

Resonant X ray Scattering study of magnetism in KCuF_3 [HE2052].

C. Mazzoli¹, F. Fabrizi¹, S. Di Matteo¹, L. Paolasini¹, F. de Bergevin¹
and P. Ghigna²

¹ European Synchrotron Radiation Facility, Grenoble, France

² Dipartimento di Fisica Chimica di Pavia, Italy

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KCuF_3 pseudo-cubic perovskite has been investigated by means of resonant X-ray diffraction. In spite of a simple crystallographic structure this compound shows a totally unexpected quasi-1D Heisenberg magnetism that orders in a 3D type A anti-ferromagnetic structure below $T_N=39\text{K}$.

It has attracted the interest of the scientific community since early sixties when it was identified as an ideal model to study strongly correlated electron systems with peculiar interplays among several interacting degrees of freedom. In fact, the low dimensional magnetic properties are traditionally attributed to the antiferro-orbital arrangement of the Cu^{2+} ion $3d^9$ electronic wave-functions (orbital ordering), resulting from an high temperature cooperative Jahn-Teller distortion.

A first series of measurements have been performed some time ago [1,2] on samples grown by aqueous solution method (A). Recently new batches of Bridgman grown samples (B) have become available. We have measured some of the new B samples on ID20 beamline, detecting a new resonant signal at magnetic reflections [3]. Fig.1 shows the typical spectrum of a magnetic reflection ($[441]_p$, 12K) of sample B (empty symbols) compared with the one detected in sample A (filled symbols). Detector counts ($\sigma - \pi$ scattering channel) have been corrected for monitor, fluorescence and absorption. Intensities are scaled to the respective maxima. Note that the ratios between non resonant scattering and the maximum of the resonant scattering are the same in both samples.

In this experiment we have focused our attention on the low energy peak ($E = 8.976 \text{ keV}$) of B sample, see fig. 1, by performing azimuthal scans and full polarisation analysis.

Fig. 2 shows the dependence of the $[005]_p$ resonant intensity as a function of the azimuthal angle ψ , in $\sigma - \pi$ polarisation channel at 12K. Filled circles are the measured data (detector intensity normalised by monitor;

non resonant contribution was subtracted). The black continuous line is the fit result with a fully E2 model including domain populations (red dashed and blue dash-dotted lines), with a weight suggested by the fit of azimuthal scans on non-resonant magnetic signal. The quality of the fit removes doubts about the possibility of dipolar contributions in the signal: for the first time a direct access to 3d Cu ion wave-functions is reported in this compound [4].

- [1]: L. Paolasini et al., Phys. Rev. Lett. 88 (2002) , 106403
- [2]: R. Caciuffo et al.: Phys. Rev. B 65 (2002), 174425
- [3]: Article accepted by Phys. B.
- [4]: Article in preparation.

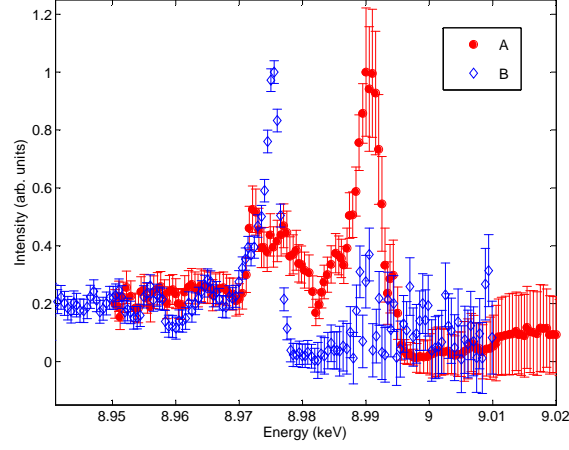


Figure 1: Energy spectrum of $[441]_p$ magnetic peak at 12K for both A and B samples (filled and empty symbols, respectively). The intensities have been collected at corresponding azimuth, in the $\sigma - \pi$ scattering configuration, and corrected as stated in the text. A sample data are published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

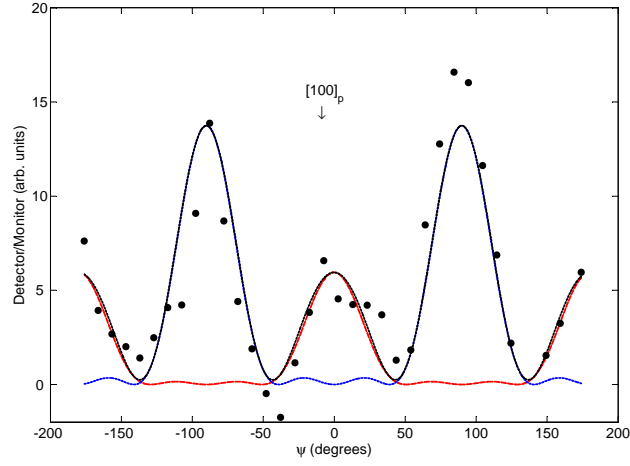


Figure 2: Azimuthal scan on $[005]_p$ magnetic reflection: $\sigma - \pi$ scattering channel, Cu-ion resonant energy ($E = 8.976$ keV) at 12K. Closed circles are experimental data, dashed and dotted lines represent the two domain contributions; continuous line is the result of the fit (see text for details).