The safety and quality of products made from different materials depend on the quality of metrological assurance used for characterization of the composition and properties of these materials. Modern diffractometric systems have new components which increase the productivity of these systems, whereas they may cause new uncertainties in the results of determining of the characteristics based on the diffraction pattern measurement data. Therefore of the considerable changes are needed in the Testing Program for Type Approval. Note that some manufacturers and users may not pay due attention to the metrological assurance, and the reliability and repeatability of characteristics. Some types of diffractometers are tested only for one and unconventional characteristic of the diffraction pattern, for example, angular position at small angles of diffraction reflections. As results is allows provide assurance for approximate phase analysis only. The accuracy for the positions of these reflections can be lower by one order of value than for the reflections whose positions are at very high values of angles, but it is based on these values that the uncertainty of crystal lattice parameters is determined just. In order to provide a more profound and overall testing of diffractometers for Russian Federation have been developed a new programs and certified measurement procedures and the system of Certified Standard Reference Materials (CSRM) of diffraction properties, based on stable physical characteristics and related to the parameters of the diffraction pattern [1-2]. Note that the results of comparative measurements show that the achieved accuracies for our CSRM and for the similar SRM systems available at NIST are alike. This CSRM system allows to conduct tests of X-ray diffractometers for conventional and new purposes: 1) a quantitative phase analysis based on the ratio of reflection intensities and on the results of measuring of a complete diffraction pattern using the Rietveld methods; 2) determining of micro-structural characteristics (grain sizes, sizes of nano-fragments and the value of micro-distortions of a crystal lattice) which are in demand especially in the machine-building, micro-electronics and bio-nanotechnology. For this purpose we use CSRM and Measures with different levels of micro-distortions and taking into account the atomic weights of components; 3) determining of the life-service of a product on the basis of residual stress. The use is made of tablet-shaped, sintered CSRMs and measures; 4) for single crystal diffractometers we have developed new relevant and required CSRMs also.


Keywords: diffractometric systems; metrological assurance; reliability and repeatability

The Bio-imaging and diffraction beamline P11 at Petra III is dedicated to Imaging and diffraction experiments of biological samples. The beamline provides two different endstations: An X-ray microscope operated between 2.4 and 10 keV and a crystallography experiment operating between 6 keV and 35 keV. The main basis of idea for the beamline design is to provide an extremely stable and flexible setup ideally suited for micro- and nano-beam applications.

The P11 X-ray optics consist of a LN2 cooled double crystal monochromator and two horizontal deflecting and one vertical deflecting X-ray mirror. All three mirrors are dynamically bendable and are used to generate an intermediate focus at 65 m from the source with a size of 16 x 96 µm rms (v x h) and a divergence of 8 x 15 µrad rms (v x h). For the design of the beamline optics special care was taken to preserve the coherence properties of the beam and to deliver most of the photons from the source into a small focal spot at the sample position.

Key element of the experimental hutch is an 8 meter long granite block with a weight of 10 tons, carrying the two experiments. The secondary source is physically located on top of the granite. A Scanning Transmission X-ray microscope (STXM) will allow structural investigations of aperiodic objects such as single cells and also small tissue sections. The crystallography endstation will provide beamsizes down to 1 micron with a photon flux of > 10^12 ph/sec for the investigation of micro crystals. The experiment is equipped with a Pilatus 6M detector and an automatic sample changer.

The presentation will provide general information of beamline P11 with special emphasis on different high precision X-ray optics and other hardware components developed for the beamline.

Keywords: Macromolecular Crystallography; X-ray optics; Instrumentation