Shape measurement by tracking topology in phase contrast and diffraction

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Atomic resolution 3D imaging of biological specimens is now possible after decades of development for phase contrast electron microscopy, cryo-techniques (cryo-EM) and crucial electron detector advancements, since the first inception of electron tomography [1]. Comprising sensitive wave interference, phase contrast imaging of weakly interacting specimens is vital in this context for overcoming noise and mitigating irradiation damage. Coupled with sophisticated pre-processing, at the heart of such 3D reconstructions is the standard back-projection algorithm of computed tomography. Transmission electron microscopy is generally renowned for nanoscale 2D imaging afforded by strong electron-matter interactions. However, interpretation of specimen shape can be marred by overlapping detail in images, a problem which can be addressed with 3D reconstruction. Apart from cryo-EM, advanced incoherent electron imaging is often necessary to ensure accurate 3D back-projection reconstruction [2], subject to certain ‘missing wedge’ distortions from inaccessible specimen tilt orientations. Recent advances have enabled atomic resolution electron tomography of small nanocrystals [3]. For specimens for which only 3D shape is of interest, simpler 3D reconstruction methods are possible.

Here we describe a 3D imaging approach that can harness sensitive phase or diffraction contrast to measure 3D shape, and demonstrate this through electron microscope experiments across a variety of materials, including nanocrystals, alloys and cryo-EM specimens [4]. There exist a wide variety of specimens for which topological features of interest reside in phase contrast images, such as ridges, valleys, hills, saddles etc., and which are sparsely distributed. Our algorithm uses a differential geometry approach to stereoscopy, to track topological features within inline electron holograms, incoherent images, or diffraction patterns.

Fig. 1 shows two distinct examples: morphology of an isolated magnetite nanocrystal on a thick carbon support (a-c) and 3D diffraction from a complex perovskite Pb(ScTa)0.5O3. Both specimen reconstructions were measured from tilt series acquired on the FEI Titan 80-300 aberration corrected transmission electron microscope (at the Monash Centre for Electron Microscopy), operating at 300kV using plane wave illumination. The tilt series of specimen rotation angles spanned ±7.5º for the magnetite, sufficient to track the pertinent features, while the perovskite tilt angles spanned ±70º to minimise the missing wedge, which appears almost vertical in Fig. 1d and Fig. 1e. The continuum of diffracted intensities in Fig. 1d was reconstructed by assuming a flat Ewald sphere using bilinear interpolation, where the Bragg peaks dominate the contrast. As shown by the 3D points in Fig. 1e, subtle diffuse streaks conveying correlated disorder were revealed by tracking topological features using our algorithm.

Figure 1. (a) magnetite nanoparticle in-line hologram with detected ridges and valleys overlayed in inverted contrast, with corresponding 3D reconstruction merging both ridges and valleys shown (b) & (c). Pb(ScTa)0.5O3 3D diffraction of Bragg intensities is rendered in (d), with the 3D tracking-based reconstruction of topological ridges projected in (e).


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