	Experiment title: Study of the layered $TbBaCo_2O_{5.5}$ by means of resonant x-ray scattering.	**Experiment number**: HE 2411
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Report:

Layered cobalt oxides $RBaCo_2O_{5+\delta}$ with R= rare-earth have been intensivily investigated the last decades due to the occurrence of coupled transitions (structural, orbital and *spin* orderings) arising from an additional degree of freedom: the electronic configuration of the cobalt ion. In particular, $TbBaCo_2O_{5.5}$ exhibits a metal to insulator transition at T_{MI}~340 K. On cooling below T_{MI}, the material exhibits a paramagnetic to ferrimagnetic transition at T_C~ 280 K with a spontaneous magnetic moment that disappears at T_N~ 250 K where an antiferromagnetic phase is formed [1]. With further cooling, a spin reorientation is realized at T_S~ 180 K. When δ=0.5, the formal Co valence is +3 and this compound shows a double perovskite structure. There is an Tb/Ba ordering along the c-axis and oxygen vacancies ordering along the b-axis. This gives rise to the linkage of CoO_6 octahedra and CoO_5 pyramids with Co^{+3} present in the two environments. It is thus thought that these various transitions are accompanied by changes either in the unit cell symmetry or in the cobalt spin state. The other striking feature observed in this compound is the metal-insulator transition, whose driving force is also subject of controversy.

We have carried out resonant x-ray scattering (RXS) experiments at the Co K-edge in a $TbBaCo_2O_{5.5}$ single crystal to probe the type of electronic anisotropy in the different phases between 90 K and 350 K [2]. This temperature range probes the metallic, insulating, ferrimagnetic and antiferromagnetic phases.

A crystal was cut and polished to have a flat (0 1 0) plane. The crystal was twinned so we observed both [h 0 0] and [0 k 0] domains. RXS experiments were performed on the BM02 beam line with the scattering vector Q perpendicular to the ac-plane. The sample was mounted with silver paint in a closed cycle refrigerator which could be rotated about the scattering vector to perform azimuthal scans in a range of ~130º. The electrical field (**E**) of the polarized beam was parallel to the a-axis for the 90º azimuthal angle (ϕ) whereas **E** was parallel to the c-axis for ϕ=0º. No polarization analysis of the scattered beam was performed so that we have contributions from both $\sigma\rightarrow\sigma'$ and $\sigma\rightarrow\pi'$ channels.

Strong resonances have been observed at the Co K edge for (0 k 0) reflections with k odd at 90 K (Figure 1). The resonant cusp is up (positive) for both, (0 3 0) and (0 7 0) reflections but it is down (negative) for (0 1 0) and (0 5 0) ones. This behavior arises from the crystal structure, specifically from the displacement of Tb and Ba ions from the ideal tetragonal positions. These resonances strongly depend on the azimuthal angle reaching the maximum and minimum value at ϕ =0º and 90º, respectively.

