The Phonon Contribution to Diffraction Patterns

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It is generally accepted that in high resolution electron microscopy (HREM), elastic image simulations have a higher lattice fringe contrast than experimental lattice images by a factor of 2-3 (the Stobbs factor) [1]. Some of the discrepancy is due to phonon scattering, which cannot be removed by present TEM energy filters and is manifest in diffraction patterns as a diffuse background between Bragg spots, most significant at higher angles. Our aim here is to compare quantitatively the phonon contribution to experimental diffraction patterns with diffraction patterns simulated using the frozen phonon model over a range of scattering angles [2].

Energy filtered convergent-beam diffraction (CBED) patterns from varying thicknesses of a clean Si sample were obtained with a condenser aperture of radius 1.11 mrad (FIG. 1a) and the phonon scattering intensity was measured between the Bragg discs as described by Boothroyd & Yeadon [3]. Diffraction patterns (FIG. 1b) were simulated using the frozen phonon multislice program TEMSIM [4]. Section averages of the phonon background and Bragg disc intensities against scattering angle are shown in FIG. 2 & 3.

The CBED disc intensities for the simulated patterns are in reasonable agreement with experimental results (FIG. 2) given that no absorption was included to account for the loss of intensity caused by plasmon and higher losses in the frozen phonon simulations. In the case of the diffuse background (FIG. 3), where the phonon contribution is observed to increase with thickness, the intensity is much higher for the measured patterns up to ~7 mrad, due to the point spread function contribution of the 000 discs. The presence of Kikuchi lines and peaks in phonon scattering at Bragg discs produces undulations in the diffuse background. Beyond 7.5 mrad, the phonon intensities for the patterns are comparable, though the measurements at present extend only to 16 mrad.

For simulating the phonon contribution to high angle annular dark-field images (HAADF) near the first order Laue zone the Einstein approximation used here should be adequate. Our intention is to match experimental phonon intensities near the first order Laue zone to Einstein approximation simulations including inelastic absorption. We can then use these to model the phonon contribution to HREM images. However, this approximation may underestimate the phonon contribution to HREM images as it does not model the increased phonon scattering around the Bragg peaks. Further work will be to determine whether the Debye phonon model is necessary for accurate simulation of the phonon contribution to HREM images.

[1] C. B. Boothroyd, *J. Microsc.* **190** (1998) 99
[2] Z. L. Wang, *Micron*, **34** (2003) 141
[3] C.B. Boothroyd, and M. Yeadon, *Ultramicroscopy*, **96** (2003) 361
[4] E. J. Kirkland, *Advanced Computing in Electron Microscopy*, Plenum Press, 1998

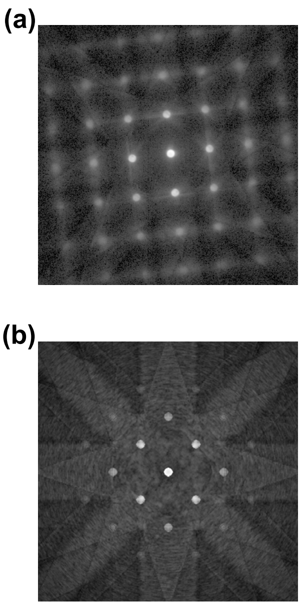

FIG. 1. CBED Patterns for Si 100 shown on a logarithmic scale, thickness 200 nm for (a) experimental and (b) simulated conditions.

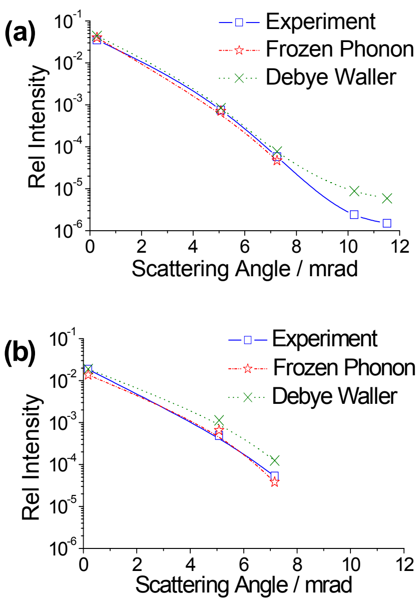

FIG. 2. Bragg disc intensities for Si 100, for experiment, frozen phonon simulations and Debye Waller simulations for thickness (a) 50 nm and (b) 200 nm.

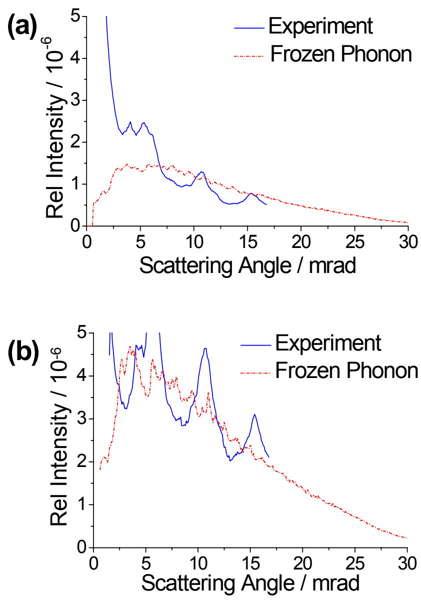

FIG. 3. TDS Background for Si 100 under experimental and frozen phonon simulated conditions for thickness (a) 50 nm and (b) 200 nm.