

The Powder Diffraction and Total Scattering Beamline P02.1 at PETRA III, DESY

[Alba San José Méndez](#)¹, Volodymyr Baran¹, Henrik Jeppesen¹, Alexander Schökel¹, Tim Schoof¹, Mario Wendt¹, Sergej Wenz¹ and Martin Etter¹

¹Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, alba.mendez@desy.de and martin.etter@desy.de, Germany

Powder Diffraction is a well-established method that allows to investigate long-range order structural properties of crystalline materials. On the other hand, Total Scattering measurements in combination with the Pair Distribution Function method is an expanding and powerful technique that allows to investigate the short-range and/or long-range order at the same time, making it possible not only to investigate crystalline materials, but also amorphous solids or liquids. Therefore, the combination of both methods provides a detailed insight into the structure of a wide range of material systems, including organic materials such as pharmaceuticals, co-crystals, covalent-organic frameworks, polymers and fibers, metal-organics such as metal-organic frameworks and inorganic materials such as nanoparticles, ceramics, cements, battery materials, metals and steels, metallic glasses, minerals and mineral glasses, superconductors, strongly (electron-)correlated materials, corrosion products, melts, liquids and so forth. For this huge range of crystalline and non-crystalline materials, structural properties, phase transitions or phase mixtures can be investigated at synchrotron facilities in *ex situ*, *in situ* or *operando* experiments utilizing either beamline-offered or user-developed sample environments.

The Powder Diffraction and Total Scattering Beamline P02.1 at the PETRA III synchrotron at the DESY facility in Hamburg, Germany, is a specialized station, where researchers from science and industry have the possibility to collect Powder Diffraction and Total Scattering data simultaneously with a fixed energy of 60 keV [1, 2]. With a custom-made tandem detector setup consisting of two large area detectors, users can, among others, perform *in situ* crystal growth experiments from the amorphous and nanocrystalline state up to the microcrystalline state, collecting simultaneously high-resolution Powder Diffraction data and Total Scattering / Pair Distribution Function data on the same sample. The P02.1 beamline offers a variety of sample environments for high-temperature (gas blowers, ceramic heater, Linkam furnace) and low-temperature (cryostreamer, cryostat) studies, as well as for mechanical treatments (stress rig, ball mills, etc.). While the aforementioned sample environments are available at the beamline, others like gas-flow cells, battery setups, etc., are provided on a collaborative basis with DESY users. Besides regular on-site synchrotron experiments, users can also apply for mail-in / rapid access services for Powder Diffraction and/or Total Scattering / Pair Distribution Function measurements of samples packed in capillaries. These measurements can be then automatically performed using a robotic system either at room-temperature or at temperatures in the range between 100 K and 1200 K, achieved by the employment of a liquid nitrogen cryostreamer and a hot-air blower.

In this presentation, we will inform the scientific community as well as industrial customers about the latest developments at beamline P02.1.

[1] Dippel A.-C. et al., Z. Anorg. Allg. Chem. 2014, 640, 3094.

[2] Dippel A.-C. et al., J. Synchrotron Radiat. 2015, 22, 675.