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Deep learning-based feature detection on 2D X-ray surface scattering data

Grazing-incidence Wide Angle X-ray scattering (GIWAXS) is a key technique for characterizing surface structures of thin films. The method can be used for in-situ experiments monitoring growth and crystallization effects in real-time, but it produces large amounts of data, frequently exceeding the capabilities of traditional data processing methods.
Feature detection in multidimensional X-ray data poses a critical challenge in automated analysis. Especially, in datasets with low signal-to-noise ratio and experimental artifacts in the data, classical peak finding methods may fail.
We demonstrate an automated pipeline for the analysis of GIWAXS images, based on the Faster Region-based Convolutional Network architecture for object detection, modified to conform to the specifics of GIWAXS data. The model exhibits high accuracy in detecting diffraction features on noisy patterns with various experimental artifacts. We demonstrate our method on real-time tracking of organic-inorganic perovskite crystallization.
We will discuss the performance of the ML peak finding approach in comparison to classical peak detection methods on the basis of a manually annotated dataset of 35 GIWAXS images.

V. Starostin et al., npj Comput Mater 8 (2022) 101
V. Starostin et al., Synchrotron Radiation News 35 (2022) 21
A. Hinderhofer et al., J. Appl. Cryst. (2023). 56, 3-11

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