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Strategy to Simulate and Fit 2D GISAXS Patterns of Nanostructured Thin Films

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Grazing-incidence small-angle X-ray scattering (GISAXS) is a widely used method for the characterization of the nanostructure of supported thin films and enables time-resolved in situ measurements. The two-dimensional (2D) scattering patterns contain detailed information about the nanostructure within the film and at its surface. Efficient and fast model fitting is often hampered because it is time-consuming to analyze the 2D patterns. Moreover, the structural information is not only distorted by the reflection of the X-ray beam at the substrate-film interface and its refraction at the film surface, but also by scattering of the substrate, the sample holder and other types of parasitic background scattering. In this work, a new, efficient strategy to simulate and fit 2D GISAXS patterns, that explicitly includes these effects, is presented and demonstrated at the example of (i) a model case nanostructured thin film on a substrate and (ii) experimental data from a microphase-separated block copolymer thin film [1]. To make the protocol efficient, characteristic line cuts through the 2D GISAXS patterns, where the different contributions dominate, are analyzed. The contributions of the substrate and the parasitic background scattering—which ideally are measured separately—are determined first and are used in the analysis of the 2D GISAXS patterns of the nanostructured, supported film. The nanostructures at the film surface and within the film are added step by step to the real-space model of the simulation, and their structural parameters are determined by minimizing the difference between simulated and experimental scattering patterns in the selected line cuts. While, in the present work, the strategy is adapted for and tested with BornAgain, it can be easily used with other types of simulation software. The strategy is also applicable to grazing-incidence small-angle neutron scattering.

1. F. Jung, C. M. Papadakis, *J. Applied Crystallogr.* **2023**, *56*, 1330.

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