

MS14-P14 | POWDER DIFFRACTION EXPERIMENTS ON A SINGLE CRYSTAL DIFFRACTION INSTRUMENT - HOW FAR CAN WE PUSH THIS?

Stuerzer, Tobias (Bruker AXS GmbH, Karlsruhe, GER); Adam, Martin (Bruker AXS GmbH, Karlsruhe, GER); Smith, Vernon (Bruker AXS GmbH, Karlsruhe, GER); Ott, Holger (Bruker AXS GmbH, Karlsruhe, GER)

Modern single crystal X-ray diffraction (SC-XRD) allows – often within minutes – the reliable structure determination from one small single crystal. Complementing SC-XRD, powder X-ray diffraction (P-XRD) is typically used on bulk material for qualitative and quantitative phase analysis, texture investigations and structure refinement.

Advances in X-ray diffraction technology are pushing the limits of what information can be extracted from more complicated samples. This development seems to go hand-in-hand with researchers working on tiny, poorly crystalized, samples which often are multiply twinned or intergrown. Many of these compounds are hardly suitable for conventional SC-XRD and only accessible with investing unreasonable amounts of time. For some of these cases P-XRD may help but often not enough sample material is available, a dedicated instrument is not accessible or the researcher is no familiar with the respective hard- and software.

We will present results from a number of experiments where we compare data obtained with typical P-XRD and SC-XRD systems. With a focus on phase identification, quick quantitative analysis and texture investigations we will discuss the impact of wavelength, beam and detector properties, particularly for tiny samples. We will also discuss whether a standard SC-XRD system can outperform a dedicated P-XRD setup. We hope to answer the question: “how far we can we push P-XRD on a SC-XRD instrument?”