

AI-Driven Advances in X-Ray Analytics

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We explore how AI is transforming X-ray analytics, enabling rapid in operando studies. This talk highlights examples of sub-millisecond-scale X-ray reflectivity (XRR) measurements during thin-film deposition, demonstrating how AI accelerates data analysis. By handling tens of thousands of datasets, we determine roughening exponents during film growth at high rates. Beyond fast scanning XRR with advanced setups, AI-driven deep reinforcement learning further speeds up XRR measurements by up to four times through adaptive scans, where the scan points are selected on the fly.

Extending beyond reflectometry, we present recent advancements in using AI for Grazing Incidence X-Ray Diffraction (GIXD) analysis. GIXD is crucial for determining thin-film structures, yet its data analysis is often complex and time-consuming. By leveraging AI, we achieve high-precision determinations of crystal unit cell parameters and the contact plane of adsorbate layers, while simplifying the experimental setup by eliminating the need for specular scans. Overall, AI tools significantly enhance the speed and reliability of X-ray analytics, paving the way for autonomous labs in crystallographic research and AI-driven materials discovery.