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Applications of Spatial Distribution Maps for Advanced Atom Probe Reconstruction and Data Analysis

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The aim of this research is to develop advanced analytical techniques to significantly refine the resolution of atom probe microscopy analyses and hence the accuracy of 3D atomistic nanostructural characterization. Due to the finite spatial resolution of the technique, crystallographic features generally appear blurred within the tomographic reconstruction. A new post-processing approach to return displaced crystalline APM data back to its original lattice configuration will be presented [1, 2]. Fundamental to this strategy is the application of spatial distribution map (SDM) techniques [3-5] to correct the reconstruction, replacing each atom back on the lattice, while at each point maintaining the integrity of the local atomic neighborhood, as illustrated in Figure 1. The algorithm utilizes the limited structural information across multiple crystallographic directions already existing in the data to identify in real space each atom's most likely lattice site. Individual lattice sites defining the local atomic neighborhoods are now clearly defined, as demonstrated in Figure 2.
Restoration of the lattice in the reconstruction provides many significant benefits to subsequent analyses of the data. Notably, nearest neighbor and radial distribution function analyses can now access information previously convoluted by the limited spatial resolution of the technique. Further, since most of the cluster identification methodologies are based on inter-atomic distances criteria [6, 7], having the atoms on a lattice permits the definition of less arbitrary criteria which will lead to a significant increase in the accuracy of the cluster characterization. This approach also represents a first step towards addressing the missing data problem inherent in every APT experiment. Vacant lattice positions in the reconstructions indicate sites where atoms have been lost to due to limited detector efficiency. Combined knowledge of global and local neighborhood distributions can conceivably be used to predict the identities of the missing atoms. The insight gained through advanced APM tomographic reconstruction techniques has exciting implications for furthering our understanding of nanostructure and its relationship to material properties and performance, and hence the design and development of new materials.

References

[1] P.P. Camus et al., Applied Surface Science 87 (1995) 305.
[2] F. Vurpillot et al., Ultramicroscopy 95 (2003) 223.
[3] T. Boll et al., Ultramicroscopy 107 (2007) 796.
[4] B.P. Geiser et al., Microsc. and Microanal. 13 (2007) 437.
[5] M.P. Moody et al., Ultramicroscopy Accepted (2009).
[6] L.T. Stephenson et al., Microsc. and Microanal. 13 (2007) 448.
[7] A.V. Ceguerra et al., Phil. Mag. Accepted (2009).

