Invited Lecture

Inspired by users: big data tools at the Swiss-Norwegian Beamlines at ESRF

V. Diadkin[1], D. Chernyshov[1]

[1]Swiss-Norwegian beamlines (SNBL) at the European Synchrotron Radiation Facilities (ESRF), 38000 Grenoble, France

diadkin@esrf.fr

The Swiss-Norwegian beamlines at the European Synchrotron Radiation Facility have now been in user operation for almost three decades. Over the last decade, the scientific activities on the beamlines have become more and more focused on solving problems in materials science and crystal chemistry, that also implies an advent of new users with little experience in synchrotron experimentation. Here we present an overview of the operational characteristics of the beamline software and the data tools developed for BM01 and BM31.

Although BM01 originally conceived as a station for single crystal diffraction, the combination of large area detector Pilatus2M and flexible goniometer provides a very versatile diffraction platform for many types of X-ray diffraction and scattering experiments: powder diffraction, diffuse scattering, high-pressure experiments, surface diffraction and many others. Currently, the diffractometer is composed of the two fast Pilatus 2M detectors for WAXS and SAXS measurements; the detectors can be used separately or simultaneously offering a necessary combination of high angular coverage with high angular resolution. We provide a few goniometer schemes including a heavy load kappa setup. The beamline also supports a variety of in-situ operando tools covering broad range of temperature, pressures, electric and magnetic fields, battery and gas cells.

The flexibility of the setup together with a large number of the experimental protocols requires a dedicated software for data acquisition and processing that has to be easy-to-use for beamline newcomers and, at the same time, must have a lot of advanced options for experts. An overview will be given to the SNBL data collection and processing pipeline: Pylatus (control software of the diffractometer), SNBL ToolBox (a set of tool for data reduction), Bubble (powder integration), Medved (data viewer) and a few other tools. A survey of high-energy diffraction (XRD/PDF) and EXAFS station BM31 will be presented as well, in particular with respect of the advanced scripting.

The software tools and applications of the diffractometers will be illustrated with examples of absolute structure determinations, diffuse scattering, multi-temperature data collections both for powder and single crystals, medium pressure studies, in-situ diffraction under controlled gas atmosphere, and also diffraction from thin films.