ESRF	**Experiment title:** **ORBITAL ORDERING AND JAHN-TELLER EFFECT IN $KCuF_3$ BY RESONANT X-RAY SCATTERING**	**Experiment number:** HE-821
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Report:

The aim of this work was the invesrtigation of the interplay between the exchange interaction and "orbital ordering" effect associated with the cooperative Jahn-Teller (J-T) distortion in $KcuF_3$, by resonant x-ray scattering method at the K-edge of Cu, in order to elucidate the controversial mechanism of dipole and quadrupole resonances observed recently in manganites and in vanadium sesquioxides, respectively [1-2]. In fact whereas in V_2O_3 the orbital peaks are visible only tuning the photon energy to the threshold of Vanadium 3d bands, which corresponds to the quadrupole resonant energy [2], in manganites the resonant signal observed in the orbital superlattice reflections is mainly associated with the anoumalous anisotropy tensor (ATS) due to the local atomic environment of edge-atom [3]. As expected, the same resonant effect of manganites appears in $KCuF_3$, as shown in the spectra reported in Fig 1. Tuning the energy across the Cu K-edge at the forbidden lattice reflection, we can distinguish the antiferromagnetic reflections corresponding to the propagation vector q_{AF}=(001) from the ATS reflections by the inspection of the energy dependence and polarization analysis of scattered signal.

$KCuF_3$ crystallizes in a pseudo-cubic perovskite and because the J-T effect, the F^- ions are displaced from the midpoint of Cu^{2+}-Cu^{2+} bonds in the basal plane, giving rise to a polytype structures associated to different orbital structure [5]. The distortion of cristal lattice give rise to the onset of Bragg peaks that obey to different extinction rules : for the twisted (a)-type a=b=8.2829, c=7.8487 the satellite reflection (hkl) appear at h≠k odd l=odd, and for the untwisted (d)-type a=b=8.2791, c=7.8606 h≠k odd l=even,, where a=b are the distances between adjacent in plane Cu-atoms. Both the polytypes can exist in a same crystal. We

have tested (using 16 bunches mode) many single crystal and select a sample in which the dominant ordered structure corresponds to the twisted (a)-type. Because the quasi-one dimensional magnetic properties and the Dzyaloshinsky-Moriya antisymmetric exchange interaction between spins on c-axis, the F atoms on the c-axis are displaced from the Cu-Cu bonding lines, and conseguentely a new set of superlattice structure can be founded, corresponding to h odd, k=even l=even or odd. The azimuthal scans around the ATS reflections show the characteristic local site symmetry due to the asphericity of atomic environment and the data are in good agreement with the extinction rules and azimuthal dependencies calculed for the actual crystal structure (space group $P2_12_12_1$) [5]. Below 38K, magnetic reflections appears at h,k even, l odd, and the energy dependence (Fig. 1a) show a complex energy dependence. Far above and below the K-edge, the magnetic non resonant signal is present in both $\sigma-\sigma$ and $\sigma-\pi$ channels, in contrast to the ATS reflections that have the enhancement centered only around the Cu K-edge (Fig. 1b-c). Closer to the absorption edge we can observe at E2=8.972 keV a sharp resonance attributed to the virtual quadrupolar transition from 1s to 3d states and a broad resonant region from 8.980 to 8.994 keV attributed to the dipolar transition 1s-4p. The complete cristallographic, orbital and antiferromagnetic cell is shown in Fig. 2.

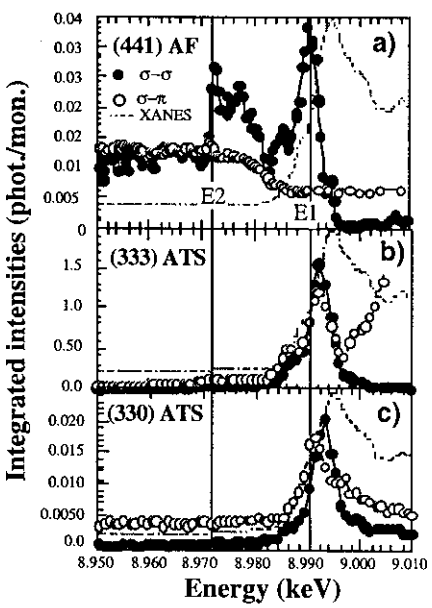

Fig. 1 Energy scans of AF reflection (441) and ATS reflections (330) and (333) recorded in $\sigma-\pi$ (black points) and $\sigma-\sigma$ (open points) polarization channels. The broken line shown the XANES around the K-edge of Cu.

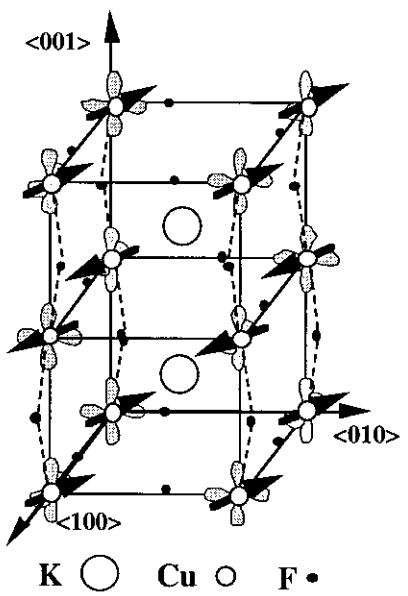

Fig. 2 Orbital and magnetic structure of $KCuF_3$. The arrows indicate the moment direction pointing along the <110> direction. The orbital ordering configuration corresponds to the a-type structure.

References

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