Poster

# Exploring the influence of imperfections on 3D electron diffraction intensities through multislice simulations

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In recent times, there have been notable advancements in refining crystal structure models using electron diffraction data [1, 2], thanks to improved experimental setups and modelling techniques. However, compared to typical R-factors observed in X-ray diffraction experiments, there remains a significant gap. This suggests that there are parameters overlooked in the model that have a notable impact on the diffracted intensities. To delve into this, we use the multislice approach [3] implemented in *ab*TEM [4] – a Python-based code capable of accurately simulating electron scattering. By comparing the intensities of reflections from perfect and imperfect models, we aim to gauge the influence of crystal defects on diffracted intensities.

In our method, we generate a supercell of suitable dimensions and specify the desired tilt angle, creating a large, non-periodic model for simulation. We then calculate diffraction patterns for a finite cropped area. Our study demonstrates that diffraction from arbitrary crystal orientations can indeed be simulated using the multislice approach with a sufficiently large, periodic crystal model. We also analyse how diffracted intensities converge with varying supercell sizes.

To validate our results, we compare diffraction patterns from defect-free structure models obtained with *ab*TEM with those from Bloch-wave calculations [5] as implemented in Dyngo/Jana2020 [6, 7] and py4DSTEM [8]. The close agreement between the two methods ensures that any changes in intensities are attributed to introduced imperfections rather than calculation methodology.

We explore various imperfections, starting with introducing point defects (vacancies) in the silicon structure, which serves as a straightforward control. We also delve into the influence of atom size on the calculated intensities, choosing an array of isostructural crystals with varying composition.

Our work demonstrates the feasibility of understanding deviations between modelled and experimental intensities in 3D electron diffraction experiments stemming from different types of crystal imperfections. Our goal is to develop more accurate methods for describing the effects of imperfections on electron diffraction data to enable precise fits and refinements even with imperfect samples.

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