SNBL BM31: towards multi probe operando XRD + XAS + PDF

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The availability of experimental methods that probe a material's structure, often complex and dynamic, at different length and time scales is key to obtain fundamental insight in technologically relevant materials and environmental geochemistry. Indeed, progress in sustainable technologies relies on the development of innovative materials utilizing an in-depth understanding of the interplay between a material's structure and its macroscopic properties. To this end, there is a need for advancing current X-ray based facilities allowing the study of materials with multiple techniques at their working state (i.e., operando methods).

The BM31 station of the Swiss Norwegian Beam Lines (SNBL) at the European Synchrotron Radiation Facility (ESRF), offers the possibility to combine X-ray absorption spectroscopy (XAS) and X-ray powder diffraction (XRD) in an alternating fashion, quasi-simultaneously, in the same experimental setup. SNBL aims at extending these capabilities, by upgrading the current setup with a new CdTe area detector and focusing capabilities. This equipment will allow to i) implement pair distribution function analysis (PDF) of total scattering data, enabling combined XRD-PDF-XAS experiments and ii) enhance appreciably both the temporal (~1 s for XAS, ~100 ms for XRD-PDF) and spatial resolution (utilizing a beam size of ~100 × 100 μm2) of the experiments. The upgraded BM31 optics and endstation will also be compatible with the implementation of a XES von Hamos spectrometer, foreseen at a later stage.

The combined XRD-PDF-XAS measurements will allow the acquisition of complementary information of a material under the relevant working conditions: covering the length-scale from short to mid-range atomic arrangements viz. ~ 1 Å to several nm by PDF, the average structure by XRD, as well as the electronic state, and geometry around the element of interest by XAS. All these data can be acquired in a temporal and spatially resolved manner in a single experiment. This will constitute a unique tool allowing the detailed study of materials for a wide range of applications, for instance: heterogeneous and electro-catalysis, CO_2 capture, gas separation, batteries and trace element reactions in environmental studies.