MS41. Advanced powder diffraction

Chairs: Radovan Černý, Michela Brunelli

MS41-O1 Multidimensional studies of heterogeneous working devices

Gavin Vaughan[1]

1. ESRF, CS40220 38043 Grenoble Cedex 9 France

email: vaughan@esrf.fr

Real working systems for chemical applications are typically highly heterogeneous, and the isolated characterization of their constituent elements, ex-situ, is typically not sufficient to understand their operation under real working conditions. Likewise, studies of model systems may capture the essential operation of these devices, but not the interaction between atomic structure and nano- and microscopic engineering which may in fact be of crucial importance in the actual functioning of these devices.

For this reason, methods have been developed to carry out three dimensional diffraction characterization, often coupled with ancillary probes or simultaneous absorption tomography, of real devices under real operational conditions. In order to understand fully the functioning of devices key to the energy economy, such as batteries, fuel cells, solar cells and hydrogen storage materials, or of reactions crucial the chemical industry, such as catalysis or large-scale syntheses, simultaneous characterization on multiple length scales is a requirement.

We will discuss the experimental means to probe via synchrotron X-ray diffraction methods the multi-dimensional space spanned by the properties of interest to understand the chemical functioning of such systems. Examples will be given, in particular for poorly crystalline or amorphous materials, for which three-dimensional volumes have been reconstructed, with each voxel characterized with respect to its atomic, microstructural and temporal evolution.

Keywords: diffraction tomography, synchrotron, in operando

MS41-O2 Femtosecond X-ray powder diffraction

Michael Woerner[1]

1. Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy Max-Born-Strasse 2A, 12489 Berlin, Germany

email: woerner@mbi-berlin.de

The spatial arrangement of valence electrons determines structural and functional properties of crystalline matter. While equilibrium electron distributions have been derived with high precision from stationary x-ray diffraction experiments, their transient changes during optically induced functional and/or relaxation processes have remained mainly unexplored. Femtosecond x-ray powder diffraction allows for determining transient electron density maps in crystals with a spatial resolution of 0.03 nm and a temporal resolution of 100 fs. Using a tabletop, laser driven, femtosecond hard x-ray source in combination with a setup for x-ray powder diffraction to record diffraction patterns consisting of several tens of reflections we study in a pump-probe approach, photo-induced structure changes in the femtosecond time domain by diffracting ultrashort hard X-ray pulses from the excited sample. Both changes of atomic arrangements, i.e. lattice geometries, and of electronic charge density are addressed. In the talk I shall discuss our measurements of transient electron density maps in a variety of ionic crystals [1-6].

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