

Closing the loop: Online reflectivity fits using neural networks integrated into beamline environments

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We present a case study of machine learning (ML) integrated into beamline control to drive autonomous x-ray reflectivity (XRR) measurements [1], which can be seen as a prototypical implementation to serve as an example for other in-situ and in-operando synchrotron and neutron experiments. ML strategies have significantly improved in the analysis of reflectometry data in recent years [2], however, there have been limitations in the robust handling of complex scenarios, that might require additional knowledge about the sample for successful XRR fitting. This work addresses these challenges by enabling the use of prior knowledge during the ML fit. During the growth of organic molecular thin films, we established a closed loop between real-time, ML-based online data analysis and the sample environment to tailor the deposition process of organic thin films on a molecular monolayer level.

[1] J. Synchrotron Rad. 30, 1064-1075 (2023), Pithan et al.

[2] J. Appl. Cryst. 56, 3-11 (2023), Hinderhofer et al.

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