

Crystal and magnetic structure determination of the oxygen deficient perovskite $\text{YBaMn}_2\text{O}_{5.5}$.

In the practical session we shall perform a complete analysis of X-ray and neutron diffraction data of the title compound, using the programs of the FullProf Suite. All the results have been published in the article:

"Crystal and magnetic structures of the Mn^{3+} orbital ordered manganite $\text{YBaMn}_2\text{O}_{5.5}$ "
C. Perca, L. Pinsard-Gaudart, A. Daoud-Aladine, M.T. Fernández-Díaz and J. Rodríguez-Carvajal.
Chemistry of Materials 17, 1835-1843 (2005)

A copy of this article is provided as a PDF file for personal use during the course.

The data files, at room temperature, corresponding to a laboratory X-ray diffraction pattern ($\text{YBaMn}_2\text{O}_{5.5}$ _RX.dat) and two neutron diffraction patterns ($\text{YBaMn}_2\text{O}_{5.5}$ _3T2.dat, $\text{YBaMn}_2\text{O}_{5.5}$ _D1A.dat) of different instruments and wavelengths will be used in the final refinement.

There are three IRF files (3t2.irf, d1a.irf and rx.irf) containing the characteristics of the instruments. In the reserved "pcr-files" directory there are three individual PCR files that are appropriate for refining individually the three diffraction patterns and another file called Multi-Pattern.PCR that allow a combined refinement of all patterns simultaneously.

First exercise

- 1: Indexing the X-ray diffraction pattern $\text{YBaMn}_2\text{O}_{5.5}$ _RX.dat (Ins=0). Use TREOR90 and DICVOL04 from WinPLOTR.
- 2: Try to determine the possible space groups using CheckGroup after refining the powder diffraction pattern using the Le Bail method.
- 3: A proposal in the literature was the space group Ammm, a PCR file is provided with this model. Refine the different patterns using this model and see the presence of additional peaks not accounted for by the unit cell provided in the Ammm-model
- 5: Starting from the model Ammm try to construct another model using the possible space groups found in the previous exercise 2. Compare with the already provided PCR files in the "pcr-files" directory.
- 6: Refine the diffraction patterns for the retained model and finally construct a single PCR file handling the three patterns simultaneously. Use the different programs for calculating Bond Valence Sums and for visualising the crystal structure.

Second exercise

- 1: A set of files, corresponding to neutron diffraction data taken on G4.1 (LLB), will be used to determine the magnetic structure of $\text{YBaMn}_2\text{O}_{5.5}$ as a function of temperature. There are 59 data files (lg34783.dat up to lg34841.dat) corresponding to different temperatures. The format of the files corresponds to Ins=5. Construct a buffer file and open it with WinPLOTR-2006 to explore the magnetic ordering.
- 2: Determining the magnetic structure of this compound at low temperature: determine the propagation vector, make a symmetry analysis and test systematically the possible solutions. A PCR file with the nuclear structure fixed is provided.
- 3: Determining the first magnetically ordered state of this compound (just below T_N).
- 4: Use of FullProf in sequential mode to treat all the diffraction patterns and visualise the behaviour of cell parameters and magnetic moments as a function of temperature.