Text blocks for the publication of powder X-ray diffraction data

Standard measurements conducted on Bruker D8

Powder X-ray diffraction (PXRD) patterns of the pulverized samples were recorded at room temperature on a D8-A25-Advance diffractometer (Bruker, Karlsruhe, Germany) in Bragg-Brentano θ-θ-geometry (goniometer radius 280 mm) with Cu $K\alpha$-radiation (λ = 154.0596 pm). A 12 µm Ni foil working as K_β filter and a variable divergence slit were mounted at the primary beam side. A LYNXEYE detector with 192 channels was used at the secondary beam side. Experiments were carried out in a 2θ range of 7 to 120° with a step size of 0.013° and a total scan time of 1h.

Standard measurements conducted on PANalytical X'Pert

Powder X-ray diffraction (PXRD) patterns of the pulverized samples were recorded at room temperature on a X'Pert MPD diffractometer (PANalytical, Almelo, Netherlands) in Bragg-Brentano θ-θ-geometry (goniometer radius 280 mm) with Cu $K\alpha$-radiation (λ = 154.0596 pm). A 12 µm Ni foil working as K_β filter and a variable divergence slit were mounted at the primary beam side. A PIXcel^{1D} detector was used at the secondary beam side. Experiments were carried out in a 2θ range of 7 to 120° with a step size of 0.013° and a total scan time of 1h.

If data evaluation was conducted add:

The recorded data was evaluated using the Bruker TOPAS 5.0 software [1], with the observed reflections being treated via single-line fits.

[1] Topas 5, Bruker AXS, Karlsruhe, Germany **2014**.

High temperature measurements conducted on Bruker D8

Powder X-ray diffraction (PXRD) patterns at elevated temperatures were recorded on a D8-A25-Advance diffractometer (Bruker, Karlsruhe, Germany) in Bragg-Brentano θ-θ-geometry (goniometer radius 280 mm) with Cu $K\alpha$-radiation (λ = 154.0596 pm) using a XRK 900 / HTK 1200N (Anton Paar GmbH**,** Graz, Austria) reactor chamber. The samples were investigated in air / vacuum in the temperature range of 30 to 220 °C with heating rates of 10 or 50 K min^{-1}, respectively. A 12 µm Ni foil working as K_β filter and a variable divergence slit were mounted at the primary beam side. The secondary beam side was equipped with a LYNXEYE detector

(192 channels). Diffraction patterns were recorded between 3 and 40° 2θ with a step size of 0.013° and a total scan time of 1h for each temperature. The thermal expansion of the reaction chamber and sample holder was determined using elemental Si (NIST Standard reference material 640f, a = 5.4311(1) nm). The obtained data were refined using the Bruker TOPAS 5.0 software package [1], keeping the lattice parameter of Si fixed while refining the height displacement. This was conducted for different temperatures from which a linear regression was determined. For the subsequent measurements, the z-height was modified by the previously determined values as a function of the temperature used.

If data evaluation was conducted add:

The recorded data was evaluated using the Bruker TOPAS 5.0 software [1], with the observed reflections being treated via single-line fits.

[1] Topas 5, Bruker AXS, Karlsruhe, Germany **2014**.

Acknowledgments (choose the applicable one)

When publishing work done at the Service Center X-ray Diffraction, please include the following acknowledgement:

Instrumentation and technical assistance for this work were provided by the Service Center X-ray Diffraction, with financial support from Saarland University and German Science Foundation (project number INST 256/349-1).

When the measurements were carried out by the members of the Service Center X-ray Diffraction, please include the following acknowledgement:

Instrumentation and technical assistance for this work were provided by the Service Center X-ray Diffraction, with financial support from Saarland University and German Science Foundation (project number INST 256/349-1). The authors thank Dr. Oliver Janka for the support in collection of the X-ray diffraction data presented in this paper.