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Contribution ID: **72** Type: **Talk**

Deep Learning-Driven Grazing Incidence Small-Angle X-ray Scattering Data Processing for Nanostructure Characterization

Nanostructured materials, particularly those formed through nanoparticle deposition or self-assembly on thin film surfaces, are critical to numerous advanced applications due to their exceptional physical and chemical properties. Grazing-incidence small-angle X-ray scattering (GISAXS) has become an indispensable technique for characterizing the morphology of these nanostructures, offering detailed insights into electron density distributions at both the surface and within the film. However, extracting structural information from GISAXS data remains challenging, largely due to the phase problem. Conventional methods typically involve fits to the experimental data using predetermined, simplified models. The process is both time-consuming and constrained by the limited variety of the available models, often resulting in oversimplified descriptions parameterized by a single size and a polydispersity parameter. Moreover, convergence difficulties become more challenging for GISAXS data fits when using traditional regression algorithms compared with SAXS data. To address these limitations, we use the distorted wave Born approximation (DWBA) method and simulate a diverse range of 2D scattering patterns to generate comprehensive, high-quality training datasets for analyzing the morphology of a self-assembled gold nanoparticle. These datasets underpin our application of deep learning techniques, specifically convolutional neural networks (CNNs), which effectively predict size distributions from the simulated and experimental GISAXS data. Our findings offer a promising and time-efficient alternative to conventional GISAXS data analysis methods.

Authors: Prof. ROTH, Stephan (DESY); ZHAI, Yufeng (DESY)

Co-authors: Prof. HEXEMER, Alexander (Lawrence Berkeley National Laboratory); Prof. STIERLE, Andreas (DSEY); Dr JEROMIN, Arno (DESY); Dr SOCHOR, Benedikt (DESY); Dr HEGER, Julian (TUM); Dr ZHOU, Jungui (DESY); Prof. MÜLLER-BUSCHBAUM, Peter (TUM); Dr VAYALIL, Sarathlal (DESY); DAN, Shachar (DESY); Prof. KELLER, Thomas (DESY); Ms WANG, Wenbo (University of Hamburg); Dr PARAK, Wolfgang (University of Hamburg)

Presenter: ZHAI, Yufeng (DESY)

Session Classification: Parallel: Materials (RT2)

Track Classification: RT2