Linking Diffraction Techniques with XRF and XAS Spectroscopy at the German CRG Beamline ROBL / ESRF

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The recent upgrade of the Rossendorf Beamline [1] at ESRF allows simultaneous collection of diffraction and spectroscopy (XRF and XANES). A 6-circle Huber diffractometer (XRD1) with Eulerian cradle geometry is used for high-resolution powder diffraction and surface diffraction (Fig. 1, left). The powder diffraction module uses an Eiger CdTe 500k detector, the surface diffraction module is equipped with a Pilatus Si 100k detector. PXRD data suitable for Rietveld refinement can be collected between 10 and 31 keV in an 2θ angular range of 0-65°. The Bragg reflexes in PXRD are extracted by radial integration using a modified pyFAI code [2]. Diffraction measurements can be combined with XRF and XAS spectroscopy using a single-element Si drift detector (Vortex X90 CUBE, 1mm SDD, 25 mm Be window) with a FalconX1 processor.

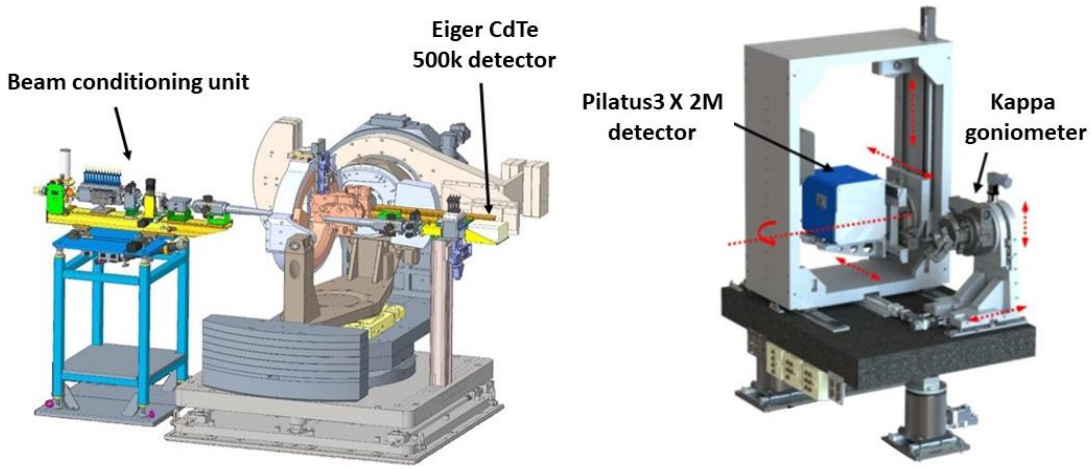

Fig. 1. The two diffractometers at ROBL: XRD1 (left) and XRD2 (right)

The second diffractometer (XRD2, Fig. 1 right) consists of a heavy optical bench with an exchangeable goniometer and a Pilatus3 X 2M detector. It is used for single crystal diffraction and *in situ* or *operando* powder diffraction. Devices for non-ambient sample conditions are a hot-air blower (RT-1100K), a heating chamber (RT-1470K), and a LN2 cryostream (90-400K). This diffractometer is controlled with the Pylatus software [3]. The single crystal data extraction is performed with CrysAlisPro [4]. The Si drift detector can be placed in different positions to combine diffraction with XRF and XAS measurements. We will present some recent results to demonstrate the experimental opportunities.

[1] Scheinost A C et al. ROBL-II at ESRF: a synchrotron toolbox for actinide research. J. Synchrotron Rad., 28, 333-349 (2021)
[2] Kieffer J, Valls V, Blanc N, Hennig C. J. New tools for calibrating diffraction setups. Synchrotron Rad., 27, 558-566, (2020)
[3] Dyadkin V, Pattison P, Dmitriev V, Chernyshov D. A new multipurpose diffractometer PILATUS @ SNBL. J. Synchrotron Rad. 23, 825-829, (2016)
[4] CrysAlisPro Software System, Rigaku Diffraction (http://www.rigaku.com).

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