

Talk for the annual ORSO meeting 2022

Title:

mlreflect – a Python-based pipeline for neutron and X-ray reflectivity data analysis using neural networks

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Abstract:

Neutron and X-ray reflectometry (NR and XRR) are powerful techniques to investigate the structural, morphological and even magnetic properties of solid and liquid thin films. This talk demonstrates the Python package *mlreflect* which implements a pipeline for the fast analysis of reflectometry data using neural networks [1]. The package combines several training and data treatment techniques discussed in previous publications. The predictions made by the neural network are accurate and robust enough to serve as good starting parameters for a subsequent least mean squares (LMS) fit of the data. The results are demonstrated for a large experimental dataset of 242 reflectivity curves from organic thin films on silicon substrates. The pipeline reliably finds an LMS minimum very close to a guided fit by a human expert within a fraction of second.

Furthermore, the differences between simulated and experimental data and their implications for the training and performance of neural networks are discussed. The experimental test set is used to determine the optimal noise level during training. Also, the extremely fast prediction times of the neural network are leveraged to compensate for systematic errors by sampling slight variations of the data.

[1] Greco, A. et al. *J. Appl. Crystallogr.* **55**, 362 (2022)