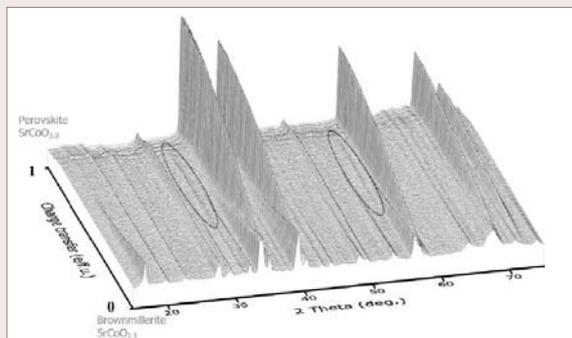


[C5. R. Le Toquin] Time-resolved in situ studies of oxygen intercalation into SrCoO_{2.5}, performed by neutron diffraction and X-ray absorption spectroscopy



Evolution of the neutron powder diffraction pattern obtained in situ during the electrochemical oxidation of SrCoO_{2.5} vs charge transfer. The diffractogram of the brownmillerite SrCoO_{2.5} is represented at the bottom, whereas that of the perovskite SrCoO_{3.0} is shown at the top. The dotted ellipsoids show the positions of the superstructure reflections.

reaction product (SrCoO_{3.0}) does not proceed continuously but gives evidence for the formation of O⁻ species for stoichiometries corresponding to SrCoO_{2.82}(0.07)[1]. The use of neutrons (vs X-rays) in the diffraction experiments and the choice of the transmission (vs fluorescence) mode in the XAFS experiment guarantee that the obtained data well represent bulk and not just surface properties.

[1] R. Le Toquin, W. Paulus, A. Cousson, C. Prestipino, C. Lamberti, JACS 128 (2006) 13161-13174

[Collaboration : R. Le Toquin, W. Paulus, Université de Rennes 1, A. Cousson, LLB, C. Prestipino, C. Lamberti, Université de Turin]

[C6. V. Paul-Boncour] Structural and magnetic properties of RMn₂D₆ compounds (R=Y, Dy, Er) synthesized under high deuterium pressure

Hydrogen absorption in RMn₂ Laves Phases (R= Rare Earth) modifies significantly their magnetic properties. For x ≈ 4.5, the RMn₂H_x hydrides crystallize in a structure derived from that of the parent intermetallic, with H atoms in tetrahedral interstitial sites. Applying a hydrogen pressure of several MPa to YMn₂ led to the formation of YMn₂H₆ [1]. According to X-ray (XRD) and neutron powder (NPD) diffraction experiments, YMn₂D₆ crystallizes in a disordered fluorite structure (K₂PtCl₆ type) with a = 6.709(1) Å at 300 K (Fig. 1). In the Fm3m space group, the Y and half of the Mn atoms (Mn1) occupy randomly the 8c site whereas the remaining Mn atoms (Mn₂ in 4a site) are surrounded by 6 H atoms (24e site). This structure is not derived from that of the C15 YMn₂ and the H atoms form covalent bonding with Mn atoms. RMn₂D₆ phases, isostructural to YMn₂D₆, were also obtained starting either from C15 (R =Dy, Ho) or C14 (R=Er) Laves phases. YMn₂D₆ displays a modified Curie Weiss behaviour and the NPD study shows the absence of long range magnetic order. The M(H) curves of the RMn₂D₆ compounds (R=Ho, Dy and Er) at 4.2 K show a ferromagnetic behaviour but the saturation magnetization is only half that of the parent compound. NPD studies on ErMn₂D₆ [2] revealed only local magnetic order of Er moment below 5 K, with ferro and antiferromagnetic correlations (Fig. 2). This has been related to the chemical disorder of R and Mn atoms on the 8c site.

[1] V. Paul-Boncour, S. M. Filipek, M. Dorogova, et al. J. Sol. State Chem., 178 (2005) 356

[2] V. Paul-Boncour, S. M. Filipek, G. André, F. Bourée et al., J. Phys. : Cond. Mat., 18 (2006) 6409

[Collaboration: V. Paul-Boncour, LCMTR Thiais; S.M. Filipek (Poland), G. André, LLB ; F. Bourée LLB]

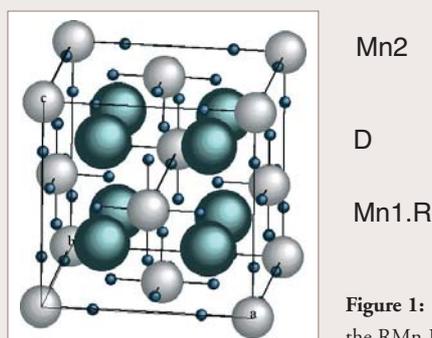


Figure 1: Structure of the RMn₂D₆ compound

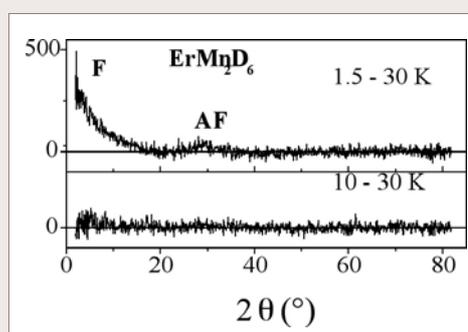


Figure 2: Difference NPD patterns of ErMn₂D₆