29th International Conference on Nanomaterials and Nanotechnology

4th Edition of International conference on

Advanced Spectroscopy, Crystallography and Applications in Modern Chemistry

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Combined analysis: XRD-XRF-raman within the EU SOLSA project

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 micro source, 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.



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Biography

Daniel Chateigner is a specialist in Combined Analysis using X-rays, electron and neutron diffraction. His main activities are two folded: i) push forward the development of Combined measurement and Analysis: texture, structure, crystallite sizes, reflectivity, residual stresses, phase analyses, fluorescence, Raman ..., in a single approach called "Combined Analysis" (ISTE-Wiley 2010). This methodology has been employed in many science fields, from high-tech materials to biomineralisation. ii) developments of Open Databases around crystallography, the largest worldwide Crystallography Open Database (COD www. crystallography.net), the Materials Properties Open Database (MPOD http://mpod.cimav.edu.mx), more recently the Raman Open Database (ROD http://solsa. crystallography.net/rod/) and Theoretical CODs, TCOD (http://www.crystallography.net/tcod/) and PCOD (http://www.crystallography.net/pcod/).

In 1996 he worked as research fellow at the University of California at Berkeley (Earth and Planetary Science department, USA) then became Maître de Conférences at Université du Maine (Le Mans, France) where he received his Habilitation diploma. Since 2001 he is Professor at Normandie Université. He gained a PhD in Physics and Crystallography from Université Joseph Fourier (Grenoble) in 1994.

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