Plenary Lecture

Calculating the intensity in electron diffraction patterns

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Quantitative calculations of electron microscope images and diffraction patterns are particularly important for high-resolution imaging and currently do not agree well with experimental results[1]. Calculating the intensity of diffraction patterns quantitatively is difficult! If the atoms in the crystal were perfectly ordered and stationary then the diffraction pattern would consist of regular spots with no intensity in-between the spots. But even for perfect crystals the atoms are vibrating and the amount of vibration increases with temperature. This vibration means the atoms are not perfectly ordered and causes weak diffuse scattering between the spots in the diffraction pattern (phonon scattering). In addition, some electrons interact with the crystal as they pass through and lose energy. The diffraction pattern is thus made up of electrons of many different energies. Calculating how all these effects add up to give the intensities in a diffraction pattern is very complex. Here we investigate how accurately the diffuse scattering can be calculated using the "frozen phonon" method[2].

We can simplify the calculation by recording the diffraction pattern through an energy filter. This will filter out all the electrons that have lost energy, meaning that only the elastic (ie no energy loss) scattering has to be calculated. But energy filtering diffraction patterns is itself difficult because the entrance aperture of the energy filter is only 3mm in diameter. This, combined with aberrations in the microscope lenses, limits the maximum scattering angle at the edge of a diffraction pattern to about 140mrad (4°). An example of an experimental energy-filtered diffraction pattern from 001 Si is shown in fig. 1.

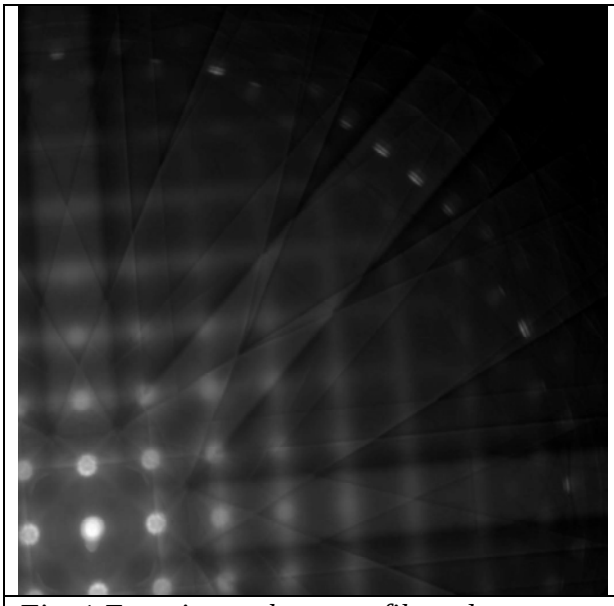

Fig. 1 Experimental energy-filtered diffraction pattern from 210nm thick 001 Si taken on a JEOL 200kV microscope.

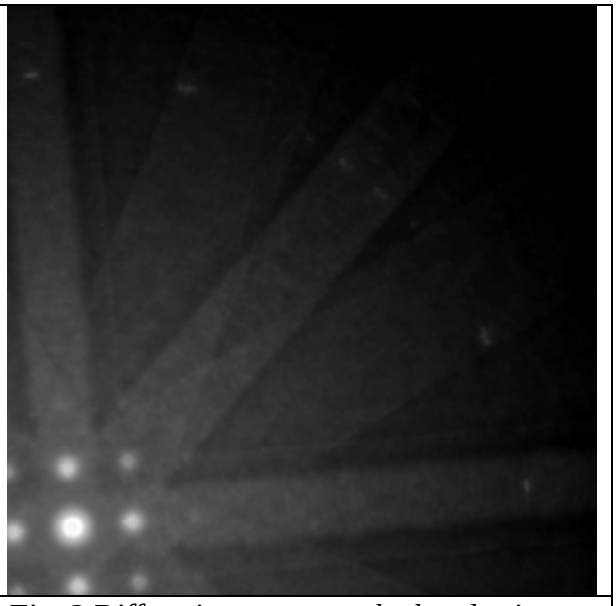

Fig. 2 Diffraction pattern calculated using the frozen phonon method for the same conditions as fig. 1 and a root mean square vibration amplitude of 0.0078nm.

The frozen phonon method for calculating the effects of vibrating atoms on electron scattering makes use of the assumption that the period of the atomic vibrations is much smaller than the time taken for electrons to pass through the crystal. Thus for each electron wave the atoms can be assumed to be "frozen" in a particular state. The final diffraction pattern is built up by adding together many diffraction patterns calculated with different random displacements of the atoms. The mean displacement of the atoms depends on the temperature of the sample. A calculated diffraction pattern for the same material as fig. 1 is shown in fig. 2[3].

In assessing the accuracy of the calculation, we compared both the intensities of the diffraction spots and the intensity of the diffuse background as a function of scattering angle. We found that the diffraction spot intensities were predicted very well for both thin samples (65nm) and thicker samples (210nm). The diffuse background intensity for very small scattering angles around the 000 beam in the experimental diffraction pattern is dominated by scattering from the very strong 000 beam (due to the point-spread function of the detector) and is thus difficult to compare. However, for larger scattering angles the calculated diffuse background agreed well with that for the experimental pattern. We thus conclude that the frozen phonon method provides a good quantitative way of calculating diffuse scattering, which can thus be applied to quantitative image simulations.

References

1. CB Boothroyd, Why don't high resolution images and simulations match? *J Microscopy*1998, 190: 99-108.
2. EJ kirkland, Advanced Computing in Electron Microscopy. *Plenum Press, 1998.*
3. A Soumyanarayanan and CB Boothroyd, The phonon contribution to diffraction patterns, *oceedings of the sixteenth international microscopy congress, volume 2, ed Hideki Ichinose and Takahisa Sasaki (Publication committee of IMC16, 2006) p 992*.