MS39. Recent advances in diffraction instruments, detectors and data processing

Chairs: Trevor Forsyth, Rosanna Rizzi

MS39-P1 Novel powder diffractometry concepts using Mo and Ag radiation: see more!

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In the vast majority of powder diffractometers, Cu K-Alpha radiation is used. For certain applications, however, the 8 keV photons are not ideal, e.g. for *in operando* studies on electrochemical cells. Also new applications, like Pair Distribution Function analysis, or X-ray imaging applications like Computed Tomography require shorter wavelength radiation. Most standard laboratory diffractometers are not optimized for 'hard' radiation, however, as this more penetrating radiation puts additional demands on the beam path (optical elements and detectors). Therefore, many of these studies are done at synchrotron beamlines.

In this contribution, we'll present the striking results that can be obtained with optimized optics and large monolithic hybrid pixel detectors with unique CdTe sensors for hard radiation, showing that the lab diffractometer can sometimes be a preferred alternative over synchrotron beam time.

Keywords: Instrumentation, detectors, powder diffraction, in operando, PDF

MS39-P2 New possibilities in structural studies using inside x-ray sources

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Traditionally, structure determination of crystalline substances is done by x-ray diffraction experiments. The source in these experiments is well separated from the sample and usually an almost parallel probe beam is used. Further, the sample has to be rotated to many orientations to fulfill Bragg condition and to measure enough reflections for structure determination. This arrangement makes the study of time dependent structural changes, and experiments at non-ambient conditions very difficult, especially in the short time scale. In addition, in these traditional diffraction experiments the phase of the scattered wave is lost, which makes structure solution non trivial. These difficulties could be overcome by using inside x-ray sources within the sample. In the early days of x-ray crystallography Max von Laue worked out the theory of diffraction for sources located in the sample [1]. At the same time this was also experimentally demonstrated by W. Kossel [2]. The pattern obtained this way is called Kossel pattern. Later, it was theoretically shown that not only the position and magnitude of Bragg reflections, but also their phase can be determined by measuring the fine structure of Kossel lines [3,4]. In spite of these advantages Kossel cone analysis is not wide spread. There are some experiments using electron microscopes for excitation of x-ray fluorescence, but almost no work using x-ray excitation. X-ray excitation is advantageous if bulk structural properties have to be determined. Further, in Kossel pattern studies no qualitative phase determination was demonstrated so far. Here we describe a setup built for the measurement of Kossel patterns, excited by synchrotron radiation. We also show that the resolution of this setup is enough for the determination of the phase of Bragg reflections.

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