**Reliability of thickness determination by position-averaged convergent beam electron diffraction**

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For quantitative analysis of atomic-resolution scanning transmission electron microscopy (STEM) imaging modes, it is often beneficial to have an independent measure of specimen thickness. Unfortunately, most thickness measurement techniques involve substantial changes in the specimen orientation and optical conditions from those under which atomic-resolution STEM images are recorded, making it difficult to connect their results to the thickness at the specific region of interest. However, averaging the diffraction pattern while the STEM probe is scanned - called position-averaged convergent beam electron diffraction (PACBED) - gives a pattern whose appearance is robust to noise and lens aberrations but still sensitive to sample structure and thickness [1]. Comparison between experimental and simulated PACBED patterns can be used to estimate such specimen properties as thickness [2], polarity [3] and composition [4].

This talk examines the influence of practical realities such as shot noise, specimen mistilt, surface roughness and inelastic scattering on the reliability of thickness determination by PACBED [5]. Our exploration combines experimental examples with systematic simulations. Automating thickness determination using as a metric the sum square difference between experimental and simulated patterns removes the subjective element of "by eye" comparisons. We present simple prescriptions for both determining thickness and estimating a precision or uncertainty bound on that determination (see Fig. 1). Using this metric, we find that most limitations of practice reduce the precision of thickness determination but do not much affect its accuracy, strengthening the case for PACBED as a robust technique. We round out the presentation with some recommendations for practical application, including that smaller probe-forming apertures generally give better precision than larger probe-forming apertures.

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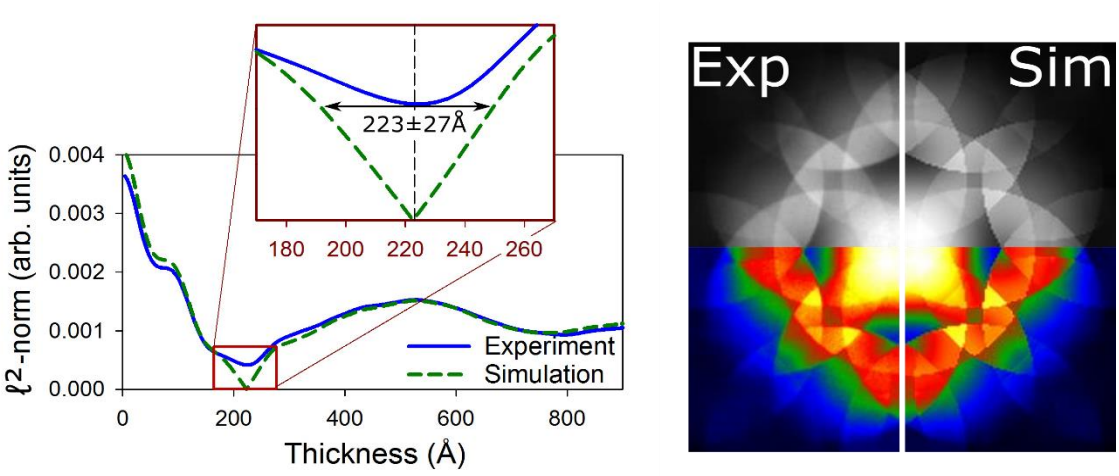


Fig. 1: Left - Root-sum-square-error ($\ell^2$-norm) plot comparing simulated PACBED patterns from different thicknesses against an experimental PACBED pattern ("Experiment") and the simulated pattern for thickness 223 Å ("Simulation"). The region around the global minimum is magnified in the inset, which also shows how an uncertainty/precision is defined. Right - comparison between the experimental PACBED pattern and the simulated pattern for thickness 223 Å, on both grey (upper half) and colour (lower half) scales.