Overview and Developments at the High-Energy Beamline P21.2, Petra III, DESY

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P21.2 is the inline branch of the Swedish Materials Science beamline and is specialized on multi-modal diffraction and imaging studies at energies between 40 and 150 keV. Flexible focusing and monochromatization options are available depending on the experimental needs for resolution and flux. Available detectors for scattering include large flat panel and low-noise photon-counting pixel detectors variants. The range of high-resolution CMOS-based imaging cameras has recently been expanded to offer higher speeds and larger field of view. Detectors for X-ray reflectometry and fluorescence as well as an assortment of sample environments, e.g. heaters, furnaces and load frames are available as well.
The beamline provides two experiment endstations. The multi-purpose endstation EH3 is in operation since 2019 and has served a variety of experiments such as combined SAXS/WAXS, surface diffraction and grain-resolved studies as well as radio- and tomography in different contrast modes. The spacious hutch is well suited for *in-situ* and *operando* studies in large setups and distributed peripherals. For precise positioning of samples and environments a Huber surface/interface diffractometer is routinely used. Individual rotation and translation stages and a high load capacity hexapod are available as well. A system of motorized portals around and downstream of the sample position provides a high degree of freedom for detector positioning. The portals are accompanied by a 15 m evacuated flight tube for SAXS measurements.
The newly furbished second endstation EH2 is under commissioning and is expected to host first user experiments in the second half of the year. It is mainly targeted at heavy and bulky equipment and sample environments. As such it prominently features a large hexapod for sample positioning with a maximum capacity of 1.5 tons and optional rotation stage. A detector table with two movable towers can host any of the available detectors. Hexapod and detector table are supported on air casters and can be flexibly repositioned for the desired measurement geometry. A portal frame for positioning close to the sample is planned as well.
The flexible detector positioning capabilities in EH3 enable a new addition to the beamline technique portfolio — combined small-, wide and total scattering (for PDF) measurements, i.e. SAXS/WAXS/PDF. Staggered placement of multiple detectors with overlapping Q-range segments allows for a simultaneous and continuous coverage over an exceptionally wide overall Q-range. We will present initial results from a first run of this setup investigating the formation and growth of Mo-based polyoxometalate (POM) clusters with a Q-range coverage from ~0.02 to ~16 $Å^{-1}$ at ~40 keV, i.e. spanning three orders of magnitude.
Furthermore, we are highlighting developments on the beamline data analysis capabilities provided to the users. Currently, diffraction experiments with our flat-panel detectors can be augmented by an automatic data integration pipeline providing fast feedback to the users for manual post-processing and decision-making during the beamtime. The scope of pipeline is being extended to support additional detectors and techniques in a modular manner to cover a larger range of experiment types. The modularity will also allow users to integrate own, bespoke data processing steps adhering to the pipeline interface protocols. To complement the online capabilities, the same analysis codes provided by the beamline are foreseen to also power a set of computational notebooks for offline usage, e.g. manually during or post beamtime at the home institute.