

Consistent atom probe representation for machine learning and data mining

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To correlate mechanical properties of Al alloys with chemical segregation in Atom Probe Tomography (APT), we have developed two approaches. In the 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 and their corresponding statistical descriptors. In the second, we employ SOAP (Smooth Overlap of Atomic Positions) descriptors to encode local chemical and structural environment around each atom in APT dataset. Upon using a pairwise similarity criteria on SOAP vectors, atoms lying in similar atomic environments (phases) are identified.

Poster title

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