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Data Mining and Informatics for Quantitative Atom Probe Tomography

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The ability to generate realistically 3-D reconstructed data that incorporates the miss sequencing caused by preferential evaporation and the resulting local magnification effects will be the key to designing the next generation 3-D reconstruction algorithms. State-of-the art analysis has shown that the interaction of the electrode-pulse with DC field evaporation can cause complicated and important effects in the resulting mass spectra. It would be useful to develop a solid simulation of the ion optical system to understand both spatial and mass resolution effects. Other processing steps like density-correction, cluster-finding and enveloping are so time demanding that intuition about handling them is very expensive to develop. As noted in many studies the quality of data in pulsed laser atom probe tomography is influenced by many instrumental parameters. It is important that we resolve these technical issues if we are to advance quantitative interpretation of atom probe data.. To do so, we need to apply a host of tools: (a) supercomputers that can process extremely large data sets, (b) data mining algorithms that can be used to make robust clustering analyses, which is critical in discriminating between atomic chemistries (Figure 1) and spatial locations [1], and (c) new visualization approaches for studying atomic scale clustering

A key concept towards extracting geometric features and classification of atom probe data from large point cloud data set is the construction of low-dimensional models that encode the available input information. In the context of constructing reduced input models and low-complexity surrogate systems, it has to be noted that linear model reduction methods have been extensively used for representing data snapshots (e.g. principal component analysis (PCA) in imaging). The PCA method uses a Euclidean distance measure; which works well if all the latent variables interact in a linear combination of each other. If the data correlation space however is such that these contributions interact in a non-linear fashion that make them invisible to PCA. One then needs to explore non-linear data dimensionality reduction techniques. In this presentation we show how atom probe data can be represented using geodesic and topological preserving distance measures (Figure 2).

The low-dimensional reduced representations can be constructed in a dynamic, data-driven and adaptive way through representation of the input data as high-dimensional points on a differential manifold. Novel graph-theoretic techniques can be utilized to construct a topologically invariant transformation of the manifold into a low dimensional region. In this talk we discuss how data-driven computational strategies for computing manifolds in high dimensional space can be applied to quantify clustering of atom probe data

References

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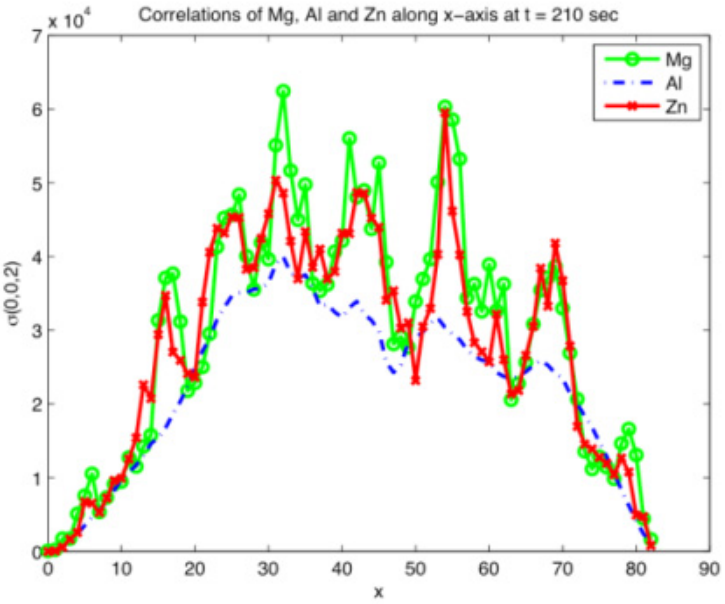

Figure 1: Autocorrelation functions for multicomponent Al-Zn-Mg developed through clustering algorithms on high performance supercomputer providing one method of representation of chemical clustering from atom probe tomography data (From Ref. 1)

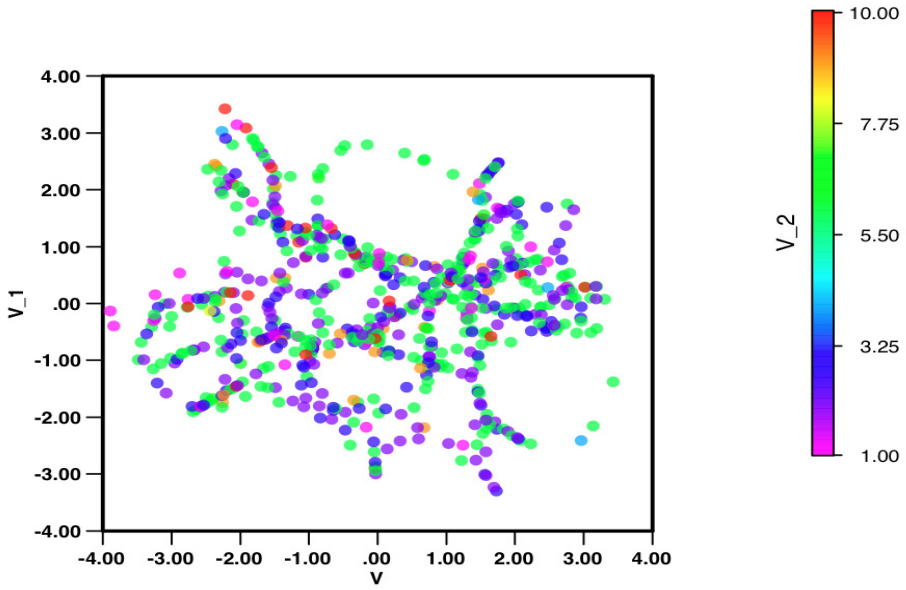

Figure 2: An alternative non-linear manifold representation of atomic clustering in multicomponent alloys.

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