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UC8: Neutron TOF diffraction

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The university group at RWTH Aachen specializes in neutron TOF powder diffraction method development, primarily driven by the new concepts of the neutron time-of-flight diffractometer POWTEX, developed in collaboration with Forschungszentrum Jülich at FRM-II/MLZ in Garching. Unfortunately, no free neutrons were available in 2024. Within the DAPHNE project, we are therefore spreading our methods to other neutron TOF diffractometers while generally aiming to allow a broader, more sustainable applicability of the new developments. This overall goal splits into the following tasks, addressing the different steps in the workflow from raw data to scientific result: 1. multidimensional data reduction using Mantid, 2. derive and include fundamental instrument description in NeXuS data files, 3. multidimensional Rietveld test-cases, 4. AIXtal, a web and cross-platform Rietveld platform for (not only) first-time users, 5. AI tools for structure solution and profile refinement of powder diffraction data.

Utilizing our Mantid routine PowderReduceP2D for high-pressure data collected from SNAP@SNS, ORNL, USA combined with the derived and iterated fundamental instrumental parameters of SNAP allowed us to test-case the multidimensional Rietveld refinement on high-pressure neutron TOF powder diffraction data of a PbNCN sample. While the details were recently published in [1], it is important to note three things: At first, it is very tedious to collect instrumental parameters from various sources while they should actually be part of the data file. At second, a detector coverage of only 1.3 sr (SNAP) vs. ≈ 9 sr (POWTEX) already allows to do multidimensional Rietveld, which is remarkable and underlines the general applicability. While the data reduction steps, with the exception of the one- or multi-dimensional binning, were as similar as possible, the scientific result of the multi-dimensional refinement does differ significantly from the conventional, one-dimensional Rietveld refinement.

Based on these results, we created a sample nexus file containing data fields for the fundamental instrumental parameters. This was presented and discussed at a workshop with the SNS diffraction department which also allowed us to collect the view from the facility perspective. Shaping the future of the Rietveld diffraction software was also recognized as a common interest, especially since the existing software has been mostly around for a long time and the future of the method needs to be clarified.

AIXtal v1 was developed as prototypic, modern web-platform, which allows first-time users to utilize the Rietveld method while partly hiding the complexity of the existing tools GSAS-II and FullProf for the case of conventional X-ray diffraction. The web interface now runs on WebAssembly, which promises performance gains, and moreover now runs not only in the WebBrowser but also natively on Windows, Linux to allow a local installation as well. The higher-performance GUI shall allow to process multidimensional neutron data in the future. While multidimensional Rietveld (GSAS-II 2D) is available as worker already, we only recently started working on GUI and plotting features for this case. The integration of AI methods into AIXtal, e.g. to predict the space group symbol or to support the refinement process, shall ease the structure solution and refinement from powder dat, not only for the unexperienced user.

[1] Y. Meinerzhagen, K. Eickmeier, P.C. Müller, J. Hempelmann, A. Houben, R. Dronskowski, J. Appl. Crystallogr. 2024, 57, 1436–1445, doi:10.1107/s1600576724007635.

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