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A Lattice-Rectified and Detection Efficiency Compensated APT Reconstruction

M. P. Moody*, A. V. Ceguerra*, A. J. Breen*, B. Gault*, L. T. Stephenson*, R. K. W. Marceau* and S. P. Ringer*

* Australian Centre for Microscopy and Microanalysis, The University of Sydney, NSW 2006, Australia

Atom probe tomography (APT) provides a unique combination of highly chemically and spatially resolved 3D atomistic information. However, the technique has two significant constraints: limited detector efficiency and imperfect spatial resolution. Detector efficiency is inhibited by the open area of the microchannel plate (MCP), leading to upwards of 40% of the atoms evaporated from the specimen being omitted from the final analysis. This design limitation is common to all commercial detectors. The spatial resolution, although imperfect, is very high, however, this can be very much material and specimen dependent. Limited spatial resolution is due to a combination of trajectory aberrations caused by local geometric and compositional variations on the specimen, surface migration, preferential evaporation effects and the simplified geometry used in the 3D reconstruction [1]. Even with improved instrumentation, the burden of improving spatial resolution will mostly fall to the development of new and improved analytical approaches. This is a critical area of research, though, the current proportion of APT research efforts devoted to this objective is somewhat limited.

Recently, two new analytical techniques have been developed to independently address each of these problems respectively: short range order driven (SRO) Monte Carlo simulations and lattice rectification. Lattice rectification is an approach whereby the perfect lattice configuration of the original specimen is restored by using the existing crystallographic structure that is resolvable within the reconstructed APT dataset (FIG 1) [2]. Likewise, SRO parameters which describe the average distribution of solutes within a system have been adapted to the characterization of APT data. In the case of atom probes with a straight ion flight path to the detector, the SRO is largely independent of detection efficiency limitations. By means of Monte Carlo algorithm driven by a set of target SRO parameters [3], complementary complete (i.e. equivalent to 100% efficient) simulated lattice-based datasets can be generated that are highly representative of the original APT reconstruction (FIG 2).

The aim of this research is to hybridize these recent advances by developing a methodology to generate the first corrected (lattice rectified) APT reconstructions in which the missing atoms due to the effects of limited detection efficiency have been accurately replaced based upon consideration of the measured SRO. These unique completed and corrected 3D atomistic representations of all atomic species within complex multi-component materials generated by microscopy can be data-mined for quantitative nanostructural information and ultimately have the potential to be seeded directly into computer simulation to predict bulk material properties of materials of industrial significance.

References

[1] B. Gault et al., *Microsc. and Microanal.* 16, (2010) 99.
[2] M. P. Moody et al., *Microsc. and Microanal.* (2011) doi: 10.1017/S1431927610094535.
[3] A. V. Ceguerra et al., *Phys. Rev. B.* 82 (2010) 132201.
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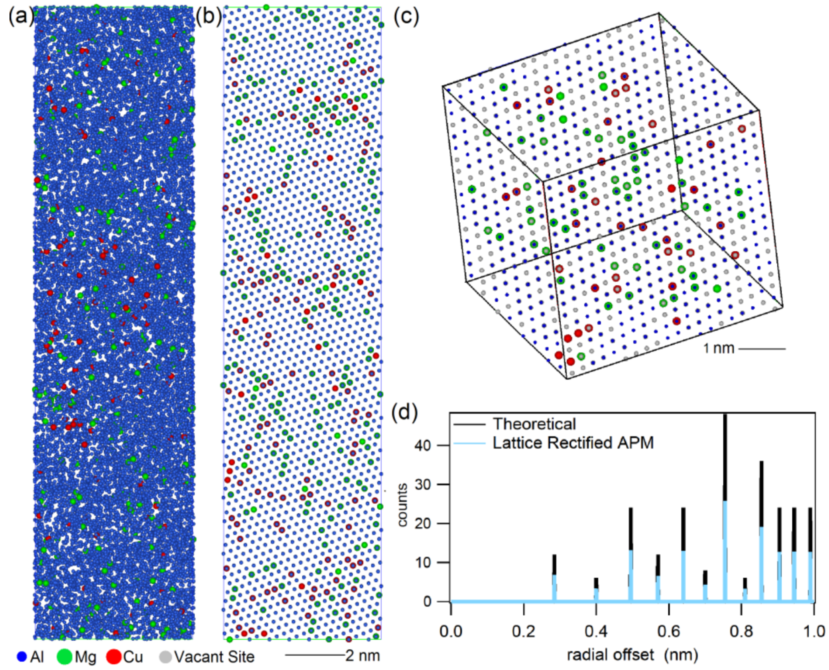

FIG 1. Lattice rectification of AQ Al-1.1Cu-1.7Mg (at. %). (a) depicts a 5 nm thick section of the raw APT data. (b) a complementary section after lattice rectification. (c) is a close-up sub-volume of (b), but now vacant lattice sites in the rectified reconstruction have also been highlighted. (d) RDF analysis of the rectified data.

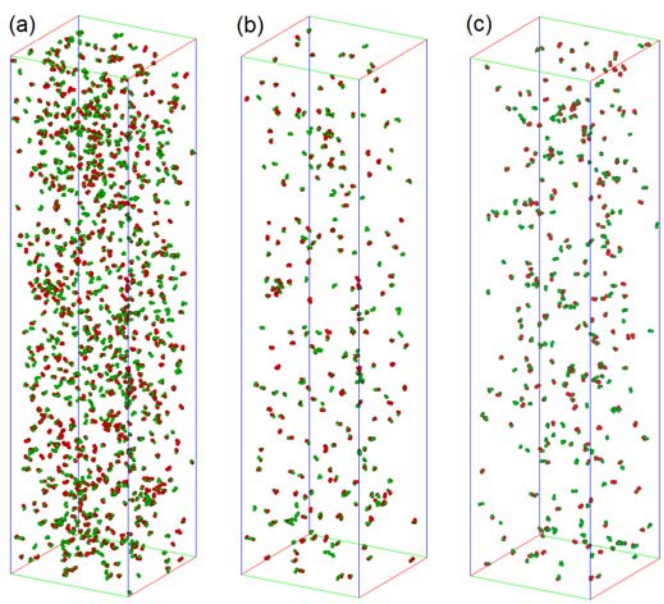

FIG 2. Atom maps of solute clusters identified within sub-volumes of APT experimental data and associated MC simulations. (a) Clusters in the complete simulated system based on GM-SRO characterization of Al-1.1Cu-1.7Mg (at. %), 60 s aged condition (b) clusters identified in the MC simulation after the stochastic removal of atoms to model 57% detector efficiency (c) cluster characterization within the original APT reconstruction of Al-1.1Cu-1.7Mg (at. %), 60 s aged condition.

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