KR 9: Recent Developments in X-ray Diffraction

Time: Thursday 10:15–11:00 Location: CHE 184

KR 9.1 Thu 10:15 CHE 184

A diffraction effect in X-ray area detectors — •Christian Gollwitzer and Michael Krumrey — Physikalisch-Technische Bundesanstalt, Berlin, Germany

When an X-ray area detector with a single-crystalline sensor layer, such as a hybrid pixel detector, is used to record a scattering or diffraction image, a pattern of lines can appear which overlays the detected images.[1] This pattern with an intensity decrease of up to 20% is caused by diffraction in the sensor layer. Experimental images of a modular PILATUS 1M detector[2] together with a theory are presented over a photon energy range from 3.4 keV to 10 keV. The effect can be exploited to measure the photon energy of the beam and angular misalignment of the detector.

[1] C Gollwitzer & M Krumrey: *A diffraction effect in X-ray area detectors*, submitted to *J. Appl. Cryst.* (2013) `arXiv:1308.6525`

[2] J Wernecke, C Gollwitzer, P Müller & M Krumrey: *Characterization of an in-vacuum PILATUS 1M detector*, submitted to *J. Synchrotron Rad.* (2013) `arXiv:1311.5082`

KR 9.2 Thu 10:30 CHE 184

Beam Conditioning in Cutting Edge X-ray Analytical Equipment — •Jörg Wiesmann, André Beerlink, Andreas Kleine, Jürgen Graf, Frank Hertlein, and Carsten Michaelsen — Incoatec GmbH, Geesthacht

Nowadays, X-ray optical components, such as multilayer mirrors or scatterless apertures, are used as beam conditioning devices in nearly all state-of-the-art X-ray analytical equipment.

Scatterless apertures, such as the scatterfree pinholes SCATEX, are usually made of oriented single crystals, and enable a beam conditioning that is free of parasitic scattering commonly associated with conventional metal apertures. Therefore, such pinholes allow a significant improvement of small angle scattering instruments as the number of necessary pinholes can be reduced while simultaneously enlarging the beam defining pinhole size. This leads to an increased flux on the sample.

Multilayer X-ray mirrors are widely used as monochromators and beam shaping devices in protein and small molecule crystallography. Beam shaping with multilayer mirrors includes the optimization of the flux on the sample and the control over the beam shape and divergence.

In this contribution, we will give an overview of current developments in multilayer optics and scatterless beam components, showing their benefit for typical applications in combination with high-brightness microfocus X-ray sources. We will be presenting selected results for protein crystallography and small angle scattering obtained with the METALJET X-ray source.

KR 9.3 Thu 10:45 CHE 184

Analyzing high pressure diffraction data of perovskites with parametric Rietveld refinement and rotational symmetry modes of a rigid body — •Martin Etter[1], Melanie Müller[1], Michael Hanfland[2], and Robert E. Dinnebier[1] — [1]Max Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]European Synchrotron Radiation Facility (ESRF), Grenoble, France

The high pressure behavior of crystals can best be observed with X-ray or neutron diffraction methods, as these methods allow the application of least square iteration processes (e.g. Rietveld method) to refine parameters, which are directly connected with structural and/or magnetic changes within the crystal. A challenge of the investigation of diffraction patterns under high pressure is that the data quality often decreases after only a few GPa, which makes it difficult for a least square iteration process to find the correct minimum. For this reason, adequate structural models are needed in order to stabilize the refinement and to decrease the number of free parameters. Such models can be provided by the application of rigid bodies, symmetry modes or the recently developed method of rotational symmetry modes of a rigid body which combines the advantages of both. Additionally, these models can be parameterized, treating different data sets simultaneously with the application of physical equations as constraints, which leads to a further reduction of refined parameters. In order to illustrate the power of this new approach, sequential and parametric Rietveld refinements of a LaFeO3 perovskite investigated with synchrotron powder X-ray diffraction under high pressure were carried out.