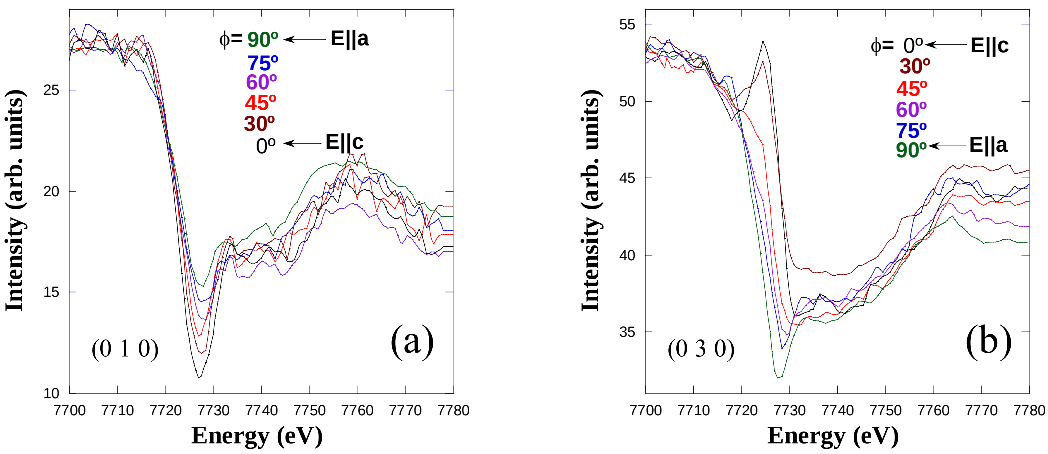

Figure 1. Energy-dependent scans collected at 90 K for the (0 1 0) and (0 3 0) reflections (panel a and b, respectively) at the azimuthal angles indicated in the figures.

The resonance occurrence and its azimuthal behavior are explained as coming from the anisotropy of the tensor of susceptibility (ATS reflections). RXS comes from the presence of two different environments for the Co ions, octahedra and pyramids of oxygens, resulted from the ordered rrangement of oxygen vacancies along the b axis.

Reciprocal lattice scans along the [0 k 0] direction were also performed between 90 and 350 K across the insulator to metal transition at different photon energies, on and out of resonance (Figure 2). Neither new nor forbidden reflections have been detected in these scans respect to the high temperature phase. This result discards differences among Co_{oct} or among Co_{pyr} in the low temperature insulating phases.

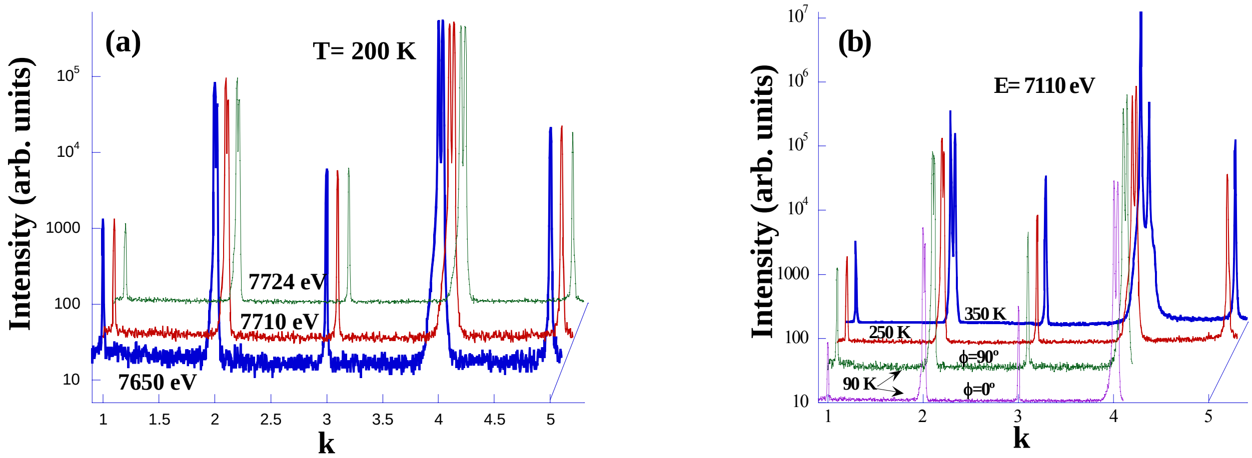

Figure 2. Reciprocal lattice scans along the [0 k 0] direction. (a): Patterns collected at 200 K with □= 0º at different energies, on and out of resonance. (b): Patterns measured E=7110 eV (pre-edge energy) with □= 0º except the curve indicated in the figure at different temperatures.

Finally, no evidence for further contributions, such as an orbital ordering, has been found in these experiments in the insulating low temperature phase.

[1] V. P. Plakhty, Yu. P. Chernenkov, S. N. Barilo, A. Podlesnyak, E. Pomjakushina, E. V. Moskvin and S. V. Gavrilov, Phys. Rev. B **71**, 214407 (2005).

[2] J. Blasco, J. García, G. Subías, H. Renevier, M. Stingaciau, K. Conder and J. Herrero-Martín, Phys. Rev. B (2008), in press.