Understanding the effect of imperfections on 3D electron diffraction intensities using multislice simulations

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Recently, the refinement of crystal structure models against electron diffraction data has improved significantly due to advances in experimental setups and modelling [1, 2], but in comparison to typical residual factors from X-ray diffraction experiments there is still a significant R-factor gap. This indicates that parameters neglected in the model influence significantly the diffracted intensities. We investigate the effect of crystal imperfections on the diffracted intensities using the multislice approach [3] implemented in abTEM [4] – a Python-based code capable of efficient and accurate simulation of electron scattering. We compare the calculated intensities of reflections obtained from perfect and imperfect models to estimate the influence of crystal defects on diffracted intensities.

In our novel approach, we generate a supercell of an appropriate size and then specify the desired tilt angle, creating a large non-periodic model that is simulated and diffraction pattern calculated for a finite cropped area. We demonstrate that diffraction from arbitrary crystal orientations can indeed be simulated within the multislice approach with a sufficiently large repeated crystal model, and we show how the diffracted intensities converge as a function of the supercell size.

To ensure that the calculated intensities are not affected by the choice of simulation parameters, we first compared diffraction patterns from defect-free structure models obtained with abTEM with those from Bloch-wave calculations [5] as implemented in Dyngo/Jana2020 [6, 7]. The high level of agreement between the two methods ensured that any changes in intensities of investigated diffraction patterns would be due to introduced imperfections and not because of the method of how intensities are calculated.

The first investigated imperfection was an introduction of point defects (vacancies) in the structure of silicon. This type of defect is straightforward to control and was used to further verify our approach. We also investigated the influence of strains in crystal structures, as well as the effect of phonons.

Our work shows that it is possible to investigate and understand deviations between modelled and experimental intensities from 3D electron diffraction experiments, originating from various types of imperfections in crystals. In future work we want to develop better and more accurate methods of describing the effects of imperfections on electron diffraction data which will allow good fits and accurate refinements even on data from imperfect samples.


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