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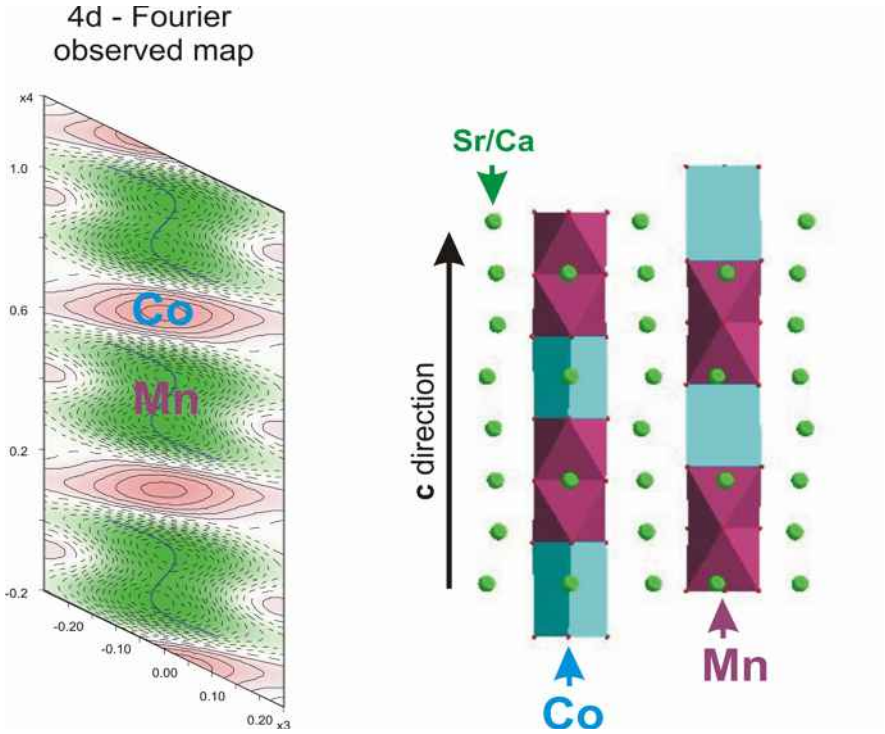
Analysis of Sr3-xCa1+xMn2CoO9 combining electron, X-ray and neutron diffraction

P. Boullay[1], O. Pérez[1], B. Raveau[1], S. Motin[1], C. Vincent[1]
[1]*CRISMAT, ENSICAEN, Caen, France*

The AxBX3 hexagonal perovskite-type compounds exhibit interesting magnetic properties such as complex magnetism or random spin chain magnetism[1,2]. Their structures are built up from infinite [BO3] chains consisting of alternating octahedral and trigonal prismatic units, separated by A infinite chains. Sr3-xCa1+xMn2CoO9 are belonging to this family of materials. X-ray powder diffraction patterns are collected for different Sr3-xCa1+xMn2CoO9 samples with different x values. Pattern matching analysis with the SG P-3 and the following cell parameters a=b=9.490(1)Å c=3xc'=3x2.57=7.732(1)Å reveals problematic groups of reflections; these reflections are shifted from one pattern to another one and, moreover, have positions preventing their indexation. Owing to the lack of spatial resolution and peaks overlapping in the powder data, the understanding of the present problem is quite impossible. Electron Diffraction Tomography (EDT) combined with Precession Electron Diffraction (PED) has been used for exploring the reciprocal space of the Sr3-xCa1+xMn2CoO9, x=0 sample. The slight deviations observed from the rational 1/3 c'* value is in agreement with the existence of aperiodicities. The structure of this family of materials has been then described using the super space formalism as a composite structure. The structural model is determined from the PED data integrated with PETS[2]; the first and second sublattices are referring to (Mn,Co)O3 and (Ca,Sr) structural parts respectively. This model is confirmed by the refinement of the X-ray powder diffraction data. Powder neutron diffraction data were then collected at PSI for different temperatures and different Sr3-xCa1+xMn2CoO9 samples. Using the previously refined model, a Co/Mn ordering is revealed thanks to the neutron scattering lengths of these two elements (see fig1). Finally, the treatment of the antiferromagnetic behavior observed bellow 25K is performed in the 4d approach using Jana2006[3].

[1] *Roussel,P., Perez, O., Quarez, E., et al., Zeitschrift für Kristallographie (2010) vol. 225, p. 1-11,* ***[2]*** *Palatinus, L. (2011). PETS – program for analysis of electron diffraction data. Institute of Physics of the AS CR, Prague, Czech Republic,* ***[3]*** *Petrıcek, V., Dusek, M. & Palatinus, L. (2006). The crystallographic computing system JANA2006. Institute of Physics, Prague, Czech Republic.*



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