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Grazing-Incidence X-ray Scattering Data for Machine Learning of Neural Networks

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Relationships between the structure and function are at the heart of material science based on functional films, which makes the knowledge of how film morphology influences its function essential. Key objectives are understanding the formation during synthesis and deposition processes as well as the degradation and the deformation during operation in devices and external stimuli. Achieving a comprehensive and statistically relevant knowledge of the film's characteristics often requires the use of indispensable tools like grazing-incidence X-ray small-angle and wide-angle scattering (GISAXS/GIWAXS). These methods enable the exploration of the film's characteristic morphology in reciprocal space, providing precious insights in a non-destructive way with high time resolution at synchrotrons. However, a challenge arises due to the loss of phase information during measurements, which inhibits a direct transformation from reciprocal space to real space via inverse Fourier transform. In addressing this obstacle, neural networks emerge as promising solutions. The data derived from GISAXS and GIWAXS conducted, e.g., in-situ during formation of functional films, alongside the evaluation utilizing established models, can serve as valuable training sets for the development and refinement of neural networks. For this, two different in-situ data sets obtained from slightly different samples measured at else exactly same conditions regarding the instrumental setup are compared. The first data set is used for training of the neural network and to identify typical features and artefacts in X-ray scattering, as well as distinguishing Poisson noise from the data of interest in complementation to simulated data and results obtained from established models. The trained network is then used to analyze the second data set accordingly and rated with respect to its uncertainty. This strategy holds the potential to enhance our understanding of the structure-function relationships within functional films by enabling the interpretation of reciprocal space data in terms of real-space morphology by neural networks.

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