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The In-Situ GIWAXS Heuristic Tool for Efficient Reduction of High-Quality Big Data

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Large-scale facilities have gained importance for extended characterization methods in the field of material sciences. In particular, structure analysis by highly brilliant X-ray beams is an ideal technique to investigate drying, crystallization, or degradation processes in-situ. These processes require a high time resolution to capture the reaction dynamics, while developments in detector resolution increase the amount of data that must be processed, ideally in real-time. This has raised the necessity to advance data-processing software tools to help the scientist extracting the essential conclusions from big data sets quickly and efficiently.

In this work, we present a self-contained, python-based tool for the analysis of in-situ grazing-incidence wide-angle X-ray scattering (GIWAXS). The focus lies on the performant and loss-free processing of GIWAXS datasets with high system compatibility for the users. In our software, the IN SItu Giwaxs Heuristic Tool (INSIGHT), we included geometrical transformation and corrections similar to GIXSGUI [1] but extended the functionality to arbitrarily positioned and oriented detectors while maintaining full access to the raw data. This allows for post-processing the original data in q-space without any quality loss.
We apply our tool to an exemplary set of in-situ GIWAXS data following the annealing and crystallization process of a thin film of methylammonium lead iodide based perovskite for the application in solar cells.

[1] "GIXSGUI: a MATLAB toolbox for grazing-incidence X-ray scattering data visualization and reduction, and indexing of buried three-dimensional periodic nanostructured films," Z. Jiang, J. Appl. Cryst. 48, pp 917-926 (2015).

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