Contribution ID: **22** Type: **Talk**

Tracking morphological changes during sputter deposition using GISAXS and machine learning

Monday, 8 April 2024 10:10 (20 minutes)

Solving inverse problems is the basis of the analysis of scattering experiments. The difficulty stems from the fact that the real-space structure has to be retrieved from reciprocal space information. With respect to thin films and interfaces, grazing incidence small- angle X-ray scattering (GISAXS) is a powerful tool for accessing their nanoscale structure formation. GISAXS allows for experiment in real time with high time resolution and high statistical relevance[1]. The two-dimensional scattering pattern is governed by the distorted-wave Born approximation (DWBA) - refraction and reflection effects have to be considered, adding further to complexity in data analysis. Hence, a model-based approach using simulations for the GISAXS pattern is necessary for elucidating the nanostructure[2,3].

Sputter deposition is an industrially-relevant method for fabricating metal-polymer nanocomposites[3]. The time resolution down to the sub-millisecond scale combined with in situ sputter deposition yields a large amount of data that requires careful analysis[4]. One way to extract quantitative information is to use a data base of model simulations of the sample. While fundamental assumptions about the system must be made in order to establish the simulations[5], the choice of appropriate inputs leads to a good approximation of the GISAXS data. A key issue is finding the simulation that best represents the system at each stage of the experiment.

Neural networks (NNs) are used to predict the behavior of a system through mathematical modeling. In our case, we use as preprocessing a background and intensity thresholding following Parente et al. [6] with the thresholding factor β being the only variable in the preprocessing stage. Additionally, we tested different network architectures using non-linear activations functions ReLU (R) and Leaky ReLU (L) in different compositions. We present the results of a multilayer perceptron and a convolutional NN (CNN) concerning the structure and morphology of the cluster growth of gold in silicon during sputter deposition. Especially the prediction of the percolation threshold is discussed.

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Session Classification: Session 1

Track Classification: MLC