

INSTRUMENT DATABASE

In-situ powder X-ray diffraction

II LT/HT X-RAY POWDER DIFFRACTOMETER STADIMP

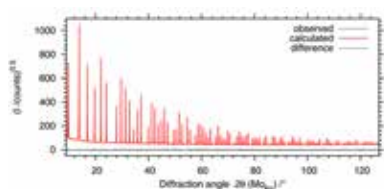


Figure 1: LaB6 Standard Reference Material (SRM), capillary transmission measurement.

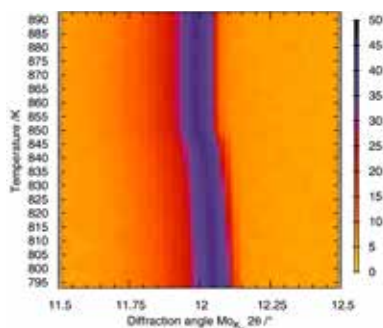


Figure 2: The (011) reflection of alpha-Quartz showing the phase transition to beta-Quartz at 847 K (in-situ HT2 high-temperature oven). Scattering data between 13° and 21° 2θ were collected between 790 K and 890 K in 2 K steps (Data collection time 1.5 h, the square-root intensity is given).

X-ray powder diffraction in combination with the Rietveld method allows for structure determination of crystalline powder samples. The knowledge about the structure of a compound is the most important step to understand its physical and chemical properties. In combination with low- and high-temperature chambers, structure examination between 12 K and 1850 K is possible. This enables a deep understanding of the thermal-expansion behaviour as well as the examination of phase transitions. The high-temperature furnace, which can be used with reaction gases and in combination with the fast detector allows for the in-situ observation of reactions.

The diffractometer enables fast switching between transmission and reflection geometry. The samples can either be prepared in capillaries or as flat samples for transmission measurements in a Debye-Scherrer geometry or as flat samples for the Bragg-Brentano set-up. The short wavelength of the molybdenum radiation enables a screening of the reciprocal space to high Q – values, enabling even the calculation of low-resolution pair distribution functions (PDF) from the obtained scattering data.

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01 II General Information

Keywords: X-ray powder diffraction, temperature-dependent structure characterization

Categories:

- Diffraction
- Structure characterization
- non-ambient X-ray powder diffraction (12 K – 1850 K)
- in-situ reaction studies (300 K – 1850 K)

Main Application: structure determination and refinement from temperature-dependent X-ray data

Measured Quantities: diffraction patterns

Year of Fabrication: 12/2017

Manufacturer: Stoe & Cie GmbH, Darmstadt

02 II Specifications

- Ge(111) monochromized Mo radiation
- Transmission (capillary and flat samples) and reflection geometry
- Dectris Mythen 1k linear detector (18° 2θ width) allowing for energy discrimination to suppress sample fluorescence and fast data collection for e.g. observation of reaction kinetics
- Stoe in situ HT2 heating chamber allows for application of different gases while heating (300 K – 1873 K)
- Oxford Cryosystems PheniX He-closed-cycle cooling chamber (12 K – 310 K)

03 II Contact

Dr. Lars Robben

Faculty 2 – Chemistry/Biology –
Institute for Inorganic Chemistry and
Crystallography

Phone +49 421 218 63142

email: lrobben@uni-bremen.de

Location: NW2/C

Principal Investigator:

Prof. Dr. habil. Thorsten M. Gesing

