Neutron powder diffraction studies of magnetic transitions in Fe-based orthorhombic perovskites

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The orthorhombic iron- and chromium-based perovskites (orthoferrites $RFeO_3$ and orthochromites $RCrO_3$, where *R* is a lanthanide) have been studied for a long time for their wide variety of magnetic properties [1, 2]. Given the flexibility in chemical composition allowed within the perovskite structure, there are plenty of opportunities for cation substitutions in the search for novel properties. In this work, several new quaternary perovskites were studied in an attempt to tune different magnetic properties. Most of these materials display a magnetic transition called spin reorientation (SR), which is outlined on Fig. 1. To evaluate the diverse magnetic transitions, neutron powder diffraction (NPD) experiments were performed in the instruments HRPT (Paul Scherrer Institute) and D1B and D2B (Institut Laue Langevin).

Among the studied compounds, the perovskites $RCr_{0.5}Fe_{0.5}O_3$ (R = Tb, Dy, Ho, Er, Tm, Yb, Lu) display magnetic properties which are mainly determined by the lanthanide cation, particularly at low temperatures. These materials also retain similarities with the corresponding orthochromites and orthoferrites, providing a framework to understand their magnetic properties. Other interesting findings in these perovskites include negative thermal expansion, metamagnetic transitions and magnetization reversal (MR) [3, 4]. The next step was assessing different strategies for the tuning of the magnetic transition temperatures, with substitutions in the A and B sites of the perovskite structure ($Sm_{1-x}Tm_xFeO_3$ and $TmCr_{1-x}Fe_xO_3$, respectively). Both systems enabled the tuning of their magnetic transitions as a function of composition. In the former, the SR transition was successfully shifted to room temperature, while in the latter, three different magnetic transition temperatures (T_{SR}, $T_{compensation}$ of MR and $T_{Néel}$) could be tuned.

This work covers a wide compositional space within the mixed orthochromite-orthoferrite system, exploring many interesting and puzzling magnetic properties. In all cases, NPD was used along extensive magnetization measurements to understand the different magnetic transitions in detail.

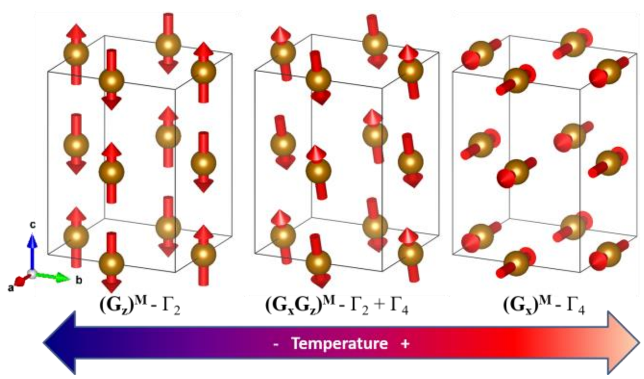

Figure 1. Outline of a spin reorientation transition in the transition metal substructure of an orthorhombic perovskite (*Pbnm* setting).

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Keywords: perovskite, magnetic structure, spin reorientation, neutron powder diffraction.

Authors want to acknowledge the valuable assistance of V. Pomjakushin (PSI), and G. Cuello, E. Suard and V. Nassif (ILL).

Acta Cryst. (2021), A**77**, C228