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Beamline P02.1: A Workhorse for High-Resolution Powder Diffraction & Total Scattering Experiments at PETRA III, DESY

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Powder diffraction is a standard tool for characterisation in a wide range of fields across the physical sciences: from materials science and metallurgy, to chemistry and solid state physics. Third generation synchrotron sources provide high fluxes of X-rays at higher energy than laboratory sources. These characteristics open the door not only to rapid data collection for high spatial-resolution structural studies, but also to time-resolved in situ/in operando measurements of functional materials under real conditions, thanks to high energy X-rays being able to penetrate operating environments. Furthermore, the use of high energy X-rays increases the region of reciprocal space which may be studied in an experiment, facilitating improved spatial resolution in total-scattering measurements.

Beamline P02.1 (PETRA III, DESY, Hamburg, Germany) is almost unique amongst high-resolution powder diffraction instruments in operating at a fixed energy of 60 keV [1],[2]. This energy is particularly well suited to the collection of powder diffraction data for Rietveld refinement (especially for high-Z materials, where absorption is a problem at lower energy) and for collection of total-scattering data (the high energy facilitating Q_{Max} of at least 20 \AA^{-1}), which may be interpreted by Pair Distribution Function (PDF) analysis. Currently two detectors are available on the beamline (a two-dimensional Perkin Elmer XRD1621 and an in-house developed 10-channel Multi-Analyser Detector), whilst additional devices are available from a shared detector pool (including a Dectris Pilatus3 CdTe 2M designed for high-energy data collection).

In addition to ambient temperature capillary measurements, P02.1 offers a range of standard sample environments (e.g. hot-air blower –RT–1100 K; cryostream –90–500 K; cryostat –10–300 K) whilst a number of others are under development (e.g. low pressure gas adsorption cell) or are maintained by the PETRA III sample environment group. Recently we have also brought a sample changing robot into operation, with capacity for 300 samples (see figure); this device is compatible with the cryostream and hot-air blower environments. Furthermore, the enormous amount of free space around the diffractometer, compared to many other powder diffraction beamlines, allows easy integration of complicated sample environments which are brought to the beamline by our users.

We report here the latest developments at P02.1 including planned changes to detector configurations, new sample environments, updates to the control software and possible remote access schemes.

[1] Dippel A.-C., Bindzus N., Saha D., Delitz J. T., Liermann H.-P., Wahlberg N., Becker J., Bøjesen E. D., Brummerstedt Iversen B., Z. Anorg. Allg. Chem. 2014, 640, 3094.

[2] Dippel A.-C., Liermann H.-P., Delitz J. T., Walter P., Schulte-Schrepping H., Seeck O. H., Franz H., J. Synchrotron Radiat. 2015, 22, 675.

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