Three-beam electron diffraction for measuring crystallographic phases

Guo, Y.[1], Nakashima, P.[1] and Etheridge, J.[1,2]

[1] Department of Materials Science and Engineering, Monash University, Australia, [2] Monash Centre for Electron Microscopy, Monash University, Australia

Due to the strong Coulomb interaction with matter, electrons are scattered multiple times when they travel through a TEM specimen. As a consequence of multiple scattering, electron diffraction patterns contain information about the phases of structure factors. However, it remains challenging to extract this information without any a priori structural knowledge and no generic approach to the direct, analytical inversion of multiple scattering exists. (Phase information is normally "lost" in X-ray diffraction patterns due to their weak interaction and resultant single-scattering.)

In this work, we derive an analytical expression for the intensity distribution in convergent beam electron diffraction (CBED) patterns which are recorded in a three-beam condition where two reflections satisfy their Bragg conditions simultaneously. Our analytical theory provides a method for measuring three-phase invariants to within 45° simply by inspection of features in the indexed CBED patterns, without any additional information about the structure itself. We demonstrate the experimental implementation of this method with two simple test cases: centrosymmetric Si and non-centrosymmetric GaAs. Our three-beam method may complement existing structure determination methods, by providing direct measurements of three-phase invariants to replace 'guessed' invariants in *ab initio* phasing methods and so provide more stringent constraints to the structure solution.

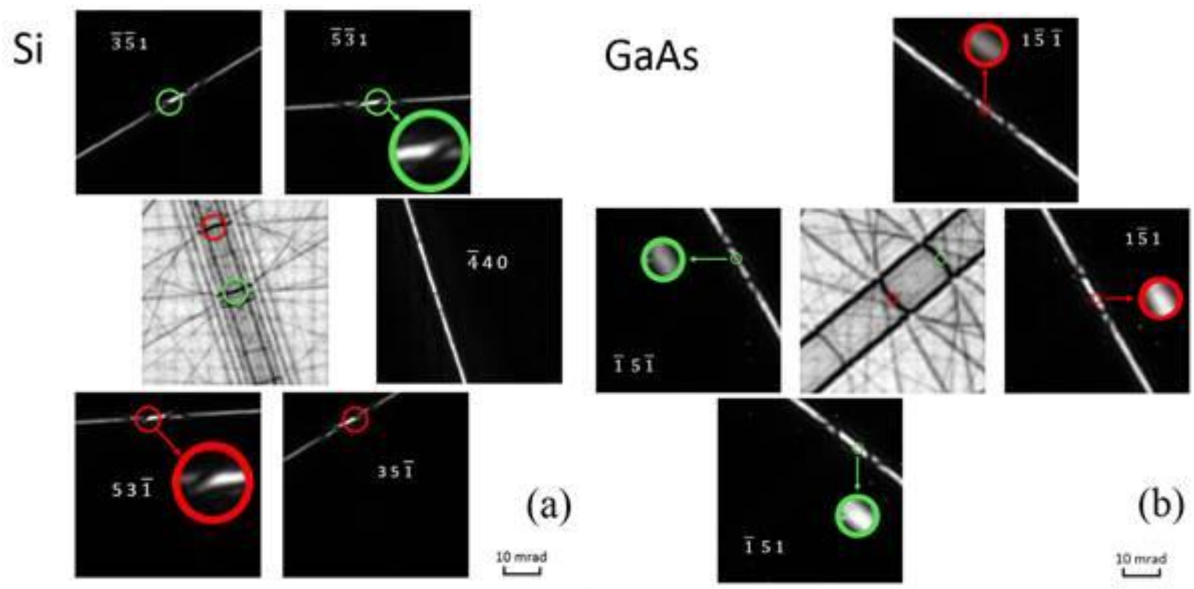

Figure 1 Reconstructed Large Angle Rocking CBED patterns of a few selected reflections for (a) Si [1 1 8] and (b) GaAs [5 1 0] at 200kV. The three-beam conditions in the Friedel pair reflections are

labelled with circles of different colours. The three-phase invariants contained in (a) $\varphi_{\bar{5},\ \bar{3},\ 1}+\varphi_{2,\ \bar{2},\ 0}-\varphi_{\bar{3},\ \bar{5},\ 1}$ and (b) $\varphi_{1,\ \bar{5},\ 1}+\varphi_{0,\ 0,\ \bar{2}}-\varphi_{1,\ \bar{5},\ \bar{1}}$ can be determined to be $0°$ and $+90°$, respectively, by observations of the features in these patterns according to the rules derived from three-beam electron diffraction theory.

Acknowledgements

The authors thank the Monash Centre for Electron Microscopy for facilities and staff support. This work was supported by the Australian Research Council grant number DP150104483. P.N.H.N. was funded by the Australian Research Council (FT110100427).