Obstacles and optimisation in weak-beam dark-field tomography of defects

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Abstract. Weak-beam dark field tomography of dislocations has so far been done in a heuristic way with little theoretical analysis of how to optimise the technique. In this paper a more quantitative analysis of the limits of WBDF tomography is summarised. It can be shown that the object reconstructed from WBDF images by a conventional tomography algorithm is the locus of dislocation images laid down as central slices at the appropriate tilt angles, as would be intuitively expected. By comparison with projections of the displacement field, a reconstruction from dark-field images gives a better indication of the dislocation’s path than a projection of the displacement field itself. Reconstruction is performed on a simulated tilt series of stacking fault images; the resulting structure follows the correct plane but is a 3D array of rods, not a flat plane. This is produced by the ‘movement’ of dynamical fringes in the stacking fault images as the sample is tilted and is an example of WBDF images being suboptimal for tomography. Finally, the influence of misalignment between the tilt axis and systematic row is modelled, and is shown to degrade the reconstruction, especially in the out-of-plane direction. This misalignment changes the excitation error with tilt, which introduces another variable to the reconstruction process and breaks the requirement that the images be a straight-ray projection of a monotonic function of the required parameter.

1. Introduction
Tomography is the reconstruction of a 3–dimensional object or structure from a tilt series of 2–D projections. In electron microscopy, tomography has mainly been used for reconstructing the shapes of samples such as particles or nanotubes, using mass-thickness contrast, for example [1]. Diffraction contrast, such as that in dark-field images of defects, has been considered too complex for use in tomography. Using weak-beam dark field (WBDF) defect images for tomography was first attempted in 2005 and was surprisingly successful [2]. To do this, the tilt axis of the tilt-rotate holder is set up parallel to the systematic row that will be used for the weak-beam condition, and the beam tilted along the systematic row to achieve the weak-beam condition. The sample is then tilted around the eucentric axis by up to 70° in each direction and a tilt series of images are recorded; ideally the weak-beam condition is kept constant during tilt. This experiment was originally done to test the feasibility of the concept; the next stage, in progress, is to consider the theoretical basis of this technique and determine its limits.

This paper summarises the results of some simulated experiments to investigate the effects of small and large changes in sample orientation while setting up tomography. On the large scale, for reconstructing stacking faults, the movement of dynamical fringes as the sample is tilted...
has an important impact on the reconstruction; an orientation must be found to minimise this movement. On the small scale, the effect of a small misorientation between the tilt axis and the $g$ used for imaging is investigated; as expected, misalignment is found to impair reconstruction quality, especially perpendicular to the film.

2. Tomography theory

When image intensity can be represented as an integral of the property of interest along straight lines through the sample [3], the Fourier slice theorem relates the object $f(x,y)$ to this parallel projection through the sample $P_\theta(t)$ along ray $t$ according to Equation 1. The Fourier transform of the object’s projection at angle $\theta$ to the $x$ axis, gives a central slice of the Fourier transform of the object taken at an angle $\theta$ to the $x$-frequency axis [4]. In this case, the object can be reconstructed by backprojection tomography. The process of backprojection is that of extending the values in the Fourier-transformed projection over the stripe of Fourier space that corresponds to the projection’s tilt angle [3]. When all the projections are backprojected across the same space, a flawed version of the object is reproduced.

$$\int_{-\infty}^{\infty} P_\theta(t) \exp[-2\pi iw t] dt = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x,y) \exp[-2\pi iw(x \cos \theta + y \sin \theta)] dx dy$$  \hspace{1cm} (1)

A WBDF dislocation image is not, however, a straightforward projection; in the kinematical approximation, the integral is not over the displacement field $\mathbf{R}$ itself, but over $\exp(-2\pi i g \cdot \mathbf{R}) \exp(-2\pi i s z)$, which is then squared in calculating intensity. By substituting the dark-field image intensity instead of the simple straight-ray projection in the Fourier slice theorem, it becomes a statement that the Fourier transform of an object taken at a tilt angle $\theta$ is equivalent to the Fourier transform of the intensity of the dark field image set at a tilt of $\theta$. We will not get a reconstruction of $|\mathbf{R}|$ from a tilt series of WBDF images; reconstruction will yield this image intensity ‘object’.

