Looking for the Potential in Digital Large Angle Electron Diffraction Patterns

Beanland, R.[1], Hubert, A.[1] and Roemer, R.[1]

[1] Department of Physics, University of Warwick, United Kingdom

Richard Beanland, Alex Hubert and Rudo Roemer

Department of Physics, University of Warwick, CV4 7AL, UK

The sensitivity of convergent beam electron diffraction (CBED) to a crystal's structure and electron density has been known for some time. The technique has the advantage of sampling material limited only by the size of the electron beam and the thickness of the specimen, i.e. a volume that can easily be a few thousand cubic nanometres. However, the small electron wavelength of high energy electrons leads to very small Bragg angles, which severely restricts the convergence angle that can be used. The problem becomes worse for materials with larger lattice parameters, often with the result that insufficient information is obtained from CBED to do anything useful.

Computer control of transmission electron microscopes and digital image capture allows hundreds, or thousands, of CBED patterns to be collected automatically. The patterns can then be combined to construct a single 'digital' large-angle convergent beam electron diffraction (D-LACBED) pattern that has no restrictions due to Bragg angle. These patterns have a wealth of detail (see e.g. Fig. 1) and, for example, symmetry determination becomes straightforward. Examples are given from materials that would be difficult or impossible using conventional CBED.

Careful experimentation and energy filtered imaging is needed for conventional CBED work, and elastically-scattered intensities must be measured with accuracies better than 1%. Analysis of CBED patterns can yield information about crystal potentials - even the redistribution of electrons between atoms (i.e. bonding effects) - but there has been less work on LACBED patterns. For D-LACBED patterns, it is now clear that the data contains regions that are very sensitive to particular parameters and have large, easily measured changes in intensity with no need for energy filtering. Thus, highly accurate measurement of crystal structure and bonding may be readily achievable using any modern TEM on a routine basis. We also find that for some materials, such as $BaTiO_3$, simulated patterns differ wildly from the experimental data, indicating a high sensitivity to local symmetries that differ from the macroscopic average structure.

Fig. 1. Montage of D-LACBED patterns from the [001] axis of tetragonal $BaTiO_3$.