Contribution ID: **51** Type: **Poster**

Neural Network based reflectometry analysis of liquid-gas interfaces

Tuesday, 9 April 2024 18:30 (20 minutes)

Researchers from the University of Kiel and Tübingen, as part of the DAPHNE4NFDI initiative, are collaborating to enhance machine learning models for analyzing X-ray and neutron reflectivity datasets, exemplified by the Python package "mlreflect" [1]. This tool, developed at the University of Tübingen, utilizes artificial neural networks trained on solid sample reflectivity data, offering rapid predictions compared to traditional iterative least mean squares fitting methods. Successful experiments at the ESRF using a closed-loop system guided by machine learning data analysis demonstrated the potential of this approach [2].

The University of Kiel's expertise in X-ray reflectivity analysis of liquid samples ([3]) complements the mlreflect package through expanded and improved training data for different layer models in respect to liquid measurements. Recent experiments at ESRF on water-air interfaces validated the ML analysis pipeline at ID10. Based on the Maxwell Cluster a similar analysis pipeline at P08 could be implemented.

One challenge is the lack of sufficient experimental data, requiring reliance on simulated reflectivity data for training. Besides, metadata standardization is vital, with DAPHNE4NFDI developing a specialized schema, while the ORSO works on a file format for reduced reflectivity data. These efforts aim to provide essential metadata for analyses, ensuring consistency and accessibility for training machine learning models. Open reflectivity data examples, such as those shown by Linus Pithan on Zenodo, facilitate testing mlreflect prediction algorithms [4].

In summary, collaborative efforts are enhancing machine learning-driven analysis of X-ray and neutron reflectivity data. Challenges, including limited experimental data for test validation and metadata standardization, are being addressed, promising improved insights with the aid of open data resources and data aggregation platforms.

[1] Neural network analysis of neutron and X-ray reflectivity data: automated analysis using mlreflect, experimental and feature enginierring, A. Greco et al., Jounal of Applied Crystallography, 55, 362 (2022).
[2] Closing the loop: Autonomous experiments enabled by machine-learning-based online data analysis in synchrotron beamline environments, L. Pithan et al., J. Synchrotron Rad., 30(Pt 6), 1064–1075 (2023).
[3] A novel X-ray diffractometer for studies of liquid-liquid interfaces, B.M. Murphy et al., J. Synchrotron Rad., 21, 45 (2014).
[4] Reflectometry curves (XRR and NR) and corresponding fits for machine learning. L. Pithan et al., Zenodo (2022). https://doi.org/10.5281/zenodo.6497438

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Session Classification: Posters

Track Classification: MLC