Combined Analysis: XRD-XRF-Raman within the EU SOLSA project

Daniel Chateigner, Professor,
CRISMAT-CNRS, Normandie Université,
Caen, FRANCE

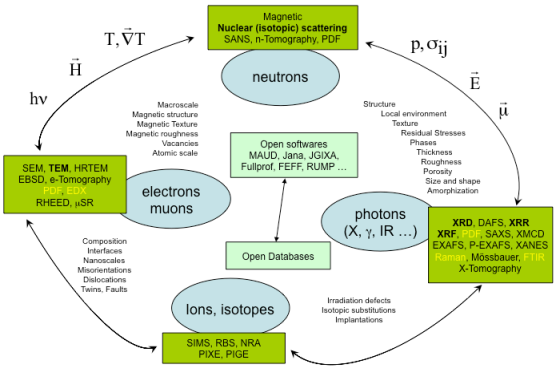
Abstract:

The SOLSA project aims to construct an analytical expert system for on-line-on-mine-real-time mineralogical and geochemical analyses on sonic drilled cores, an unprecedented challenge both in terms of instrumental, methodological and software developments.

Two instrumental developments will be carried out during this European project, one at the laboratory scale (ID1) deserving methodological testing, the other at the operational on-mine scale (ID2). At present, only ID1 is achieved for first tests. This instrument will perform simultaneously x-ray diffraction experiments, coupled to x-ray fluorescence, Raman and IR spectroscopies. It consists in a 4-circles diffractometer equipped with a curved position sensitive detector and a Cu microsource, a fluorescence detector, and an innovative system of fiber optics and mirrors to achieve Raman and IR probing. All the four experiments are able to probe a flat surface sample within approximately the same sampled volume.

In order to benefit of the complementarity of the four techniques, an expert system able to refine all datasets has to be developed. For the x-ray diffraction and fluorescence parts, the actual Combined Analysis methodology is operational for structure, microstructure, texture, stress, phases and element analyses. Complementing the Combined Analysis approach by Raman and IR spectroscopies is targeted in this project to help phase identifications and quantifications. In this aim the expert system will use Open Databases, either already existing like the Crystallography Open Database, or under development like the Raman Open Database.

We will illustrate the actual state-of-the-art Combined Analysis, and envision its near-future developments within the spectroscopies context.



Recent Publications:

- D. Chateigner (Ed.) (2010): Combined analysis, Wiley-ISTE, 496p. ISBN: 978-1-84821-198-8
- L. E. Fuentes-Cobas, D. Chateigner, M. E. Fuentes-Montero, G. Pepponi, S. Grazulis (2017). The representation of coupling interactions in the Material Properties Open Database (MPOD). *Advances in Applied Ceramics* **116** 428-433
- M. Freire, N.V. Kosova, C. Jordy, D. Chateigner, O.I. Lebedev, A. Maignan, V. Pralong (2016). A new active Li–Mn–O compound for high energy density Li-ion batteries. *Nature Materials* **15** 173-177
- Boullay P., Lutterotti, L., Chateigner D., Sicard, L. (2014). Fast microstructure and phase analyses of nanopowders using combined analysis of transmission electron microscopy scattering patterns. *Acta Crystallographica A* **70** 448-456
- Chateigner D. (2014). Crystallography Open Databases and Preservation: a World-Wide Initiative. In *Scientific Data Preservation*, Diaconou Ed., 20-25, CNRS Editions
- E.-P. Ng, D. Chateigner, T. Bein, V. Valtchev, S. Mintova (2012). Capturing ultra-small EMT zeolite from template-free systems. *Science* **335** 70-73