Experimental report

30/11/2023

Proposal: 5-31-2924 **Council:** 10/2022

Title: Lattice and spin structure investigation from Perovskite to Brownmillerite in La0.7Sr0.3MnO3-¿ powder

Research area: Physics

This proposal is a new proposal

Main proposer: Chenyang YIN

Experimental team: Chenyang YIN

Local contacts: Maria Teresa FERNANDEZ DIAZ

Samples: La0.7Sr0.3MnO3-¿

Instrument	Requested days	Allocated days	From	To
D2B	7	1	31/05/2023	01/06/2023

Abstract:

In complex oxides, oxygen vacancy plays a crucial role in determining the physical properties and enables various applications. The Perovskite (PV) to Brownmillerite (BM) topotactic phase transition can be triggered by deoxygenation in the La0.7Sr0.3MnO3-¿ (LSMO) system. Previously, we investigated the influence of oxygen off-stoichiometry in LSMO thin films during the PV-BM topotactic phase transition. However, the properties of thin films are strongly influenced by the strain induced from the substrate. In contrast, bulk-like powder constitutes a strain-free system. Comparing such a strain-free system with the thin film system is highly interesting in order to elucidate the role of the strain onto the topotactic phase transition. Especially, neutron powder diffraction allows a detailed determination of both crystal and spin structure, which can enable a comprehensive understanding of how oxygen vacancies influence the lattice and spin structure during the phase transition.

Experimental report for proposal 5-31-2924
Proposal title: “Lattice and spin structure investigation from Perovskite to Brownmillerite in $La_{0.7}Sr_{0.3}MnO_{3-\delta}$ powder“

Results:
For this proposal, we were allocated for one day of beamtime at D2B on 31.05.2023. This allows us to measure one sample at different temperatures. One Al-assisted thermal vacuum annealed $La_{0.7}Sr_{0.3}MnO_{3-\delta}$ (LSMO) powder sample exhibiting antiferromagnetism with Curie-Weiss temperature of θ = 7K (verified by SQUID-magnetometry) was measured at 2K, 250K, and 400K at D2B. Compared with the neutron diffraction pattern measured at 400K three new magnetic peaks were observed in the pattern measured at 2K, shown in Figure 1a. After Rietveld refinement (Figure 1b), we determined the crystal and magnetic structure for this sample. The refinement was done via the software Mag2pol and Fullprof [1, 2]. As illustrated in Figure 1c., the alternating oxygen octahedron (green) and tetrahedron (grey) structure indicate this sample is a Brownmillerite type LSMO. This monoclinic structure at 2K is with lattice parameters: a= 17.3667Å, b= 5.466Å, c=11.2087 Å, α=90°, β=108.86°, γ=90°. The corresponding magnetic structure is demonstrated in Figure 1d. This brownmillerite type LSMO shows a commensurate type of antiferromagnetic spin structure with the propagation vector of (0.5, 0, 0) which has been determined for the first time.

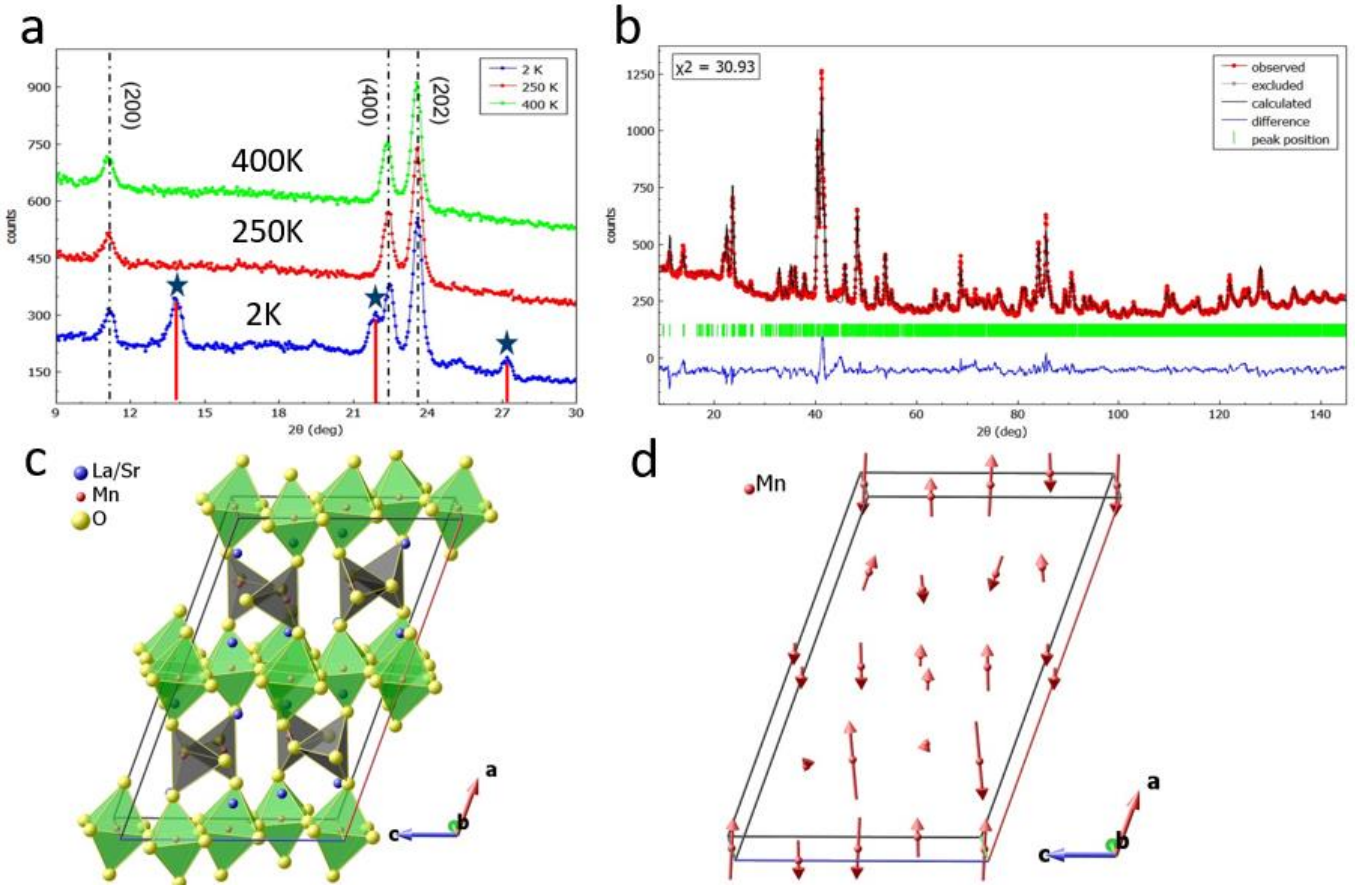

Figure 1 (a) powder neutron diffraction patterns at 2K, 250K, and 400K. The new magnetic peaks are labelled with stars. (b) Rietveld refinement of the neutron diffraction pattern at 2K. (c) Refined crystal structure at 2K. (d) Refined magnetic structure at 2K.

[1] Qureshi, N., Mag2Pol: a program for the analysis of spherical neutron polarimetry, flipping ratio and integrated intensity data. J. Appl. Cryst., 2019.52: p.175-185.
[2] Rodriguez-Carvajal, J., PHYSICA Recent advances in magnetic structure determination neutron powder diffraction. Physica B, 1993.192(93): p.55-69.