



Contribution ID: 113

Type: **Contributed talk**

Pydidas: An Integrated Tool for Diffraction Data Analysis

Friday 30 August 2024 12:00 (15 minutes)

Synchrotron X-ray diffraction (XRD) experiments are a versatile tool in understanding material properties and processes, for example alloy development for lightweight materials or additive manufacturing and for generating data to create digital twin models. The analysis of XRD data, however, is often still the domain of experts because software tools were designed for flexibility with full access to numerous parameters which, in turn, made them not very user-friendly for non-experts.

The python ecosystem includes powerful tools for generic data processing (e.g. fitting) and also for integration of area detector data (pyFAI [1], azint [2]) as well as tools for the visualization (e.g. silx [3]) of (integrated) diffraction data. While some tools also offer graphical user interfaces (e.g. pyAI calibration) or full integrations of specific analyses (e.g. dioptas [4]), our user community was missing a tool both versatile and easy to use. Helmholtz-Zentrum Hereon's new software pydidas [5] is designed to broaden the user base for our XRD experiments by delivering a user-friendly and fast processing tool. It is designed to inherently use container data formats (e.g. hdf5) and make use of parallelization. Data browsing and display, experiment calibration, workflow setup, processing and visualization are all available from within pydidas. Emphasis has been placed on an intuitive user interface and accessibility also for non-experts.

To make pydidas useful to a broad community with different analysis requirements, pydidas workflows are based on individual plugins which allows to modify workflows to a high degree. In addition, custom-made plugins can be easily integrated into pydidas to allow also for highly specific workflows which are not covered with its generic functionality.

While pydidas has reached a stable state, we intend to extend the functionality further. For example, a project to include residual stress analysis in pydidas is currently ongoing.

Pydidas is open source software and publicly available.

[1] <https://github.com/silx-kit/pyFAI>

[2] <https://github.com/maxiv-science/azint>

[3] <https://github.com/silx-kit/silx>

[4] <https://github.com/Dioptas/Dioptas>

[5] <http://pydidas.hereon.de>

I plan to submit also conference proceedings

No

Primary author: STORM, Malte (Helmholtz Zentrum Hereon)

Co-authors: Dr KRYWKA, Christina (Helmholtz-Zentrum Hereon); STARON, Peter (Helmholtz-Zentrum Hereon)

Presenter: STORM, Malte (Helmholtz Zentrum Hereon)

Session Classification: Mikrosymposium 3/3: Data, Automation and the Use of AI

Track Classification: 3. Data, Automation and the Use of AI