



Application of Multidimensional Rietveld Refinement of Neutron Data

Dienstag, 17. September 2024 21:20 (1 h 40m)

We showcase a method development in neutron powder diffraction, primarily driven by the future time-of-flight diffractometer POWTEX, developed in collaboration with Forschungszentrum Jülich at FRM-II in Garching. Within the DAPHNE project, we are expanding these methods for wider applications, emphasizing sustainability.

There is significant interest in actively researching multidimensional data-reduction and Rietveld refinement techniques, applicable not only to POWTEX but also to instruments such as POWGEN and SNAP at SNS, ORNL, USA, and future TOF diffractometers at ESS, Sweden. Recent advancements enable multidimensional data reduction with the Mantid program package. As of today, multidimensional refinement routines are being incorporated into a customized GSAS-II version, currently undergoing testing with real-world samples. The first successful application of the aforementioned methods dealt with POWTEX data collected at SNS, ORNL [1]. Herein, we report the first multidimensional refinement of a two-phase sample using high-pressure diffraction data from SNAP, also at SNS, ORNL. The results are illustrated by a comparison between conventional and multidimensional data refinement and discussed based on the structural peculiarities of PbNCN under pressure [2].

[1] Houben, A., Meinerzhagen, Y., Nachtigall, N., Jacobs, P., Dronskowski, R., POWTEX visits POWGEN, *J. Appl. Cryst.* **2023**, *56*, 633–642.

[2] Meinerzhagen, Y., Eickmeier, K., Müller, P.C., Hempelmann, J., Houben, A., Dronskowski, R., Multidimensional Rietveld Refinement of High-Pressure Neutron-Diffraction Data of PbNCN, *J. Appl. Cryst.*, submitted.

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Sitzung Einordnung: Mounting Posters, Beer and light Dinner

Track Klassifizierung: Condensed Matter