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A New Approach to Electron Tomography for The *ATOM* Project

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Atom probe tomography (APT) is a technique whereby atoms are successively removed from the surface of a sharp needle-shaped specimen by pulsed field evaporation. The diverging electric field at the apex of the needle ionizes the atoms, emitting them from the specimen towards a position-sensitive detector, producing a signal that yields the identity and position of the atom. As atoms are ionized and field evaporated onto the detector, one-by-one, a 3D tomographic reconstruction is generated [1-2]. These striking reconstructions can span ~0.2×0.2×0.5 µm and contain hundreds of millions of atoms with atomic resolution, the origins of which have recently been identified in detail [3]. Nevertheless, this technique falls short of perfect 3D atomic-resolution microscopy, due to aberrations and limitations in detector efficiency. The ATOM project is a joint initiative of Oak Ridge National Laboratory (ORNL), Cameca, Nion, ISU and the University of Sydney and involves the design and construction of a new concept microscope – the *Atomscope* – that addresses these shortcomings by integrating scanning transmission electron microscopy and APT. This enables one of the key issues in APT to be addressed: accurate measurement of tip shape for the purposes of accurate tomographic reconstruction. The approach in the *Atomscope* will be to use a new method for electron tomography, discussed below, whilst simultaneously collecting atom probe data.

The filtered back-projection (FBP) algorithm continues to be very successful and is widely used in the electron tomography community. It assumes that the recorded intensities are (at least) monotonically related to the projected 3D scattering density. This assumption can fail for crystalline materials because diffraction introduces complex intensity modulations near crystal zone axes. The incoherence of HAADF and energy-filtered electrons suppresses – but does not eliminate – these diffraction effects. Such issues can be minimized by avoiding strong diffraction conditions or by removing unwanted images which may diminish angular sampling. Algorithms such as the algebraic reconstruction technique can also be successfully applied to improve electron tomograms for crystals examined over a limited tilt range [6]. For studying mere 3D morphology, it is possible to use an alternative differential approach for reconstruction, which is less sensitive to problematic diffraction phenomena and does not rely upon the physical validity of the Radon transform. Recently, the prospects of such an approach were tested for electron tomography, whereby a 'surface-tangent algorithm' (STA) was developed and implemented [7, 8].

Basic upon geometric principles more closely related to stereoscopy [9], the STA crudely ignores complex electron/specimen interactions and assumes only that strong gradients in the 3D scattering density are preserved upon projection. In the presence of strong absorption contrast, non-linear Fresnel fringes or fickle diffraction effects, the angular variation of these projected gradients can be robustly measured to estimate the 3D morphology. Since the STA is a *local* tomography algorithm, 'missing wedge' artifacts due to limited angular range merely present as missing data in the reconstruction, without any morphological distortion which can appear in non-local reconstructions. The ideal application of the

STA is to measure the convex outer shape of atom probe specimens. Since atom probe tips are almost cylindrically symmetric, the slow angular variation of the 3D morphology can be used to great advantage. Here we demonstrate that the missing wedge can be accurately filled in to estimate the entire 3D shape of an atom probe tip. Furthermore, using 2nd order partial derivatives of the 3D morphology, it is possible to robustly compute the 1st and 2nd fundamental forms for a complete differential-geometric characterization of the atom probe tip shape, from which quantities such as principle curvatures can be estimated in 3D. Such measurements are essential for quantitative estimates of shank angles and local radii of curvature. Fig. 1a shows the apex of a field-evaporated Al atom probe tip, reconstructed with the STA from 161 images over a tilt range of ±80°. The raw point cloud on the left shows ridges which we interpret as crystal facets running along the specimen shank. Colors on the right of Fig. 1a indicate the standard errors estimated in the STA reconstruction of each point in the projection image, which are larger near the ridges. Figure 1b shows the same STA point cloud, where the missing wedge was filled in by computing roughly 1000 Taylor series to estimate the slow angular variation of the Al specimen about the tip axis, which was closely aligned with the TEM tilt axis. The colors in Fig. 1b represent one of the principle radii of curvatures, which were computed by fitting two localized and orthogonal Taylor series expansions to every point in the wedge-filled STA tomogram.

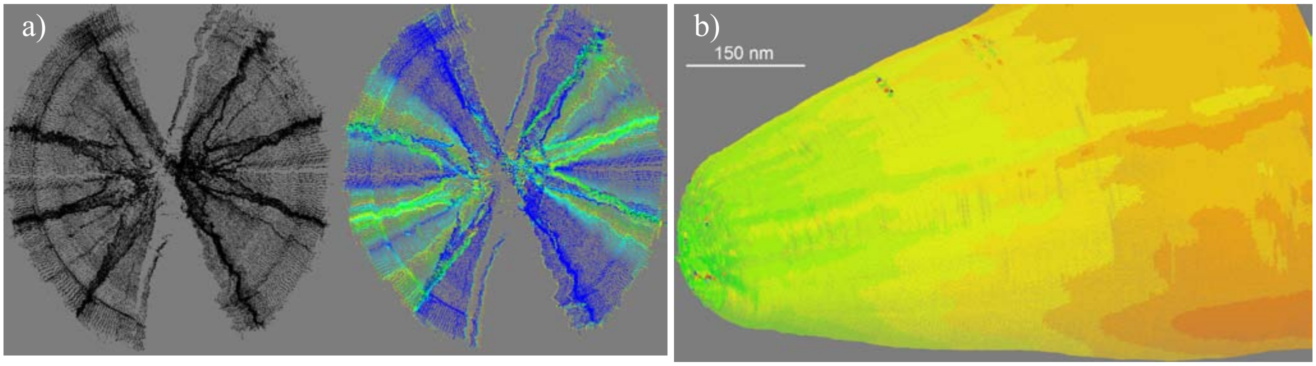

Fig. 1a: STA reconstructed point cloud of an atom probe tip, colors indicate standard errors. Fig. 1b: Data of Fig. 1a structured with missing wedge filled in. Colors indicate principle curvature.

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