Figure 1 compares a projection of the magnitude of the dislocation displacement field, and a dark-field image calculated using R. Schäublin’s CUFOUR program [5]. The parallel-sided Al crystal is oriented with [111] beam direction pointing directly down; the screw dislocation intersects the top of the 100 nm thick foil on the left and runs down with line direction [110] and Burgers vector $\mathbf{b} = \frac{1}{4}[110]$. The image is calculated using the systematic row $n(20\overline{2})$ in $g(3.5g)$ weak-beam condition, with image taken from $g = 20\overline{2}$. The dark-field image shows the familiar narrow line, dotted with oscillations from Bloch wave interference. The projection of the displacement field gives an image that becomes more diffuse as the dislocation approaches the bottom surface, becoming a low intensity region around a high-intensity core.
3. Stacking faults

When WBDF tomography is attempted on defects containing stacking faults, the reconstruction quality is found to depend on the choice of tilt axis/imaging reflection. This may be due to the difficulty of tilt series alignment with fringes present, or a basic property of stacking fault contrast. Two tilt series of g(3g) weak-beam images were simulated using CUFOUR, changing the beam direction to achieve tilt. This simulated tilt series starts with perfect alignment, because the defect is placed at the same point relative to the centre of the image every time. The defect modelled was in Al, on a stacking fault with displacement \( \frac{1}{3}(111) \) bounded by partial dislocations running along [011] from top to bottom of the 100 nm thick crystal, with Burgers vectors \( \frac{1}{6}[211] \) and \( \frac{1}{6}[121] \) according to the Thompson tetrahedron convention [6]. A partial dislocation separation of 50 nm was used, which is larger than would be found in nature but allowed the fringes to be more easily observed. Images were simulated from 45° to −45° for \( g = 200 \) and reconstruction done using conventional SIRT, 30 iterations, using FEI’s Inspect3D™. Adaptations were made so that the image became appropriately longer and shorter as the sample was ‘tilted’, as for an experimental tomography series.

The tilt axis was along the projected width of the stacking fault, so the depth range of the stacking fault changed and the fringes changed position along the length as the tilt angle changed — they appeared to ‘move’ along the stacking fault through the tilt series. The simple projection object that would give this behaviour is an array of rods, and this is what is reconstructed; this is apparent when viewed parallel to the [211] direction, from which a (111) stacking fault should appear as a flat plane. Unlike for the case of a dislocation, this shows that WBDF contrast is detrimental to tomography of defects containing stacking faults, and another technique such as STEM LAADF imaging would be better [7].

4. Tilt axis misalignment

To test the effect of misalignment between the tilt axis and the systematic row, three tilt series of weak-beam images were modelled using CUFOUR, applying different amounts of misalignment. A mixed dislocation was used, \( b = \frac{1}{3}[110] \) along [011] in an Al crystal of foil normal [001]; it passed through the crystal at 45° to the surfaces. A tilt range of −45° to +45° was used for \( g = 200 \) and reconstruction done using SIRT 30 iterations as before. The measure of tilt
Figure 3. Reconstructions of misaligned weak-beam dark-field tilt series of a single dislocation inclined at 45° to the foil plane. Left: no misalignment. Centre: \( \Delta n = 1 \) (see text). Right: \( \Delta n = 2 \). The dislocation’s apparent midline is rotated by misalignment, and its shape and thickness change. This rotation has been seen in threading dislocations in experimental reconstructions [2].

axis misalignment \( \Delta n \) for weak-beam condition \( g(n g) \) is the difference in \( n \) between the two ends of the tilt series. Simulations were done for \( \Delta n = 1, \Delta n = 2 \) and perfectly aligned, for zero tilt image conditions \( g/3.5g \) (as used previously for experimental WBDF tomography). As the diffraction condition is changed, the excitation errors change also, making the images more inconsistent. The results, shown in Figure 3, show that misalignment of the tilt axis has a profound effect on the reconstruction. The perfectly aligned tilt series produces a dislocation of the correct shape, though with dynamical fringes; as the misalignment increases, the intensity deviates more in shape, and the inclination of the dislocation is no longer accurately found. It is therefore important to carefully align the tilt axis along the systematic row before taking a tilt series.

5. Conclusions
Weak-beam dark field tomography of defects is described by an adapted Fourier slice theorem and reconstructs an ‘object’ corresponding to the dark field tilt series image intensity, not the displacement field of the defect; this is a better function for showing the path of a dislocation core. Simulations show WBDF stacking fault images are less suitable, giving a reconstruction that is an array of rods, not a flat planar fault. Misalignment of the tilt axis with the systematic row causes changes in excitation error that break the projection requirement, giving a dislocation reconstruction of impaired resolution and changed direction.

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7. References
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