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A materials informatics framework to discover patterns in atom probe tomography data.

Tuesday, 14 September 2021 19:00 (2 hours)

To quantify chemical segregation at multiple length scales in APT in a semi-automatic way, we propose a multi-stage strategy. First, we collect composition statistics from APT datasets for 2x2x2 nm voxels. These voxel compositions are then clustered in compositional space using Gaussian mixture models to automatically identify key phases. Next, based on this compositional classification we employ DBSCAN in physical space at voxel resolution to detect individual precipitates at a small fraction of the effort needed for single-atom-based algorithms. This framework was used to identify and disentangle plate-like Zr-rich and topologically complex Cu-rich precipitates in two APT datasets from Fe-doped Sm-Co magnets, each containing approximately 500 million ions. Upon segmentation of each precipitate using DBSCAN a new approach based on principle component analysis (PCA) is applied to 2D slices of the complex Cu-rich precipitates to further decompose them into approximate planar regions along with their junctions. For each precipitate, the actual distribution of atomic fractions is compared to the expected distribution of a random alloy. This step helps to quantitatively assess clustering within a given precipitate for each atomic species. Finally, for each quasi-planar precipitate, a triangular grid is superimposed to investigate in-plane compositional fluctuations, thickness, and 1D composition profiles.

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