The High Resolution Powder Diffraction Beamline P02.1 at PETRA III is a high-energy station that provides fixed energy photons of 60 keV. It is dedicated to in situ analysis of complex polycrystalline, disordered, and nanocrystalline materials during synthesis or under realistic operating conditions. In November 2010, P02.1 started operations with the first x-ray beam in the experimental hutch. About a month later, the first diffraction pattern was collected using a temporary setup that consisted of a pair of slit systems, a sample positioning stage, and an area detector. This temporary setup was gradually upgraded during the next months by e.g. a 2-circle diffractometer and sample environments for heating and cooling. At the same time, the beamline optics were commissioned for user operation. Since August 2011, medium resolution experiments are performed at P02.1 using the PerkinElmer XRD1621 area detector and standard as well as user-specific sample setups. Concurrently, the rebuilding of the beamline to the final high resolution station was prepared.

As a first step, the optical elements such as slit systems, absorbers, and small shutter were placed onto a granite block concrete-cast to the floor. In July 2012, the high resolution powder diffractometer was ready for installation at the beamline. The 3-circle diffractometer with a diameter of ~2000 mm of the largest detector plate was funded by the German federal ministry for education and research (BMBF, grant no. 05KS7OD2) and manufactured by Rotary Precision Instruments UK. The diffractometer was designed to carry sample environments up to a weight of 50 kg and two different types of detectors: a 10-channel multi-analyser detector (MAD) for high resolution diffraction measurements (funded and constructed by the above BMBF project), and a microstrip detector array covering a large angular range for very fast parallel data collection. While the microstrip detector suitable for high-energy x-rays is under development, the MAD was installed end of 2012 and is being commissioned for routine operation.

The PerkinElmer detector, on the other hand, was re-implemented immediately after the high resolution instrument was initially set up. The table tracks for the detector translation were designed to maximise the range of movement parallel and perpendicular to the beam. Basically, the sample to detector distance (SDD) may now be varied between approx. 200 and 3000 mm provided that the experimental setup does not restrict the detector movement in any other way. Laterally, the detector can be moved off-center by a whole width of the active area, i.e. 400 mm, so that the direct beam is not recorded on the image. This setup enables the collection of diffraction data to more than 30 Å⁻¹ in q-space at short SDD as well as a high resolution setup at large SDD. Most experiments that were performed at P02.1 until the end of 2012 made use of the PerkinElmer area detector. Detailed analysis of the instrumental resolution function that takes into account the individual geometrical contributions e.g. by the beam, the sample, and the pixel size is in progress. This function will yield the boundary conditions for crystallite size and strain determination when using the area detector.

In Fig. 1, the 3d model of the final experimental setup and a picture of the actual status at the end of 2012 are displayed. The temporary sample environment table will be replaced by the customised table on rails in 2013. On the whole, this beamline layout provides large flexibility to accommodate bulky and heavy sample environments either on the inner circle of the diffractometer or on the support table in front. Even very complex experiment setups can be implemented that require all-in-vacuum or specific optical elements. Further upgrades include the installation of an automated sample changer robot and focusing optics. These features will enhance the beamline performance with respect to high-throughput measurements under standard conditions as well as applications that require a small x-ray beam, such as spatially resolved scans over inhomogeneous samples and thin film analysis.
Fig. 1: Sketch (a) and photograph (b) of the experimental setup at beamline P02.1, final and current state respectively.