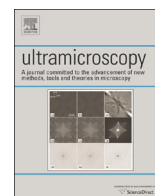




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Mining information from atom probe data

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ABSTRACT

Whilst atom probe tomography (APT) is a powerful technique with the capacity to gather information containing hundreds of millions of atoms from a single specimen, the ability to effectively use this information creates significant challenges. The main technological bottleneck lies in handling the extremely large amounts of data on spatial–chemical correlations, as well as developing new quantitative computational foundations for image reconstruction that target critical and transformative problems in materials science. The power to explore materials at the atomic scale with the extraordinary level of sensitivity of detection offered by atom probe tomography has not been fully harnessed due to the challenges of dealing with missing, sparse and often noisy data. Hence there is a profound need to couple the analytical tools to deal with the data challenges with the experimental issues associated with this instrument. In this paper we provide a summary of some key issues associated with the challenges, and solutions to extract or “mine” fundamental materials science information from that data.

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1. Introduction

Atom probe is a powerful characterisation tool that provides three-dimensional reconstructed maps that show the position and species of tens or even hundreds of millions of individual atoms with atomic resolution [1–6]. Such datasets are rich in information that is of great use to materials scientists, who are interested in the relationship between structure and properties of materials, but it is a major challenge to convert this data to quantitative and meaningful information about the microstructure of the specimen being examined.

A needle-shaped specimen is biased at a high voltage and the resulting electrostatic field causes ionisation and desorption of the surface atoms. By partially pulsing the field, a few ions at a time are projected onto a position-sensitive, single atom detector. The position at which they hit the detector is used to reconstruct the

x – y coordinates, and the sequence in which the ions are detected is used to reconstruct the z coordinate. The time-of-flight is used to identify the atomic species. A typical dataset, once reconstructed, is in the form of a point cloud containing the 3D position and mass-to-charge state of each ion. Visualisation may be carried out by using either dedicated commercial software, such as IVAS (from CAMECA), or by other software (e.g. Blender or 3Depict) that has the capability of rendering the point cloud data as points or spheres and colouring the atoms according to the mass-to-charge ratio, and therefore the identified species. Many of these software packages already provide sophisticated tools for the quantitative analysis of data, such as grid-based atomic distributions [7] and rendering of iso-surfaces, concentration profiles, proximity histograms [8], cluster analysis tools [1–9] and the analysis of multiple hit detector events [11–13]. The purpose of this paper is to outline some outstanding issues and describe some of the more recent developments for mining information from atom probe data, based on a “data mining” workshop held at the Atom Probe Tomography and Microscopy (APT&M) meeting in Stuttgart, August, 2014.

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2. Defining and assessing randomness

A true nanoscale characterisation technique, atom probe enables clusters of solute/dopants/impurities consisting of mere handfuls of atoms to be identified and characterised [14]. Of course, the natural inclination is to push this capacity to its limits. A prominent example is the investigation of nucleation during the early stages of phase transformations in materials [15–19]. Other popular applications include the onset of segregation of solute ions to defects in materials subject to extreme environments, such as ion/neutron irradiation [20–23], and the clustering of solute ions in semiconductor devices [24–27].

At these limits of APT sensitivity and resolution, researchers are examining the distribution of very fine-scale clusters of atoms and effectively asking – *is this distribution of atoms random?* More precisely, is it probable that this distribution could be observed in a completely randomly arranged configuration of atoms? Although this might seem like a straightforward proposition, given the intrinsic limitations of experimental data, this interpretation requires careful consideration.

Visual inspection of the reconstruction is nearly always the first course of action. In many systems chemical–spatial inhomogeneity is readily apparent. However, discriminating very slight deviations from random by eye is simply impossible. Iso-concentration surfaces provide significant enhancement to visual inspection. Iso-concentration surfaces can identify regions of irregular chemical composition that may differ only very slightly from the bulk of the reconstruction. However, this information alone is not sufficient to determine whether these regions are statistically significant, i.e. are they evidence of the first stages of the nucleation of an entirely new phase, or simply a random fluctuation?

