Artificial Intelligence Co-Refinement of X-Ray Reflectivity Data Enables Faster and Lower Dose Measurements

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We present an approach for analysis of real-time X-ray reflectivity (XRR) process data not just as a function of the reciprocal space vector q as is commonly done, but as a function of both q and time. We restrict the real-space structures extracted from the XRR curves to be solutions of a physics-informed growth model, and use state-of-the-art convolutional neural networks (CNNs) and differential evolution fitting to co-refine multiple time-dependent XRR curves R(q,t) of a thin film growth experiment. Thereby it becomes possible to correctly analyze XRR data with a fidelity corresponding to standard fits of individual XRR curves even if they are sparsely sampled with a 7-fold reduction of XRR datapoints, or if the data is noisy due to a 200-fold reduction in counting times. Our approach of using a CNN analysis and of including prior information through a kinetic model is not limited to growth studies, but can be easily extended to other kinetic X-ray or neutron reflectivity data to enable faster measurements with lower beam damage.