

Binary and Ternary oxides phases diagrams studied via solid-solid state reaction and X-ray powder diffraction.

Q. Ye, M. Barré, K. Adil, A. Rousseau and F. Goutenoire

UMR6283, IMMM (Institute of Molecules and Materials of le Mans),

University of the Maine, 72085 Le Mans, Cedex 9, France
francois.goutenoire@univ-lemans.fr

Keywords: x-ray, powder, diffraction

In the solid-state nature, the X-ray diffraction is a common analysis for crystallized compounds in many fields (metallurgic, inorganic and organic chemistry and mineralogy). X-ray diffraction is also used to investigate phase diagrams in their solid part. Nevertheless, there is a large number of known phase diagrams where there is a lack of structure data due to “the impossibility to obtain single crystal”.

Since few decades, the structural determination from powder diffraction becomes easier [1]. This is mainly due to the improvement of the laboratory X-ray powder diffractometer and also the developments of new methods and computer programs (Real space Monte Carlo [2] and Super Flip [3]).

Few examples of different cases will be present. The binary phase diagrams $\text{La}_2\text{O}_3\text{-MoO}_3$ and the case of the new compound $\text{La}_6\text{Mo}_8\text{O}_{33}$ [4], the binary phase diagrams $\text{La}_2\text{O}_3\text{-WO}_3$ [5]. And more recently, our results on some ternary phase diagrams. In these last cases, the difficulty is increase due to the possibility to have three phases in equilibrium. Hopefully, new computer analysis namely PCA (Principal Component Analysis) could help to detect new phase.

[1] W.I.F David, K. Shankland, L.B. McCusker and Ch. Baerlocher, **Structure determination from powder diffraction data**, IUCR Monographs on crystallography.

[2] A. Le Bail, **Program Espoir 3.5**, <http://www.cristal.org/sdpd/espoir/>.

[3] L. Palatinus, **The charge flipping algorithm in crystallography**, Acta Cryst B, vol 69, 2013.

[4] V Brize et al., **$\text{La}_6\text{Mo}_8\text{O}_{33}$ a new ordered defect scheelite superstructure**, JSSC, 177, 2004.

[5] M.H. Chambrier and F. Goutenoire, **Structural exploration on powder diffraction a nice tool for reexamination of phase diagram**, , JEEP, 00022(2009), DOI:10.1051/Jeepp/200900022

JEEP 2023

October 4-6, 2023

Preferred type of contribution:

☐ **Poster**

☐ **Oral**

NB : The final decision belongs to the Scientific Committee