Deutsche Neutronenstreutagung



Beitrag ID: 26

Typ: Contributed Talk

POWTEX: Angular- and Wavelength-Dispersive High-Intensity Neutron TOF Diffractometer

Dienstag, 17. September 2024 10:50 (20 Minuten)

POWTEX is a TOF neutron powder diffractometer [1] under construction at MLZ. Funded by the Federal Ministry of Education and Research (BMBF, 05K22PA2), it is built by RWTH Aachen University and Forschungszentrum Jülich. Dedicated texture sample environments are contributed from Geo Science Centre at Göttingen University.

Several new concepts have been developed and components built. The two double-elliptic neutron-guides featuring octagonal cross sections with graded super-mirror coating are focusing on the sample, resulting in Gaussian intensity and divergence distributions [2]. Their common focal point at the pulse-chopper serves as "eye of a needle" in time and space, optimizing time-resolution and reducing the source background. The innovative, solid ¹⁰B jalousie volume detector was tailormade for POWTEX [3] and achieves high efficiency for a remarkably large coverage of nine steradians with almost no blind spots. The current status of components, their tests and implementation at MLZ will be shown.

POWTEX aims for short measurement times and in situ chemical experiments, e.g., phase-transitions as a function of *T*, *p*, and *B*₀. For texture-analysis, in situ deformation, annealing, simultaneous stress, etc., the large angular coverage drastically reduces the need for sample tilting/rotation.

As regards theoretical concepts, multidimensional data-reduction algorithms handling angular- and wavelengthdispersive data-sets have been developed and implemented, e.g. in Mantid [6], plotting intensity as function of the newly introduced orthogonal coordinate-system *d*, *d*_{\perp} [4,5] as alternative to λ , 2 θ coordinates. This very procedure, in addition to analytical instrument parametrizations based on fundamental design values, has allowed for multidimensional Rietveld analysis using a modified version of GSAS-II for various TOF diffractometers (POWGEN@ORNL, POWTEX@POWGEN@ORNL, SNAP@ORNL) and various samples (powdered diamond, BaZn(NCN)₂, PbNCN, Fe(dca)₂(py)₂), hence demonstrating the applicability of the method.

[1] Conrad H., Brückel Th., Schäfer W. and Voigt J., J. Appl. Cryst., 2008, 41, 836.

[2] Houben A., Schweika W., Brückel Th. and Dronskowski R., Nucl. Instr. and Meth. A, 2012, 680, 124.

[3] Modzel G., Henske M., Houben A., Klein M., Köhli M., Lennert P., Meven M., Schmidt C. J., Schmidt U. and Schweika W., *Nucl. Instr. Meth. A*, **2014**, *743*, 90.

[4] Jacobs P., Houben A., Schweika W., Tchougréeff A.L. and Dronskowski R., J. Appl. Cryst., 2015, 48, 1627.

[5] Jacobs P., Houben A., Schweika W., Tchougréeff A.L. and Dronskowski R., J. Appl. Cryst., 2017, 50, 866.

[6] PowderReduceP2D, Mantid 6.8, October 2023, dx.doi.org/10.5286/Software/Mantid6.8.

[7] Houben, A.; Jacobs, P.; Meinerzhagen, Y.; Nachtigall, N.; Dronskowski, R., J. Appl. Cryst., **2023**, *56*, 633–642.

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Sitzung Einordnung: Session 4: Instrumentation and Data Management I (Chairs: Tobias Neuwirth & Artur Gregor Glavic)

Track Klassifizierung: Instrumentation & Data Management