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Improving Spatial Accuracy in Atom Probe Tomography through a Crystallography-Mediated Reconstruction (CMR)

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Reconstruction is a critical step in the analysis workflow in atom probe tomography (APT) to transform detected ion hit coordinates (mm scale) in 2-dimensions, to a set of rich set of 3-dimensional point-cloud coordinates that reveal material structures at the atomic scale. By improving the precision of the atom probe reconstruction process, a greater accuracy of atomic neighborhood relationships is available. This is critical in modern materials science and engineering, where knowledge of a materials atomic-scale architecture is a key input in our understanding of microstructure-property relationships.

The current standard procedure for reconstruction implemented in the commercial software IVAS™ [1] is based on a geometric simplification of the field-evaporation process using a pseudo-stereographic projection model. However, recent efforts have confirmed an equidistant-azimuthal model is a more accurate representation of the projection of ions in APT [2,3]. In any case, these models are startingly simple in their assumptions and ultimately reduce to a set of four required input parameters: evaporation field 'F_e' (material specific), detection efficiency 'η' (instrument specific), image compression factor (ICF) 'ξ' (or equivalent equidistant-azimuthal magnification factor 'ρ', experiment specific) and the geometric field factor 'k_f' (experiment specific).

Gault et al. [4] defined a calibration procedure for these parameters based on observable crystallographic information and the known crystallographic structure of the analysis material. However, the crystallographic information used in this application is limited to the distance between observed poles at the detector to calibrate the ICF and observed planar-spacing to calibrate 'k_f'. Furthermore, the calibration procedure is often performed at a discrete interval in the evaporation history, thus assuming the reconstruction parameters remain static throughout the entire evaporation. As this process fails to account for the dynamic changes of the reconstruction parameters throughout both the analysis depth, and across the specimen surface [5], it is common to produce results that exhibit substantial distortions throughout the analysis depth, as measured by observed planar-spacing and angles between poles [6]

In this work, we present a crystallography-mediated reconstruction (CMR) [7] protocol to improve the spatial accuracy and dramatically improve measured in-depth distortions. To achieve this, we developed a geometric transform framework to translate atomic positions from 'detector space' to 'reconstructed space' through a barycentric transform, without necessary input of pseudo-empirical reconstruction factors ICF or k_f. The barycentric transform is mediated by novel crystallographic analysis techniques including: (1) a method to calculate the orientation of the evaporated crystal directly from the field evaporation map, (2) a method to identify and track the pole locations throughout the evaporation sequence using an input from the OIM software implemented in IVAS™ 3.8 and (3) calculating the radius evolution by accounting for the number of atoms evaporated between each successive plane visible in the reconstruction. We apply the CMR method to both a pure aluminum dataset and compare the spatial-accuracy to a reconstruction made in IVAS™, measured by the observed planar-spacing and angles

between poles as a function of analysis depth (Figure 1). It is observed that the average error for the CMR method decreases from 15.51 ± 0.069% to 3.86 ± 0.06% for interplanar spacings and 8.52 ± 0.024% to 1.53 ± 0.13% for interplanar angles. Furthermore, we present an adaptation to the CMR method for datasets that exhibit only a single crystallographic direction (pole). Here, we use a metric derived from the DF-Fit algorithm (8) to assess the 'flatness' of observed planes to calibrate the equidistant-azimuthal magnification factor (Figure 2) as a function of the in-depth direction, to be used in the CMR method [9].

References:
[1] B Geiser et al., Microscopy and Microanalysis (Suppl 2) **15** (2009) pp. 292-293.
[2] F De Geuser and B Gault, Microscopy and Microanalysis **23.2** (2017) pp. 238-246.
[3] R Forbes, Atom Probe Tomography and Microscopy Symposium (APT&M) (2014).
[4] B Gault et al., J Appl Phys **105.3** 034913.
[5] S Loi et al., Ultramicroscopy **132** (2013) pp. 107-113.
[6] A Ceguerra, A Day, S Ringer, Microscopy and Microanalysis (2019) in print.
[7] A Day, A Ceguerra, S Ringer, Microscopy and Microanalysis (2019) in print.
[8] D Haley, P Bagot, M Moody, Microscopy and Microanalysis (2019) in print.
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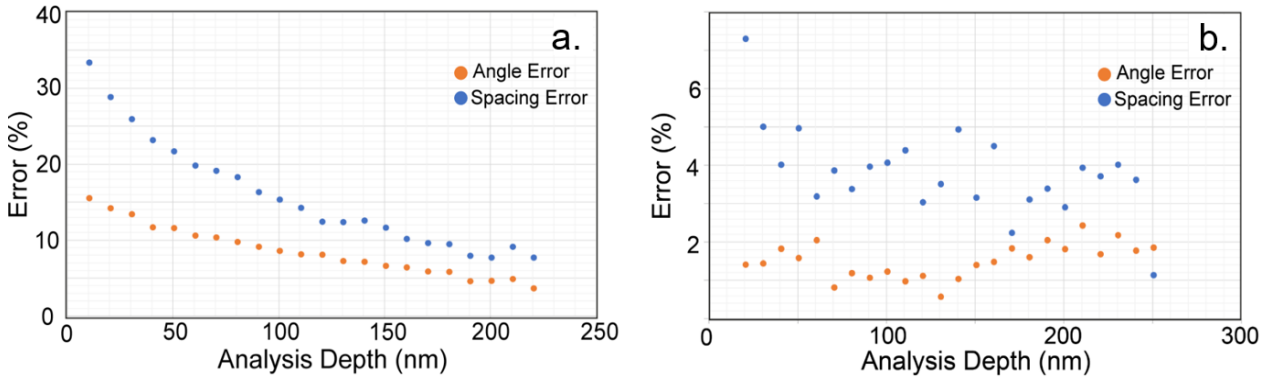

Figure 1. Errors in observed planar-spacing and interplanar angles as a function of analysis depths for reconstructions made using **a.** IVAS™ and **b.** CMR protocol

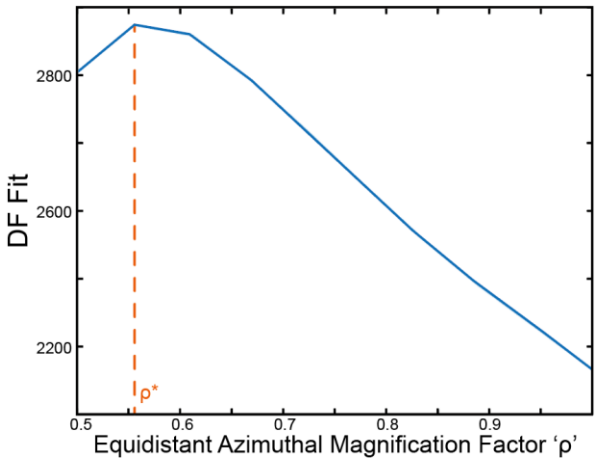

Figure 2. DF-Fit metric (8) for flatness of observed crystallographic planes for a single crystallographic direction, charted against 'ρ', to determine calibrated magnification factor 'ρ^*'.

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