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# AI Analysis of Grazing Incidence X-Ray Diffraction

*Tuesday, 16 July 2024 12:00 (20 minutes)*

In this study, we introduce cutting-edge neural network algorithms that precisely predict crystal unit cell parameters and contact planes from Grazing Incidence X-Ray Diffraction (GIXD) data. Our method processes a list of $q$-positions and delivers predictions of the unit cell with exceptional accuracy—better than 0.1 Angstrom in dimensional precision and sub-degree in angular measurements. It eliminates the necessity to measure the 'missing wedge' in a specular scan, simplifying the experimental setup. Our AI method facilitates the rapid, autonomous processing of complex GIXD patterns without user intervention. It enables a detailed evaluation of the analysis's sensitivity to missing or spurious peaks due to its ability to predict structures for a large number of GIXD patterns quickly. Indeed the analysis copes well with patterns that miss peaks or contain only few peaks in total. These advancements present a substantial improvement in efficiency and reliability for researchers utilizing intricate GIXD patterns in crystallographic surface science studies.

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Instrumentation and methods

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