For example, a computer-generated face centred cubic solid-solution model system has been generated, and is shown in Fig. 1. The simulated system consists of two types of solutes, solute A (8.0 at%) and solute B (1.5 at%). Both types of solute atoms have been randomly distributed throughout the matrix. Even so, application of an iso-concentration surface to this system highlights discrete regions of high solute composition. Indeed the spatial distribution of these regions around the reconstruction appears very much like what might be expected for a population of secondary phase clusters homogeneously nucleating within the material. Further, secondary analyses such as proxigrams can easily be applied that ostensibly strengthen the notion that this is evidence for fine scale thermodynamically-driven solute clustering.

However, in this example we already know that this is not true. The fluctuations are simply random variations in the composition. The key point is that without some kind of statistical analysis to support the hypothesis that clustering is present, the iso-concentration surface is meaningless. Conventionally, frequency distribution analyses, often colloquially referred to as binomial analyses, have been applied as a first test for randomness [28,29]. Frequency distribution analyses essentially divide the APT data into a 3D grid of voxels of similar size, all containing the same number of atoms. The frequency of occurrence of a specific element per voxel is assessed. Ultimately a histogram of these frequencies is constructed. If an element is randomly distributed throughout the reconstruction, the histogram should closely match a corresponding theoretical binomial distribution. Hence, non-randomness can be assessed by quantifying the departure of the experimentally observed distribution from that expected theoretically. Often a χ^2 test is applied to obtain a *p*-value and test the significance of this deviation. However, the sensitivity of this

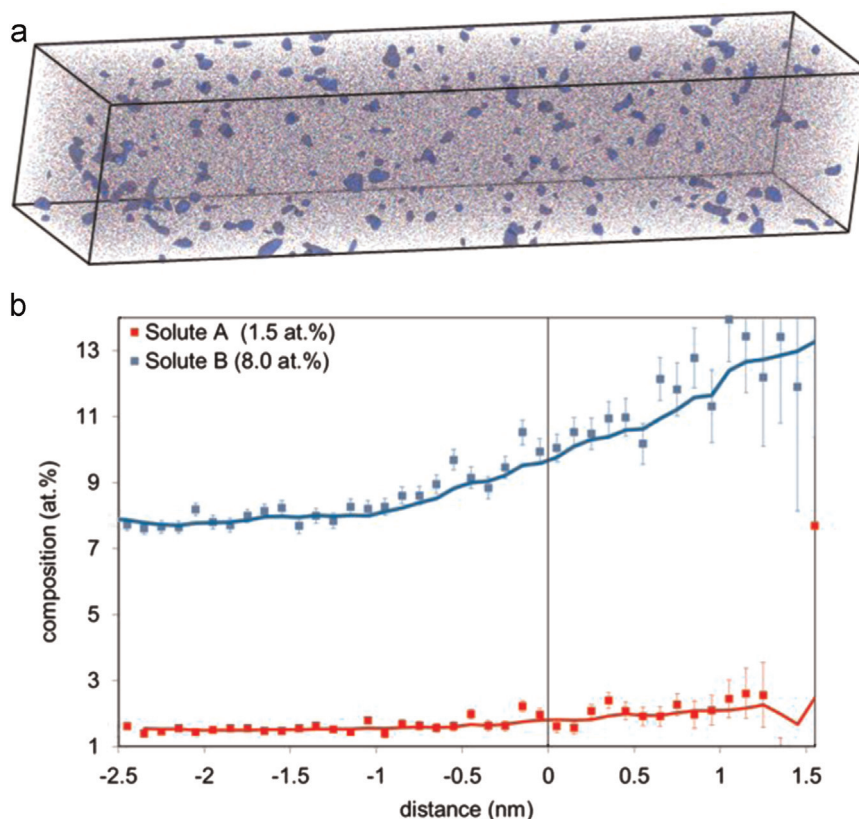


Fig. 1. (a) Simulated APT-like data ($200 \times 40 \times 40 \text{ nm}^3$) representing a ternary alloy with solute A at a composition of 1.5 at% and solute B at 8.0 at%. Solute atoms are randomly arranged in the system. The blue isoconcentration surface is defined by a total solute concentration of 10.9 at%. (b) Proxigram analysis averaged over several interfaces defined by 10.9 at% isoconcentration. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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