical spectrum of a magnetic reflection ([441], 12K) of sample B (empty symbols) compared with the one detected in sample A (filled symbols). As in the previous figure detector counts (π channel) have been corrected for monitor, fluorescence and absorption. Intensities are scaled to the respective maxima. Note that the ratio between non resonant scattering and the maximum of the resonant scattering are the same in both samples.

As in the case of orbital peak shown in fig.1, magnetic peak spectra are different in the two samples: the low energy feature only, E$\sim$8.976 keV corresponding to quadrupolar transition 1s core state to 3d empty state, has survived in the B sample and there is absolutely no detectable trace of 4p magnetism, predominant in the A sample.

The preliminary investigation of the new samples (B batch) has revealed completely new resonant spectra for both magnetic and orbital Bragg forbidden reflections, in spite of slight changes in magnetic bulk properties. Conversely a so strong change in the 4p components of both orbital and magnetic resonances is expected to strongly affect the macroscopic magnetic properties via the fluorine covalence [3].

[1]: L. Paolasini et al., Phys. Rev. Lett. 88 (2002) , 106403
[2]: R. Caciuffo et al.: Phys. Rev. B 65 (2002), 174425
[3]: N. Binggeli and M. Altarelli, Phys Rev. B 70 (2004), 085117

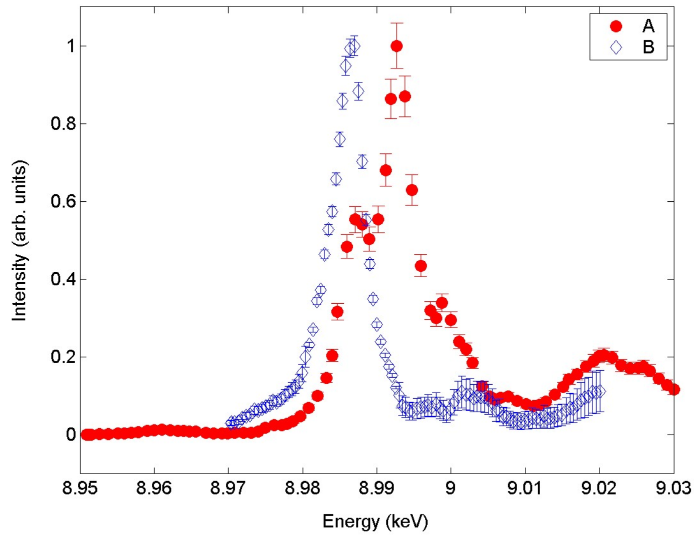

Figure 1: Energy spectrum of [331] orbital peak at 12K for both A and B samples (filled and empty symbols, respectively). The intensities have been collected at corresponding azimuth, in the $\sigma - \pi$ scattering configuration, and corrected as stated in the text. A sample data are published in [1,2].

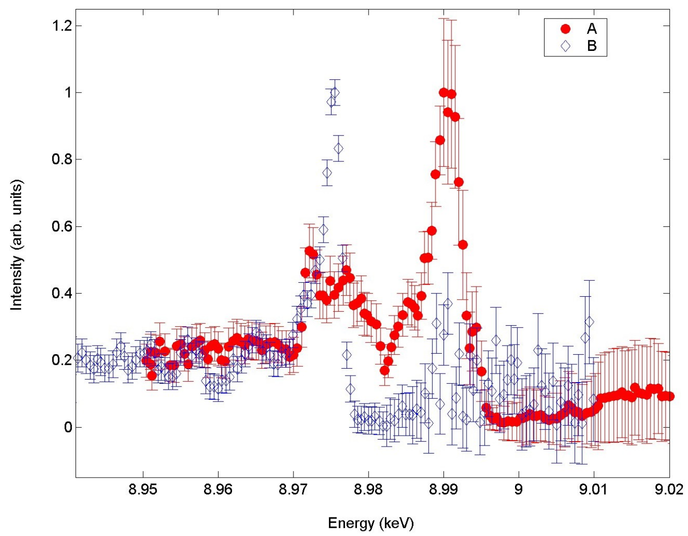

Figure 2: Energy spectrum of [441] magnetic peak at 12K for both A and B samples (filled and empty symbols, respectively). The intensities have been collected at corresponding azimuth, in the $\sigma - \pi$ scattering configuration, and corrected as stated in the text. A sample data are published in [1,2].