Crystallography in Atom Probe Tomography

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Atom Probe Tomography (APT) has the capacity to account for the five macroscopic degrees of freedom (dof) to fully describe grain boundaries with chemical sensitivity [1]. These 5dof consist of 3 parameters to characterise the misorientation axis-angle pair, and 2 to describe the grain boundary plane orientation. To inform the complete 5dof, an APT dataset must meet stringent criteria; including observable crystallographic planes, accurate calibration of reconstruction parameters, and the ability to distinguish grain boundary topology. APT analysis methodologies must be further developed to elucidate the required information, and to funnel the large volume of data into the minimal set of information required to perform a crystallographic analysis.

In this work, we focus on specific case studies, highlighting the advantages of using APT for performing crystallographic analyses, and discuss the challenges in extracting required information from raw data. Furthermore, crystallographic relationships are often used to inform reconstruction parameters. Therefore, crystallographic analyses in APT are highly sensitive to the reconstruction process. We use prior knowledge of a twin boundary, with a well-known orientation relationship, to inform the reconstruction process and to explore the limits in accuracy of APT as a crystallographic tool.

[1] Yao, Lan, et al. "The anatomy of grain boundaries: Their structure and atomic-level solute distribution." *Scripta Materialia* 69.8 (2013): 622-625.