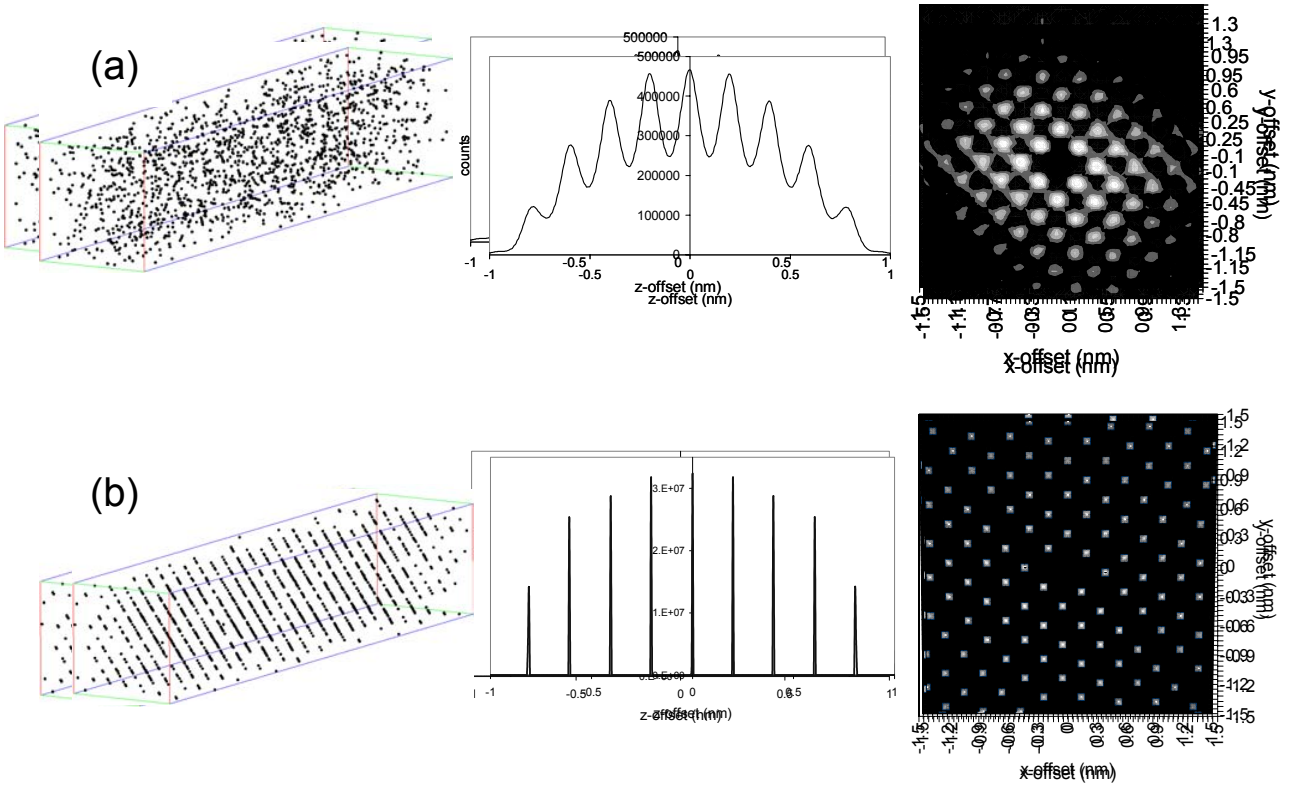

FIG. 1. (a) Sub-volume of an Al APT reconstruction and accompanying *z-SDM* and *xy-SDM* reveal crystallographic information characteristic of the (002) direction not visually apparent in the reconstruction. (b) Perfect lattice has been restored within the above reconstruction. The crystalline structure of the data is now readily observable and is confirmed by the associated SDM analysis.

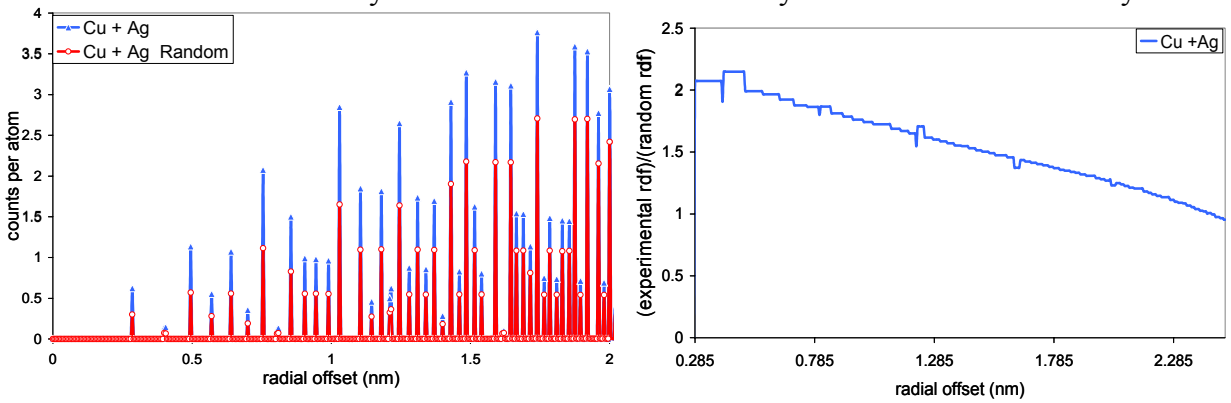

FIG. 2. Radial distribution function of Cu and Ag solute atoms in a lattice-restored APT reconstruction of an AlCuAg dataset. Individual lattice sites defining the local atomic neighbourhood are clearly defined. A strong co-segregation of solute ions is demonstrated via comparison with the RDF of a corresponding randomized distribution. This clustering phenomenon is further qualified by the ratio of the experimental RDF relative to the values measured for randomly labeled reconstruction.

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