	Experiment title: Spin-state, charge-order and orbital-order transitions in RBaCo ₂ O _{5+d}	Experiment number: HE-1612
Beamline: ID 20	Date of experiment: from: 25/02/2004 to: 02/03/2004	Date of report: 02/03/2004
Shifts: 18	Local contact(s): Luigi Paolasini	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): V. Scagnoli*, Dr. U. Staub*, Dr. M. Janousch*, Dr. A. Mulders* Paul Scherrer Institut, Swiss Light Source, CH-5232 Villigen PSI Dr. E. Brück Van Der Waals Institute, Amsterdam, Netherlands		

Cobaltites systems are particularly interesting since they display a large variety of magnetic and transport properties, which depend on the tuneable oxygen concentration. It is believed that the magnetic and transport behaviours are driven by the mixed valence state of the cobalt ions and possible orbital ordering and therefore by the $\text{Co}^{2+}/\text{Co}^{3+}$ ($\text{Co}^{4+}/\text{Co}^{3+}$) ratio determined by the oxygen content of the material.

Particularly interesting is the $\square=0.5$ oxygen concentration, where RO_x (R= rare earth ion) layers order into alternating filled and empty rows along the a -axis (see fig 1a). This produces a significant change in the local environment of the Co ions, which differentiate in octahedral (Co_I) and tetragonal (Co_II) coordination. The nominal valence of the Co ions is expected to be 3+. At $T \square 350$ K, the material exhibits a metal-insulator (MI) transition associated with a change in the volume. In addition, susceptibility measurements indicate that a spin state transition occurs at T_MI . A ferromagnetic component appears below approximately 300K, which suddenly vanishes at 260 K may indicate a paramagnetic-ferromagnetic-antiferromagnetic transition [1].

Recently, a model for the magnetic structure has been proposed [1] for $\text{GdBaCo}_2\text{O}_{5.5}$, based on magnetization measurements, which suggests an Ising-like behaviour for the spin system. The two inequivalent Co ions become either intermediate spin state (IS: $t_{2g}^5 e_g^1$; $S=1$ for Co_II) or low spin state (LS: $t_{2g}^6 e_g^0$; $S=0$ for Co_I). In the case of IS $d_{3z^2-\square^2}$ or $d_{x^2-\square^2}$ e_g orbitals can be occupied. Therefore, it has been proposed that the Co_II ions give rise to orbital ordering along the a and c axis direction.

We performed resonant X-ray scattering on the Co K-edge on a $\text{GdBaCo}_2\text{O}_{5.5}$ single crystal. This technique is well suited to obtain information on charge and orbital ordering of such perovskite systems [2-4].

We have measure the energy dependence, in the $\sigma\sigma$ charge channel, of a reflection probing along a and b axis (see figure 1). It is clearly visible the contrast along the b axis coming from the different coordination of the Co ions, respectively octahedral and pyramidal. No contrast is coming from the Co ions along the a axis, but the presence of the $(1/2\ 0\ 8)$ reflections tells that the unit cell is doubled also along the a direction. The different energy behaviour excludes the possibility of twins.

An azimuthal scan about the $(0\ 1\ 6)$ in the $\sigma\sigma$ channel reflection has been measured (fig. 2). The orbital contribution to the anisotropy tensor $\langle T_{\sigma}^K \rangle$ can be calculate and compared with the measured values.

This can help to understand the role of the orbitals in determining the singular properties of this material.

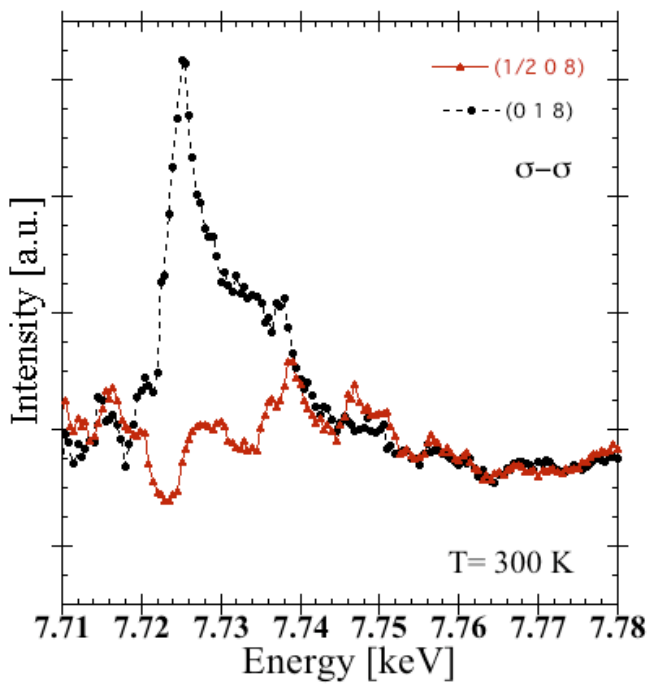


fig.1 Energy dependence of the $(1/2\ 0\ 8)$ and the $(0\ 1\ 8)$ reflections in $\sigma\sigma$.

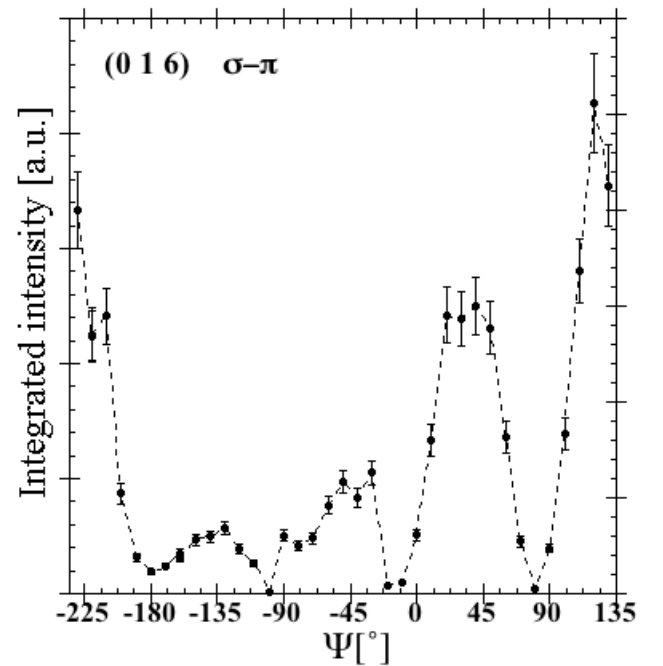


fig.2 Azimuthal scan about the $(0\ 1\ 6)$ reflection.

Reference

- [1] A.A. Taskin *et al*, Phys. Rev. Lett. **90**, 227201 (2003)
- [2] Y. Murakami *et al*, Phys. Rev. Lett. **81**, 582 (1998).
- [3] L. Paolasini *et al*, Phys. Rev. Lett. **82**, 4719 (1999).
- [4] U. Staub *et al*, Phys. Rev. Lett. **88**, 126402 (2002).